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Quantum Mechanics (046241) - Lecture Notes

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Technion
Preface

The dynamics of a quantum system is governed by the celebrated Schrödinger equation

\[ i\hbar \frac{d}{dt} |\psi\rangle = \mathcal{H} |\psi\rangle , \tag{0.1} \]

where \( i = \sqrt{-1} \) and \( \hbar = 1.05457266 \times 10^{-34} \text{ J s} \) is Planck’s h-bar constant. However, what is the meaning of the symbols \( |\psi\rangle \) and \( \mathcal{H} \)? The answers will be given in the first part of the course (chapters 1-4), which reviews several physical and mathematical concepts that are needed to formulate the theory of quantum mechanics. We will learn that \( |\psi\rangle \) in Eq. (0.1) represents the ket-vector state of the system and \( \mathcal{H} \) represents the Hamiltonian operator. The operator \( \mathcal{H} \) is directly related to the Hamiltonian function in classical physics, which will be defined in the first chapter. The ket-vector state and its physical meaning will be introduced in the second chapter. Chapter 3 reviews the position and momentum operators, whereas chapter 4 discusses dynamics of quantum systems. The second part of the course (chapters 5-7) is devoted to some relatively simple quantum systems including a harmonic oscillator, spin, Hydrogen atom and more. Finally, in chapter 8 we will study quantum systems in thermal equilibrium and in chapter 9 we will study the time-independent perturbation theory. Most of the material in these lecture notes is based on the textbooks [1] and [2].
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1. Hamilton’s Formalism of Classical Physics

In this chapter the Hamilton’s formalism of classical physics is introduced, with a special emphasis on the concepts that are needed for quantum mechanics.

1.1 Action and Lagrangian

Consider a classical physical system having $N$ degrees of freedom. The classical state of the system can be described by $N$ independent coordinates $q_n$, where $n = 1, 2, \ldots, N$. The vector of coordinates is denoted by

$$ Q = (q_1, q_2, \ldots, q_N). \quad (1.1) $$

Consider the case where the vector of coordinates takes the value $Q_1$ at time $t_1$ and the value $Q_2$ at a later time $t_2 > t_1$, namely

$$ Q(t_1) = Q_1, \quad (1.2) $$

$$ Q(t_2) = Q_2. \quad (1.3) $$

The *action* $S$ associated with the evolution of the system from time $t_1$ to time $t_2$ is defined by

$$ S = \int_{t_1}^{t_2} dt \mathcal{L}, \quad (1.4) $$

where $\mathcal{L}$ is the Lagrangian function of the system. In general, the Lagrangian is a function of the coordinates $Q$, the velocities $\dot{Q}$ and time $t$, namely

$$ \mathcal{L} = \mathcal{L} \left( Q, \dot{Q}; t \right), \quad (1.5) $$

where

$$ \dot{Q} = (\dot{q}_1, \dot{q}_2, \ldots, \dot{q}_N) \quad (1.6) $$

and where overdot denotes time derivative. The time evolution of $Q$, in turn, depends of the trajectory taken by the system from point $Q_1$ at time $t_1$.
Chapter 1. Hamilton’s Formalism of Classical Physics

1.2 Principle of Least Action

For any given trajectory $Q(t)$ the action can be evaluated using Eq. (1.4). Consider a classical system evolving in time from point $Q_1$ at time $t_1$ to point $Q_2$ at time $t_2$ along the trajectory $Q_{\Gamma}(t)$. The trajectory $Q_{\Gamma}(t)$, which is obtained from the laws of classical physics, has the following unique property known as the principle of least action:

**Proposition 1.2.1 (principle of least action).** Among all possible trajectories from point $Q_1$ at time $t_1$ to point $Q_2$ at time $t_2$ the action obtains its minimal value by the classical trajectory $Q_{\Gamma}(t)$.

In a weaker version of this principle, the action obtains a local minimum for the trajectory $Q_{\Gamma}(t)$. As the following theorem shows, the principle of least action leads to a set of equations of motion, known as Euler-Lagrange equations.

**Theorem 1.2.1.** The classical trajectory $Q_{\Gamma}(t)$, for which the action obtains its minimum value, obeys the Euler-Lagrange equations of motion, which are given by

$$Q(t) = Q_{\Gamma}(t).$$ (1.7)
1.2. Principle of Least Action

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} = \frac{\partial L}{\partial q_n}, \]

(1.8)

where \( n = 1, 2, \ldots, N \).

**Proof.** Consider another trajectory \( Q_{\Gamma'} (t) \) from point \( Q_1 \) at time \( t_1 \) to point \( Q_2 \) at time \( t_2 \) (see Fig. 1.2). The difference

\[ \delta Q = Q_{\Gamma'} (t) - Q_{\Gamma} (t) = (\delta q_1, \delta q_2, \ldots, \delta q_N) \]

(1.9)

is assumed to be infinitesimally small. To lowest order in \( \delta Q \) the change in the action \( \delta S \) is given by

\[
\delta S = \int_{t_1}^{t_2} dt \delta L
= \int_{t_1}^{t_2} dt \left[ \sum_{n=1}^{N} \frac{\partial L}{\partial q_n} \delta q_n + \sum_{n=1}^{N} \frac{\partial L}{\partial \dot{q}_n} \delta \dot{q}_n \right]
= \int_{t_1}^{t_2} dt \left[ \sum_{n=1}^{N} \frac{\partial L}{\partial q_n} \delta q_n + \sum_{n=1}^{N} \frac{\partial L}{\partial \dot{q}_n} \frac{d}{dt} \delta q_n \right].
\]

(1.10)

Integrating the second term by parts leads to

\[
\delta S = \int_{t_1}^{t_2} dt \sum_{n=1}^{N} \left( \frac{\partial L}{\partial q_n} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} \right) \delta q_n
+ \sum_{n=1}^{N} \left[ \frac{\partial L}{\partial q_n} \delta q_n \right]_{t_1}^{t_2}.
\]

(1.11)

The last term vanishes since

\[ \delta Q (t_1) = \delta Q (t_2) = 0. \]

(1.12)

The principle of least action implies that

\[ \delta S = 0. \]

(1.13)

This has to be satisfied for *any* \( \delta Q \), therefore the following must hold

\[ \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_n} = \frac{\partial L}{\partial q_n}. \]

(1.14)
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Fig. 1.2. The classical trajectory $Q_{\Gamma}(t)$ and the trajectory $Q_{\Gamma'}(t)$.

In what follows we will assume for simplicity that the kinetic energy $T$ of the system can be expressed as a function of the velocities $\dot{Q}$ only (namely, it does not explicitly depend on the coordinates $Q$). The components of the generalized force $F_n$, where $n = 1, 2, \cdots, N$, are derived from the potential energy $U$ of the system as follows

$$F_n = -\frac{\partial U}{\partial q_n} + \frac{d}{dt} \frac{\partial U}{\partial \dot{q}_n}.$$  \hspace{1cm} (1.15)

When the potential energy can be expressed as a function of the coordinates $Q$ only (namely, when it is independent on the velocities $\dot{Q}$), the system is said to be conservative. For that case, the Lagrangian can be expressed in terms of $T$ and $U$ as

$$\mathcal{L} = T - U.$$  \hspace{1cm} (1.16)

Example 1.2.1. Consider a point particle having mass $m$ moving in a one-dimensional potential $U(x)$. The Lagrangian is given by

$$\mathcal{L} = T - U = \frac{m\dot{x}^2}{2} - U(x).$$  \hspace{1cm} (1.17)

From the Euler-Lagrange equation

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} = \frac{\partial \mathcal{L}}{\partial x},$$  \hspace{1cm} (1.18)

one finds that

$$m\ddot{x} = -\frac{\partial U}{\partial x}.$$  \hspace{1cm} (1.19)
1.3 Hamiltonian

The set of Euler-Lagrange equations contains \( N \) second order differential equations. In this section we derive an alternative and equivalent set of equations of motion, known as Hamilton-Jacobi equations, that contains twice the number of equations, namely \( 2N \), however, of first, instead of second, order.

**Definition 1.3.1.** The variable canonically conjugate to \( q_n \) is defined by

\[
p_n = \frac{\partial L}{\partial \dot{q}_n}.
\]

(1.20)

**Definition 1.3.2.** The Hamiltonian of a physical system is a function of the vector of coordinates \( Q \), the vector of canonical conjugate variables \( P = (p_1, p_2, \cdots, p_N) \) and time, namely

\[
H = H(Q, P; t),
\]

(1.21)

is defined by

\[
H = \sum_{n=1}^{N} p_n \dot{q}_n - \mathcal{L},
\]

(1.22)

where \( \mathcal{L} \) is the Lagrangian.

**Theorem 1.3.1.** The classical trajectory satisfies the Hamilton-Jacobi equations of motion, which are given by

\[
\dot{q}_n = \frac{\partial H}{\partial p_n},
\]

(1.23)

\[
\dot{p}_n = -\frac{\partial H}{\partial q_n},
\]

(1.24)

where \( n = 1, 2, \cdots, N \).

**Proof.** The differential of \( H \) is given by

\[
dH = d \sum_{n=1}^{N} p_n \dot{q}_n - d\mathcal{L}
\]

\[
= \sum_{n=1}^{N} \left( \dot{q}_n dp_n + p_n d\dot{q}_n - \frac{\partial \mathcal{L}}{\partial q_n} dq_n - \frac{\partial \mathcal{L}}{\partial \dot{q}_n} d\dot{q}_n \right) - \frac{\partial \mathcal{L}}{\partial t} dt
\]

\[
= \sum_{n=1}^{N} \left( \dot{q}_n dp_n - \dot{p}_n dq_n \right) - \frac{\partial \mathcal{L}}{\partial t} dt.
\]

(1.25)
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Thus the following holds

\[ \dot{q}_n = \frac{\partial H}{\partial p_n}, \quad (1.26) \]

\[ \dot{p}_n = -\frac{\partial H}{\partial q_n}, \quad (1.27) \]

\[ \frac{\partial L}{\partial t} = \frac{\partial H}{\partial t}. \quad (1.28) \]

Corollary 1.3.1. The following holds

\[ \frac{dH}{dt} = \frac{\partial H}{\partial t}. \quad (1.29) \]

Proof. Using Eqs. (1.23) and (1.24) one finds that

\[ \frac{dH}{dt} = \sum_{n=1}^{N} \left( \frac{\partial H}{\partial q_n} \dot{q}_n + \frac{\partial H}{\partial p_n} \dot{p}_n \right) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}. \quad (1.30) \]

The last corollary implies that \( H \) is time independent provided that \( H \) does not depend on time explicitly, namely, provided that \( \frac{\partial H}{\partial t} = 0 \). This property is referred to as the law of energy conservation. The theorem below further emphasizes the relation between the Hamiltonian and the total energy of the system.

Theorem 1.3.2. Assume that the kinetic energy of a conservative system is given by

\[ T = \sum_{n,m} \alpha_{nm} \dot{q}_n \dot{q}_m, \quad (1.31) \]

where \( \alpha_{nm} \) are constants. Then, the Hamiltonian of the system is given by

\[ H = T + U, \quad (1.32) \]

where \( T \) is the kinetic energy of the system and where \( U \) is the potential energy.

Proof. For a conservative system the potential energy is independent on velocities, thus

\[ p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial T}{\partial \dot{q}_i}, \quad (1.33) \]

where \( L = T - U \) is the Lagrangian. The Hamiltonian is thus given by
1.4. Poisson’s Brackets

\[ \mathcal{H} = \sum_{i=1}^{N} p_i \dot{q}_i - \mathcal{L} = \sum_{l} \frac{\partial T}{\partial \dot{q}_l} \dot{q}_l - (T - U) = \sum_{l,n,m} \alpha_{nm} \left( \dot{q}_m \frac{\partial \dot{q}_n}{\partial \dot{q}_l} + \dot{q}_n \frac{\partial \dot{q}_m}{\partial \dot{q}_l} \right) \dot{q}_l - T + U \]
\[ = 2 \sum_{n,m} \alpha_{nm} \dot{q}_n \dot{q}_m - T + U = T + U. \]

(1.34)

1.4 Poisson’s Brackets

Consider two physical quantities \( F \) and \( G \) that can be expressed as a function of the vector of coordinates \( Q \), the vector of canonical conjugate variables \( P \) and time \( t \), namely
\[ F = F(Q, P; t) , \quad (1.35) \]
\[ G = G(Q, P; t) , \quad (1.36) \]

The Poisson’s brackets are defined by
\[ \{ F, G \} = \sum_{n=1}^{N} \left( \frac{\partial F}{\partial \dot{q}_n} \frac{\partial G}{\partial p_n} - \frac{\partial F}{\partial p_n} \frac{\partial G}{\partial \dot{q}_n} \right) , \quad (1.37) \]

The Poisson’s brackets are employed for writing an equation of motion for a general physical quantity of interest, as the following theorem shows.

**Theorem 1.4.1.** Let \( F \) be a physical quantity that can be expressed as a function of the vector of coordinates \( Q \), the vector of canonical conjugate variables \( P \) and time \( t \), and let \( \mathcal{H} \) be the Hamiltonian. Then, the following holds
\[ \frac{dF}{dt} = \{ F, \mathcal{H} \} + \frac{\partial F}{\partial t} . \]

(1.38)

**Proof.** Using Eqs. (1.23) and (1.24) one finds that the time derivative of \( F \) is given by
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\[
\frac{dF}{dt} = \sum_{n=1}^{N} \left( \frac{\partial F}{\partial q_n} \dot{q}_n + \frac{\partial F}{\partial p_n} \dot{p}_n \right) + \frac{\partial F}{\partial t} \\
= \sum_{n=1}^{N} \left( \frac{\partial F}{\partial q_n} \frac{\partial H}{\partial p_n} - \frac{\partial F}{\partial p_n} \frac{\partial H}{\partial q_n} \right) + \frac{\partial F}{\partial t} \\
= \{F,H\} + \frac{\partial F}{\partial t} .
\]

(1.39)

**Corollary 1.4.1.** If \( F \) does not explicitly depend on time, namely if \( \frac{\partial F}{\partial t} = 0 \), and if \( \{F,H\} = 0 \), then \( F \) is a constant of the motion, namely

\[
\frac{dF}{dt} = 0 .
\]

(1.40)

1.5 Problems

1. Consider a particle having charge \( q \) and mass \( m \) in electromagnetic field characterized by the scalar potential \( \varphi \) and the vector potential \( \mathbf{A} \). The electric field \( \mathbf{E} \) and the magnetic field \( \mathbf{B} \) are given by

\[
\mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} ,
\]

(1.41)

and

\[
\mathbf{B} = \nabla \times \mathbf{A} .
\]

(1.42)

Let \( \mathbf{r} = (x, y, z) \) be the Cartesian coordinates of the particle.

a) Verify that the Lagrangian of the system can be chosen to be given by

\[
\mathcal{L} = \frac{1}{2} m \dot{\mathbf{r}}^2 - q\varphi + \frac{q}{c} \mathbf{A} \cdot \dot{\mathbf{r}} ,
\]

(1.43)

by showing that the corresponding Euler-Lagrange equations are equivalent to Newton’s 2nd law (i.e., \( \mathbf{F} = m\mathbf{\ddot{r}} \)).

b) Show that the Hamilton-Jacobi equations are equivalent to Newton’s 2nd law.

c) **Gauge transformation** – The electromagnetic field is invariant under the gauge transformation of the scalar and vector potentials

\[
\mathbf{A} \rightarrow \mathbf{A} + \nabla \lambda ,
\]

(1.44)

\[
\varphi \rightarrow \varphi - \frac{1}{c} \frac{\partial \lambda}{\partial t}
\]

(1.45)

where \( \lambda = \lambda(\mathbf{r},t) \) is an arbitrary smooth and continuous function of \( \mathbf{r} \) and \( t \). What effect does this gauge transformation have on the Lagrangian and Hamiltonian? Is the motion affected?
2. Consider an LC resonator made of a capacitor having capacitance \( C \) in parallel with an inductor having inductance \( L \) (see Fig. 1.3). The state of the system is characterized by the coordinate \( q \), which is the charge stored by the capacitor.

a) Find the Euler-Lagrange equation of the system.

b) Find the Hamilton-Jacobi equations of the system.

c) Show that \( \{q,p\} = 1 \).

3. Show that Poisson brackets satisfy the following relations

\[
\{q_j, q_k\} = 0 , \quad (1.46)
\]

\[
\{p_j, p_k\} = 0 , \quad (1.47)
\]

\[
\{q_j, p_k\} = \delta_{jk} , \quad (1.48)
\]

\[
\{F,G\} = -\{G,F\} , \quad (1.49)
\]

\[
\{F,F\} = 0 , \quad (1.50)
\]

\[
\{F,K\} = 0 \text{ if } K \text{ constant or } F \text{ depends only on } t , \quad (1.51)
\]

\[
\{E + F,G\} = \{E,G\} + \{F,G\} , \quad (1.52)
\]

\[
\{E,FG\} = \{E,F\} G + F \{E,G\} . \quad (1.53)
\]

4. Show that the Lagrange equations are coordinate invariant.

5. Consider a point particle having mass \( m \) moving in a 3D central potential, namely a potential \( V(r) \) that depends only on the distance \( r = \sqrt{x^2 + y^2 + z^2} \) from the origin. Show that the angular momentum \( L = r \times p \) is a constant of the motion.

1.6 Solutions

1. The Lagrangian of the system (in Gaussian units) is taken to be given by

\[
\mathcal{L} = \frac{1}{2} m \dot{r}^2 - q \varphi + \frac{q}{c} \mathbf{A} \cdot \dot{\mathbf{r}} . \quad (1.54)
\]
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a) The Euler-Lagrange equation for the coordinate $x$ is given by

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x},$$

where

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = m \ddot{x} + \frac{q}{c} \left( \frac{\partial A_x}{\partial t} + \dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_x}{\partial y} + \dot{z} \frac{\partial A_x}{\partial z} \right),$$

and

$$\frac{\partial L}{\partial x} = -q \frac{\partial \phi}{\partial x} + \frac{q}{c} \left( \dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_y}{\partial x} + \dot{z} \frac{\partial A_z}{\partial x} \right),$$

thus

$$m \ddot{x} = -q \frac{\partial \phi}{\partial x} + \frac{q}{c} \left( \frac{\partial A_x}{\partial x} \right),$$

or

$$m \ddot{x} = q E_x + \frac{q}{c} (\dot{r} \times B)_x.$$  \hfill (1.59)

Similar equations are obtained for $\ddot{y}$ and $\ddot{z}$ in the same way. These 3 equations can be written in a vector form as

$$m \ddot{r} = q \left( E + \frac{1}{c} \dot{r} \times B \right).$$  \hfill (1.60)

b) The variable vector canonically conjugate to the coordinates vector $r$ is given by

$$p = \frac{\partial L}{\partial \dot{r}} = m \dot{r} + \frac{q}{c} A.$$  \hfill (1.61)

The Hamiltonian is thus given by
\( \mathcal{H} = p \cdot \dot{p} - L \)
\[= \dot{r} \cdot \left( p - \frac{1}{2} m \dot{r} - \frac{q}{c} \dot{A} \right) + q \varphi \]
\[= \frac{1}{2} m \dot{r}^2 + q \varphi \]
\[= \frac{(p - \frac{q}{c} A)^2}{2m} + q \varphi . \]

The Hamilton-Jacobi equation for the coordinate \( x \) is given by
\[ \dot{x} = \frac{\partial \mathcal{H}}{\partial p_x} , \] 
thus
\[ \dot{x} = \frac{p_x - \frac{q}{c} A_x}{m} , \] 
or
\[ p_x = m \dot{x} + \frac{q}{c} A_x \] .

The Hamilton-Jacobi equation for the canonically conjugate variable \( p_x \) is given by
\[ \dot{p}_x = -\frac{\partial \mathcal{H}}{\partial x} , \]
where
\[ \dot{p}_x = m \ddot{x} + \frac{q}{c} \left( \dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_y}{\partial x} + \dot{z} \frac{\partial A_z}{\partial x} \right) + \frac{q}{c} \frac{\partial A_x}{\partial t} , \] 
and
\[ -\frac{\partial \mathcal{H}}{\partial x} = \frac{q}{c} \left( \frac{p_x - \frac{q}{c} A_x}{m} \frac{\partial A_x}{\partial x} + \frac{p_y - \frac{q}{c} A_y}{m} \frac{\partial A_y}{\partial x} + \frac{p_z - \frac{q}{c} A_z}{m} \frac{\partial A_z}{\partial x} \right) - \frac{q}{c} \frac{\partial \varphi}{\partial x} \]
\[= \frac{q}{c} \left( \dot{x} \frac{\partial A_x}{\partial x} + \dot{y} \frac{\partial A_y}{\partial x} + \dot{z} \frac{\partial A_z}{\partial x} \right) - \frac{q}{c} \frac{\partial \varphi}{\partial x} , \]
thus
\[ m \ddot{x} = -q \frac{\partial \varphi}{\partial x} - q \frac{\partial A_x}{\partial t} + \frac{q}{c} \left[ \dot{y} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) - \dot{z} \left( \frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z} \right) \right] . \]

The last result is identical to Eq. (1.59).
c) Clearly, the fields $E$ and $B$, which are given by Eqs. (1.41) and (1.42) respectively, are unchanged since
\[ \nabla \left( \frac{\partial \lambda}{\partial t} \right) - \frac{\partial (\nabla \lambda)}{\partial t} = 0 , \] (1.70)

and
\[ \nabla \times (\nabla \lambda) = 0 . \] (1.71)

Thus, even though both $\mathcal{L}$ and $\mathcal{H}$ are modified, the motion, which depends on $E$ and $B$ only, is unaffected.

2. The kinetic energy in this case $T = Lq^2/2$ is the energy stored in the inductor, and the potential energy $U = q^2/2C$ is the energy stored in the capacitor.

a) The Lagrangian is given by
\[ \mathcal{L} = T - U = \frac{Lq^2}{2} - \frac{q^2}{2C} . \] (1.72)

The Euler-Lagrange equation for the coordinate $q$ is given by
\[ \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q} , \] (1.73)

thus
\[ \ddot{L}q + \frac{q}{C} = 0 . \] (1.74)

This equation expresses the requirement that the voltage across the capacitor is the same as the one across the inductor.

b) The canonical conjugate momentum is given by
\[ p = \frac{\partial \mathcal{L}}{\partial \dot{q}} = L\dot{q} , \] (1.75)

and the Hamiltonian is given by
\[ \mathcal{H} = p\dot{q} - \mathcal{L} = \frac{p^2}{2L} + \frac{q^2}{2C} . \] (1.76)

Hamilton-Jacobi equations read
\[ \dot{q} = \frac{p}{L} , \] (1.77)
\[ \dot{p} = -\frac{q}{C} , \] (1.78)

thus
\[ \ddot{L}q + \frac{q}{C} = 0 . \] (1.79)
1.6. Solutions

c) Using the definition (1.37) one has
\[
\{q, p\} = \frac{\partial q}{\partial q} \frac{\partial p}{\partial p} - \frac{\partial q}{\partial p} \frac{\partial p}{\partial q} = 1. \tag{1.80}
\]

3. All these relations are easily proven using the definition (1.37).

4. Let \( \mathcal{L} = \mathcal{L}(Q, \dot{Q}; t) \) be a Lagrangian of a system, where \( Q = (q_1, q_2, \cdots) \) is the vector of coordinates, \( \dot{Q} = (\dot{q}_1, \dot{q}_2, \cdots) \) is the vector of velocities, and where overdot denotes time derivative. Consider the coordinates transformation
\[
x_a = x_a(q_1, q_2, \ldots, t), \tag{1.81}
\]
where \( a = 1, 2, \cdots \). The following holds
\[
\dot{x}_a = \frac{\partial x_a}{\partial q_b} \dot{q}_b + \frac{\partial x_a}{\partial t}, \tag{1.82}
\]
where the summation convention is being used, namely, repeated indices are summed over. Moreover
\[
\frac{\partial \mathcal{L}}{\partial q_a} = \frac{\partial \mathcal{L}}{\partial x_b} \frac{\partial x_a}{\partial q_b} + \frac{\partial \mathcal{L}}{\partial \dot{x}_b} \frac{\partial \dot{x}_a}{\partial q_b}, \tag{1.83}
\]
and
\[
\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_a} \right) = \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{x}_b} \frac{\partial \dot{x}_a}{\partial q_b} \right). \tag{1.84}
\]
As can be seen from Eq. (1.82), the second term vanishes since
\[
\frac{\partial \dot{x}_b}{\partial \dot{q}_a} = \frac{\partial x_b}{\partial q_a}, \tag{1.85}
\]
Thus, using Eqs. (1.83) and (1.84) one finds
\[
\frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_a} \right) - \frac{\partial \mathcal{L}}{\partial q_a} = \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial x_b} \frac{\partial x_a}{\partial q_b} \right) - \frac{\partial \mathcal{L}}{\partial x_b} \frac{\partial \dot{x}_a}{\partial q_b} - \frac{\partial \mathcal{L}}{\partial \dot{x}_b} \frac{\partial \dot{x}_a}{\partial q_b} = \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial x_b} \right) \frac{\partial x_a}{\partial q_b} + \left[ \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial x_b} \right) \frac{\partial x_a}{\partial q_b} \right] \frac{\partial \dot{x}_b}{\partial q_a} + \frac{\partial \dot{x}_b}{\partial q_a} \frac{\partial \mathcal{L}}{\partial \dot{x}_b}. \tag{1.86}
\]
As can be seen from Eq. (1.82), the second term vanishes since
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\[ \frac{\partial x_b}{\partial q_a} = \frac{\partial^2 x_b}{\partial q_a \partial q_c} \dot{q}_c + \frac{\partial^2 x_b}{\partial t \partial q_a} = \frac{d}{dt} \left( \frac{\partial x_b}{\partial q_a} \right), \]

thus

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_a} \right) - \frac{\partial L}{\partial q_a} = \left[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_b} \right) - \frac{\partial L}{\partial x_b} \right] \frac{\partial x_b}{\partial q_a}. \] (1.87)

The last result shows that if the coordinate transformation is reversible, namely if \( \det \left( \frac{\partial x_b}{\partial q_a} \right) \neq 0 \) then Lagrange equations are coordinate invariant.

5. The angular momentum \( \mathbf{L} \) is given by

\[ \mathbf{L} = \mathbf{r} \times \mathbf{p} = \text{det} \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{pmatrix}, \] (1.88)

where \( \mathbf{r} = (x, y, z) \) is the position vector and where \( \mathbf{p} = (p_x, p_y, p_z) \) is the momentum vector. The Hamiltonian is given by

\[ \mathcal{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}). \] (1.89)

Using

\[ \{x_i, p_j\} = \delta_{ij}, \]
\[ L_z = xp_y - yp_x, \]

one finds that

\[ \{p^2, L_z\} = \{p_x^2, L_z\} + \{p_y^2, L_z\} + \{p_z^2, L_z\} \]
\[ = \{p_x^2, xp_y\} - \{p_y^2, yp_x\} \]
\[ = -2p_xp_y + 2p_yp_x \]
\[ = 0, \] (1.92)

and

\[ \{r^2, L_z\} = \{x^2, L_z\} + \{y^2, L_z\} + \{z^2, L_z\} \]
\[ = -y \{x^2, p_x\} + \{y^2, p_y\} x \]
\[ = 0. \] (1.93)

Thus \( \{f(r^2), L_z\} = 0 \) for arbitrary smooth function \( f(\mathbf{r}^2) \), and consequently \( \{\mathcal{H}, L_z\} = 0 \). In a similar way one can show that \( \{\mathcal{H}, L_y\} = \{\mathcal{H}, L_x\} = 0 \), and therefore \( \{\mathcal{H}, \mathbf{L}^2\} = 0 \).
2. State Vectors and Operators

In quantum mechanics the state of a physical system is described by a state vector $|\alpha\rangle$, which is a vector in a vector space $\mathcal{F}$, namely

$$|\alpha\rangle \in \mathcal{F}.$$  \hfill (2.1)

Here, we have employed the Dirac’s ket-vector notation $|\alpha\rangle$ for the state vector, which contains all information about the state of the physical system under study. The dimensionality of $\mathcal{F}$ is finite in some specific cases (notably, spin systems), however, it can also be infinite in many other cases of interest. The basic mathematical theory dealing with vector spaces having infinite dimensionality was mainly developed by David Hilbert. Under some conditions, vector spaces having infinite dimensionality have properties similar to those of their finite dimensionality counterparts. A mathematically rigorous treatment of such vector spaces having infinite dimensionality, which are commonly called Hilbert spaces, can be found in textbooks that are devoted to this subject. In this chapter, however, we will only review the main properties that are useful for quantum mechanics. In some cases, when the generalization from the case of finite dimensionality to the case of arbitrary dimensionality is nontrivial, results will be presented without providing a rigorous proof and even without accurately specifying what are the validity conditions for these results.

2.1 Linear Vector Space

A linear vector space $\mathcal{F}$ is a set $\{|\alpha\rangle\}$ of mathematical objects called vectors. The space is assumed to be closed under vector addition and scalar multiplication. Both, operations (i.e., vector addition and scalar multiplication) are commutative. That is:

1. $|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle \in \mathcal{F}$ for every $|\alpha\rangle \in \mathcal{F}$ and $|\beta\rangle \in \mathcal{F}$
2. $c|\alpha\rangle = |\alpha\rangle c \in \mathcal{F}$ for every $|\alpha\rangle \in \mathcal{F}$ and $c \in \mathbb{C}$

where $\mathbb{C}$ is the set of complex numbers. A vector space with an inner product is called an inner product space. An inner product of the ordered
Chapter 2. State Vectors and Operators

pair $|\alpha\rangle , |\beta\rangle \in \mathcal{F}$ is denoted as $\langle \beta | \alpha \rangle$. The inner product is a function $\mathcal{F}^2 \to \mathbb{C}$ that satisfies the following properties:

$$\langle \beta | \alpha \rangle \in \mathbb{C} ,$$  \hspace{1cm} (2.2)

$$\langle \beta | \alpha \rangle = \langle \alpha | \beta \rangle^* ,$$  \hspace{1cm} (2.3)

$$\langle \alpha | (c_1 | \beta_1 \rangle + c_2 | \beta_2 \rangle) = c_1 \langle \alpha | \beta_1 \rangle + c_2 \langle \alpha | \beta_2 \rangle , \text{ where } c_1, c_2 \in \mathbb{C} ,$$  \hspace{1cm} (2.4)

$$\langle \alpha | \alpha \rangle \in \mathbb{R} \text{ and } \langle \alpha | \alpha \rangle \geq 0. \text{ Equality holds iff } |\alpha\rangle = 0 .$$  \hspace{1cm} (2.5)

Note that the asterisk in Eq. (2.3) denotes complex conjugate. Below we list some important definitions and comments regarding inner product:

- The real number $\sqrt{\langle \alpha | \alpha \rangle}$ is called the norm of the vector $|\alpha\rangle \in \mathcal{F}$.
- A normalized vector has a unity norm, namely $\langle \alpha | \alpha \rangle = 1$.
- Every nonzero vector $0 \neq |\alpha\rangle \in \mathcal{F}$ can be normalized using the transformation

$$|\alpha\rangle \to \frac{|\alpha\rangle}{\sqrt{\langle \alpha | \alpha \rangle}} .$$  \hspace{1cm} (2.6)

- The vectors $|\alpha\rangle \in \mathcal{F}$ and $|\beta\rangle \in \mathcal{F}$ are said to be orthogonal if $\langle \beta | \alpha \rangle = 0$.
- A set of vectors $\{|\phi_n\rangle\}_n$, where $|\phi_n\rangle \in \mathcal{F}$ is called a complete orthonormal basis if
  - The vectors are all normalized and orthogonal to each other, namely

$$\langle \phi_m | \phi_n \rangle = \delta_{nm} .$$  \hspace{1cm} (2.7)

  - Every $|\alpha\rangle \in \mathcal{F}$ can be written as a superposition of the basis vectors, namely

$$|\alpha\rangle = \sum_n c_n |\phi_n\rangle ,$$  \hspace{1cm} (2.8)

where $c_n \in \mathbb{C}$.
- By evaluating the inner product $\langle \phi_m | \alpha \rangle$, where $|\alpha\rangle$ is given by Eq. (2.8) one finds with the help of Eq. (2.7) and property (2.4) of inner products that

$$\langle \phi_m | \alpha \rangle = \langle \phi_m \left( \sum_n c_n |\phi_n\rangle \right) = \sum_n c_n \langle \phi_m | \phi_n \rangle = c_m \cdot \delta_{nm} .$$  \hspace{1cm} (2.9)

- The last result allows rewriting Eq. (2.8) as

$$|\alpha\rangle = \sum_n c_n |\phi_n\rangle = \sum_n |\phi_n\rangle c_n = \sum_n |\phi_n\rangle \langle \phi_n | \alpha \rangle . \hspace{1cm} (2.10)$$
2.2 Operators

Operators, as the definition below states, are function from $\mathcal{F}$ to $\mathcal{F}$:

**Definition 2.2.1.** An operator $A : \mathcal{F} \to \mathcal{F}$ on a vector space maps vectors onto vectors, namely $A(|\alpha\rangle) \in \mathcal{F}$ for every $|\alpha\rangle \in \mathcal{F}$.

Some important definitions and comments are listed below:

- The operators $X : \mathcal{F} \to \mathcal{F}$ and $Y : \mathcal{F} \to \mathcal{F}$ are said to be equal, namely $X = Y$, if for every $|\alpha\rangle \in \mathcal{F}$ the following holds
  \[ X|\alpha\rangle = Y|\alpha\rangle. \]  
  (2.11)

- Operators can be added, and the addition is both, commutative and associative, namely
  \[ X + Y = Y + X, \]  
  (2.12)
  \[ X + (Y + Z) = (X + Y) + Z. \]  
  (2.13)

- An operator $A : \mathcal{F} \to \mathcal{F}$ is said to be linear if
  \[ A(c_1|\gamma_1\rangle + c_2|\gamma_2\rangle) = c_1A|\gamma_1\rangle + c_2A|\gamma_2\rangle \]  
  (2.14)
  for every $|\gamma_1\rangle, |\gamma_2\rangle \in \mathcal{F}$ and $c_1, c_2 \in \mathbb{C}$.

- The operators $X : \mathcal{F} \to \mathcal{F}$ and $Y : \mathcal{F} \to \mathcal{F}$ can be multiplied, where
  \[ XY|\alpha\rangle = X(Y|\alpha\rangle) \]  
  (2.15)
  for any $|\alpha\rangle \in \mathcal{F}$.

- Operator multiplication is associative
  \[ X(YZ) = (XY)Z = XYZ. \]  
  (2.16)

- However, in general operator multiplication needs not be commutative
  \[ XY \neq YX. \]  
  (2.17)

2.3 Dirac’s notation

In Dirac’s notation the inner product is considered as a multiplication of two mathematical objects called ‘bra’ and ‘ket’

\[ \langle \beta | \alpha \rangle = \langle \beta | \rangle \langle \rangle_\text{bra} \langle \rangle_\text{ket}. \]  
(2.18)

While the ket-vector $|\alpha\rangle$ is a vector in $\mathcal{F}$, the bra-vector $\langle \beta \rangle$ represents a functional that maps any ket-vector $|\alpha\rangle \in \mathcal{F}$ to the complex number $\langle \beta | \alpha \rangle$. 

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While the multiplication of a bra-vector on the left and a ket-vector on the right represents inner product, the *outer product* is obtained by reversing the order
\[ A_{\alpha\beta} = |\alpha\rangle \langle \beta| . \] (2.19)

The outer product \( A_{\alpha\beta} \) is clearly an operator since for any \( |\gamma\rangle \in \mathcal{F} \) the object \( A_{\alpha\beta} |\gamma\rangle \) is a ket-vector
\[ A_{\alpha\beta} |\gamma\rangle = (|\beta\rangle \langle \alpha|) |\gamma\rangle = |\beta\rangle \sum_{\epsilon \in \mathbb{C}} \langle \alpha| |\gamma\rangle \in \mathcal{F} . \] (2.20)

Moreover, according to property (2.4), \( A_{\alpha\beta} \) is linear since for every \( |\gamma_1\rangle, |\gamma_2\rangle \in \mathcal{F} \) and \( c_1, c_2 \in \mathbb{C} \) the following holds
\[ A_{\alpha\beta}(c_1 |\gamma_1\rangle + c_2 |\gamma_2\rangle) = |\alpha\rangle \langle \beta| (c_1 |\gamma_1\rangle + c_2 |\gamma_2\rangle) \]
\[ = |\alpha\rangle (c_1 \langle \beta| |\gamma_1\rangle + c_2 \langle \beta| |\gamma_2\rangle) \]
\[ = c_1 A_{\alpha\beta} |\gamma_1\rangle + c_2 A_{\alpha\beta} |\gamma_2\rangle . \] (2.21)

With Dirac’s notation Eq. (2.10) can be rewritten as
\[ |\alpha\rangle = \left( \sum_n |\phi_n\rangle \langle n| \right) |\alpha\rangle . \] (2.22)

Since the above identity holds for any \( |\alpha\rangle \in \mathcal{F} \) one concludes that the quantity in brackets is the identity operator, which is denoted as 1, namely
\[ 1 = \sum_n |\phi_n\rangle \langle n| . \] (2.23)

This result, which is called the closure relation, implies that any complete orthonormal basis can be used to express the identity operator.

### 2.4 Dual Correspondence

As we have mentioned above, the bra-vector \( \langle \beta| \) represents a functional mapping any ket-vector \( |\alpha\rangle \in \mathcal{F} \) to the complex number \( \langle \beta| |\alpha\rangle \). Moreover, since the inner product is linear [see property (2.4) above], such a mapping is linear, namely for every \( |\gamma_1\rangle, |\gamma_2\rangle \in \mathcal{F} \) and \( c_1, c_2 \in \mathbb{C} \) the following holds
\[ \langle \beta| (c_1 |\gamma_1\rangle + c_2 |\gamma_2\rangle) = c_1 \langle \beta| |\gamma_1\rangle + c_2 \langle \beta| |\gamma_2\rangle . \] (2.24)

The set of linear functionals from \( \mathcal{F} \) to \( \mathbb{C} \), namely, the set of functionals \( F : \mathcal{F} \to \mathbb{C} \) that satisfy
2.4. Dual Correspondence

\[ F (c_1 \gamma_1 + c_2 \gamma_2) = c_1 F (\gamma_1) + c_2 F (\gamma_2) \quad (2.25) \]

for every \( \gamma_1, \gamma_2 \in \mathcal{F} \) and \( c_1, c_2 \in \mathcal{C} \), is called the dual space \( \mathcal{F}^* \). As the name suggests, there is a dual correspondence (DC) between \( \mathcal{F} \) and \( \mathcal{F}^* \), namely a one to one mapping between these two sets, which are both linear vector spaces. The duality relation is presented using the notation

\[ h \alpha \left| \alpha \right> \leftrightarrow \left| \alpha \right> \quad (\text{2.26}) \]

where \( \left| \alpha \right> \in \mathcal{F} \) and \( h \alpha \left| \alpha \right> \in \mathcal{F}^* \). What is the dual of the ket-vector

\[ \left| \gamma \right> = c_1 \left| \gamma_1 \right> + c_2 \left| \gamma_2 \right> \]

where \( \left| \gamma_1 \right>, \left| \gamma_2 \right> \in \mathcal{F} \) and \( c_1, c_2 \in \mathcal{C} \)? To answer this question we employ the above mentioned general properties (2.3) and (2.4) of inner products and consider the quantity \( \langle \gamma | \alpha \rangle \) for an arbitrary ket-vector \( \left| \alpha \right> \in \mathcal{F} \)

\[ \langle \gamma | \alpha \rangle = \langle \alpha | \gamma \rangle^* = (c_1 \langle \alpha | \gamma_1 \rangle + c_2 \langle \alpha | \gamma_2 \rangle)^* = (c_1^* \langle \gamma_1 | \alpha \rangle + c_2^* \langle \gamma_2 | \alpha \rangle) \left| \alpha \right>. \quad (2.27) \]

From this result we conclude that the duality relation takes the form

\[ c_1^* \langle \gamma_1 | + c_2^* \langle \gamma_2 | \leftrightarrow c_1 \left| \gamma_1 \right> + c_2 \left| \gamma_2 \right> \quad (2.28) \]

The last relation describes how to map any given ket-vector \( \left| \beta \right> \in \mathcal{F} \) to its dual \( F = \langle \beta | : \mathcal{F} \to \mathcal{C} \), where \( F \in \mathcal{F}^* \) is a linear functional that maps any ket-vector \( \left| \alpha \right> \in \mathcal{F} \) to the complex number \( \langle \beta | \alpha \rangle \). What is the inverse mapping? The answer can take a relatively simple form provided that a complete orthonormal basis exists, and consequently the identity operator can be expressed as in Eq. (2.23). In that case the dual of a given linear functional \( F : \mathcal{F} \to \mathcal{C} \) is the ket-vector \( \left| F_D \right> \in \mathcal{F} \), which is given by

\[ \left| F_D \right> = \sum_n (F (\phi_n))^* \phi_n \quad (2.29) \]

The duality is demonstrated by proving the two claims below:

Claim. \( \left| \beta_{DD} \right> = \left| \beta \right> \) for any \( \left| \beta \right> \in \mathcal{F} \), where \( \left| \beta_{DD} \right> \) is the dual of the dual of \( \left| \beta \right> \).

Proof. The dual of \( \left| \beta \right> \) is the bra-vector \( \langle \beta | \), whereas the dual of \( \langle \beta | \) is found using Eqs. (2.29) and (2.23), thus
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\[ |\beta_{DD}\rangle = \sum_n \langle \beta | \phi_n \rangle^* |\phi_n\rangle = \sum_n |\phi_n\rangle \langle \phi_n | \beta \rangle = \sum_n |\phi_n\rangle \langle \phi_n | |\beta\rangle = |\beta\rangle . \]  

\textit{Claim}. \( F_{DD} = F \) for any \( F \in F^* \), where \( F_{DD} \) is the dual of the dual of \( F \).

\textit{Proof}. The dual \( |F_D\rangle \in F \) of the functional \( F \in F^* \) is given by Eq. (2.29). Thus with the help of the duality relation (2.28) one finds that dual \( F_{DD} \in F^* \) of \( |F_D\rangle \) is given by

\[ F_{DD} = \sum_n F (|\phi_n\rangle) \langle \phi_n | . \]  

Consider an arbitrary ket-vector \( |\alpha\rangle \in F \) that is written as a superposition of the complete orthonormal basis vectors, namely

\[ |\alpha\rangle = \sum_m c_m |\phi_m\rangle . \]

Using the above expression for \( F_{DD} \) and the linearity property one finds that

\[ F_{DD} |\alpha\rangle = \sum_{n,m} c_m F (|\phi_n\rangle) \langle \phi_n | |\phi_m\rangle \delta_{mn} = \sum_n c_n F (|\phi_n\rangle) = F \left( \sum_n c_n |\phi_n\rangle \right) = F |\alpha\rangle , \]

therefore, \( F_{DD} = F \).

\[ \]  

\textbf{2.5 Matrix Representation}

Given a complete orthonormal basis, ket-vectors, bra-vectors and linear operators can be represented using matrices. Such representations are easily obtained using the closure relation (2.23).
2.5. Matrix Representation

- The inner product between the bra-vector $\langle \beta \vert$ and the ket-vector $\vert \alpha \rangle$ can be written as

$$\langle \beta \vert \alpha \rangle = \sum_n \langle \beta \vert \phi_n \rangle \langle \phi_n \vert \alpha \rangle = \left( \frac{\langle \phi_1 \vert \alpha \rangle}{\langle \phi_2 \vert \alpha \rangle} \right) \cdot \cdot \cdot ,$$

(2.34)

Thus, the inner product can be viewed as a product between the row vector

$$\langle \beta \vert \equiv \left( \begin{array}{c} \langle \phi_1 \vert \\ \langle \phi_2 \vert \\ \vdots \end{array} \right) ,$$

(2.35)

which is the matrix representation of the bra-vector $\langle \beta \vert$, and the column vector

$$\vert \alpha \rangle \equiv \left( \begin{array}{c} \langle \phi_1 \vert \\ \langle \phi_2 \vert \\ \vdots \end{array} \right) ,$$

(2.36)

which is the matrix representation of the ket-vector $\vert \alpha \rangle$. Obviously, both representations are basis dependent.

- Multiplying the relation $\vert \gamma \rangle = X \vert \alpha \rangle$ from the right by the basis bra-vector $\langle \phi_m \vert$ and employing again the closure relation (2.23) yields

$$\langle \phi_m \vert \gamma \rangle = \langle \phi_m \vert X \vert \alpha \rangle = \langle \phi_m \vert X \vert \phi_n \rangle \langle \phi_n \vert \alpha \rangle ,$$

(2.37)

or in matrix form

$$\left( \begin{array}{c} \langle \phi_1 \vert \\ \langle \phi_2 \vert \\ \vdots \end{array} \right) = \left( \begin{array}{c} \langle \phi_1 \vert X \vert \phi_1 \rangle \langle \phi_1 \vert \phi_2 \rangle \cdot \cdot \cdot \\ \langle \phi_2 \vert X \vert \phi_1 \rangle \langle \phi_2 \vert \phi_2 \rangle \cdot \cdot \cdot \\ \vdots \end{array} \right) \cdot \left( \begin{array}{c} \langle \phi_1 \vert \alpha \rangle \\ \langle \phi_2 \vert \alpha \rangle \\ \vdots \end{array} \right) .$$

(2.38)

In view of this expression, the matrix representation of the linear operator $X$ is given by

$$X \equiv \left( \begin{array}{c} \langle \phi_1 \vert X \vert \phi_1 \rangle \langle \phi_1 \vert X \vert \phi_2 \rangle \cdot \cdot \cdot \\ \langle \phi_2 \vert X \vert \phi_1 \rangle \langle \phi_2 \vert X \vert \phi_2 \rangle \cdot \cdot \cdot \\ \vdots \end{array} \right) .$$

(2.39)

Alternatively, the last result can be written as

$$X_{nm} = \langle \phi_n \vert X \vert \phi_m \rangle ,$$

(2.40)

where $X_{nm}$ is the element in row $n$ and column $m$ of the matrix representation of the operator $X$. 
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- Such matrix representation of linear operators can be useful also for multiplying linear operators. The matrix elements of the product $Z = XY$ are given by

$$
\langle \phi_m | Z | \phi_n \rangle = \langle \phi_m | XY | \phi_n \rangle = \sum_l \langle \phi_m | X | \phi_l \rangle \langle \phi_l | Y | \phi_n \rangle.
$$

(2.41)

- Similarly, the matrix representation of the outer product $|\beta\rangle \langle \alpha|$ is given by

$$
|\beta\rangle \langle \alpha| = \begin{pmatrix}
\langle \phi_1 | \beta \rangle \\
\langle \phi_2 | \beta \rangle \\
\vdots
\end{pmatrix}
\begin{pmatrix}
\langle \alpha | \phi_1 \rangle \\
\langle \alpha | \phi_2 \rangle \\
\vdots
\end{pmatrix}
= \begin{pmatrix}
\langle \phi_1 | \beta \rangle \langle \alpha | \phi_1 \rangle & \langle \phi_1 | \beta \rangle \langle \alpha | \phi_2 \rangle & \cdots \\
\langle \phi_2 | \beta \rangle \langle \alpha | \phi_1 \rangle & \langle \phi_2 | \beta \rangle \langle \alpha | \phi_2 \rangle & \cdots \\
\vdots & \vdots & \ddots
\end{pmatrix}.
$$

(2.42)

2.6 Observables

Measurable physical variables are represented in quantum mechanics by Hermitian operators.

2.6.1 Hermitian Adjoint

**Definition 2.6.1.** The Hermitian adjoint of an operator $X$ is denoted as $X^\dagger$ and is defined by the following duality relation

$$
\langle \alpha | X^\dagger \leftrightarrow X | \alpha \rangle.
$$

(2.43)

Namely, for any ket-vector $|\alpha\rangle \in \mathcal{F}$, the dual to the ket-vector $X |\alpha\rangle$ is the bra-vector $\langle \alpha | X^\dagger$.

**Definition 2.6.2.** An operator is said to be Hermitian if $X = X^\dagger$.

Below we prove some simple relations:

**Claim.** $\langle \beta | X | \alpha \rangle = \langle \alpha | X^\dagger | \beta \rangle^*$

**Proof.** Using the general property (2.3) of inner products one has

$$
\langle \beta | X | \alpha \rangle = \langle \beta | (X | \alpha \rangle) = \langle (\langle \alpha | X^\dagger | \beta \rangle)^* = \langle \alpha | X^\dagger | \beta \rangle^*.
$$

(2.44)

Note that this result implies that if $X = X^\dagger$ then $\langle \beta | X | \alpha \rangle = \langle \alpha | X | \beta \rangle^*$. 

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Claim. \((X^\dagger)^\dagger = X\)

Proof. For any \(|\alpha\rangle, |\beta\rangle \in \mathcal{F}\) the following holds
\[
\langle \beta | X | \alpha \rangle = (\langle \beta | X | \alpha \rangle^\dagger)^* = (\langle \alpha | X^\dagger | \beta \rangle)^* = \langle \beta | (X^\dagger)^\dagger | \alpha \rangle ,
\]
thus \((X^\dagger)^\dagger = X\).

Claim. \((XY)^\dagger = Y^\dagger X^\dagger\)

Proof. Applying \(XY\) on an arbitrary ket-vector \(|\alpha\rangle \in \mathcal{F}\) and employing the duality correspondence yield
\[
XY |\alpha\rangle = X (Y |\alpha\rangle) \leftrightarrow (\langle \alpha | Y^\dagger\rangle X^\dagger = \langle \alpha | Y^\dagger X^\dagger ,
\]
thus
\[
(XY)^\dagger = Y^\dagger X^\dagger .
\]

Claim. If \(X = |\beta\rangle \langle \alpha|\) then \(X^\dagger = |\alpha\rangle \langle \beta|\)

Proof. By applying \(X\) on an arbitrary ket-vector \(|\gamma\rangle \in \mathcal{F}\) and employing the duality correspondence one finds that
\[
X |\gamma\rangle = (|\beta\rangle \langle \alpha|) |\gamma\rangle = |\beta\rangle (\langle \alpha |\gamma\rangle) \leftrightarrow (\langle \alpha | \gamma\rangle)^* |\beta\rangle = \langle \gamma | \alpha\rangle \langle \beta| = \langle \gamma | X^\dagger ,
\]
where \(X^\dagger = |\alpha\rangle \langle \beta|\).

### 2.6.2 Eigenvalues and Eigenvectors

Each operator is characterized by its set of eigenvalues, which is defined below:

**Definition 2.6.3.** A number \(a_n \in \mathbb{C}\) is said to be an eigenvalue of an operator \(A : \mathcal{F} \rightarrow \mathcal{F}\) if for some nonzero ket-vector \(|a_n\rangle \in \mathcal{F}\) the following holds
\[
A |a_n\rangle = a_n |a_n\rangle .
\]

The ket-vector \(|a_n\rangle\) is then said to be an eigenvector of the operator \(A\) with an eigenvalue \(a_n\).

The set of eigenvectors associated with a given eigenvalue of an operator \(A\) is called eigensubspace and is denoted as
\[
\mathcal{F}_n = \{|a_n\rangle \in \mathcal{F} \text{ such that } A |a_n\rangle = a_n |a_n\rangle \} .
\]
Clearly, $\mathcal{F}_n$ is closed under vector addition and scalar multiplication, namely $c_1 |\gamma_1\rangle + c_2 |\gamma_2\rangle \in \mathcal{F}_n$ for every $|\gamma_1\rangle, |\gamma_2\rangle \in \mathcal{F}_n$ and for every $c_1, c_2 \in \mathbb{C}$ Thus, the set $\mathcal{F}_n$ is a subspace of $\mathcal{F}$. The dimensionality of $\mathcal{F}_n$ (i.e., the minimum number of vectors that are needed to span $\mathcal{F}_n$) is called the level of degeneracy $g_n$ of the eigenvalue $a_n$, namely

$$g_n = \dim \mathcal{F}_n \ .$$

(2.51)

As the theorem below shows, the eigenvalues and eigenvectors of a Hermitian operator have some unique properties.

**Theorem 2.6.1.** The eigenvalues of a Hermitian operator $A$ are real. The eigenvectors of $A$ corresponding to different eigenvalues are orthogonal.

**Proof.** Let $a_1$ and $a_2$ be two eigenvalues of $A$ with corresponding eigenvectors $|a_1\rangle$ and $|a_2\rangle$

$$A |a_1\rangle = a_1 |a_1\rangle \ ,$$

(2.52)

$$A |a_2\rangle = a_2 |a_2\rangle \ .$$

(2.53)

Multiplying Eq. (2.52) from the left by the bra-vector $\langle a_2 |$, and multiplying the dual of Eq. (2.53), which since $A = A^\dagger$ is given by

$$\langle a_2 | A = a_2^* \langle a_2 | \ ,$$

(2.54)

from the right by the ket-vector $|a_1\rangle$ yield

$$\langle a_2 | A |a_1\rangle = a_1 \langle a_2 | a_1\rangle \ ,$$

(2.55)

$$\langle a_2 | A |a_1\rangle = a_2^* \langle a_2 | a_1\rangle \ .$$

(2.56)

Thus, we have found that

$$(a_1 - a_2^*) \langle a_2 | a_1\rangle = 0 \ .$$

(2.57)

The first part of the theorem is proven by employing the last result (2.57) for the case where $|a_1\rangle = |a_2\rangle$. Since $|a_1\rangle$ is assumed to be a nonzero ket-vector one concludes that $a_1 = a_1^*$, namely $a_1$ is real. Since this is true for any eigenvalue of $A$, one can rewrite Eq. (2.57) as

$$(a_1 - a_2) \langle a_2 | a_1\rangle = 0 \ .$$

(2.58)

The second part of the theorem is proven by considering the case where $a_1 \neq a_2$, for which the above result (2.58) can hold only if $\langle a_2 | a_1\rangle = 0$. Namely eigenvectors corresponding to different eigenvalues are orthogonal.

Consider a Hermitian operator $A$ having a set of eigenvalues $\{a_n\}_n$. Let $g_n$ be the degree of degeneracy of eigenvalue $a_n$, namely $g_n$ is the dimension of the corresponding eigensubspace, which is denoted by $\mathcal{F}_n$. For simplicity, assume that $g_n$ is finite for every $n$. Let $\{|a_{n,1}\rangle, |a_{n,2}\rangle, \ldots, |a_{n,g_n}\rangle\}$ be
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an orthonormal basis of the eigensubspace $F_n$, namely $\langle a_{n,i'} | a_{n,i} \rangle = \delta_{i'i'}$. Constructing such an orthonormal basis for $F_n$ can be done by the so-called *Gram-Schmidt process*. Moreover, since eigenvectors of $A$ corresponding to different eigenvalues are orthogonal, the following holds

$$\langle a_{n,i'} | a_{n,i} \rangle = \delta_{i'i'}.$$  \hspace{1cm} (2.59)

In addition, all the ket-vectors $|a_{n,i} \rangle$ are eigenvectors of $A$

$$A |a_{n,i} \rangle = a_n |a_{n,i} \rangle.$$  \hspace{1cm} (2.60)

**Projectors.** Projector operators are useful for expressing the properties of an observable.

**Definition 2.6.4.** An Hermitian operator $P$ is called a projector if $P^2 = P$.

Claim. The only possible eigenvalues of a projector are 0 and 1.

**Proof.** Assume that $|p \rangle$ is an eigenvector of $P$ with an eigenvalue $p$, namely $P |p \rangle = p |p \rangle$. Applying the operator $P$ on both sides and using the fact that $P^2 = P$ yield $P^2 |p \rangle = p^2 |p \rangle$, thus $p(1-p) |p \rangle = 0$, therefore since $|p \rangle$ is assumed to be nonzero, either $p = 0$ or $p = 1$.

A projector is said to project any given vector onto the eigensubspace corresponding to the eigenvalue $p = 1$.

Let $\{ |a_{n,1} \rangle, |a_{n,2} \rangle, \cdots, |a_{n,g_n} \rangle \}$ be an orthonormal basis of an eigensubspace $F_n$ corresponding to an eigenvalue of an observable $A$. Such an orthonormal basis can be used to construct a projection $P_n$ onto $F_n$, which is given by

$$P_n = \sum_{i=1}^{g_n} |a_{n,i} \rangle \langle a_{n,i}|.$$  \hspace{1cm} (2.61)

Clearly, $P_n$ is a projector since $P_n^\dagger = P_n$ and since

$$P_n^2 = \sum_{i,i'=1}^{g_n} |a_{n,i} \rangle \langle a_{n,i'}| \delta_{i'i'} = \sum_{i=1}^{g_n} |a_{n,i} \rangle \langle a_{n,i}| = P_n.$$  \hspace{1cm} (2.62)

Moreover, it is easy to show using the orthonormality relation (2.59) that the following holds

$$P_n P_m = P_m P_n = P_n \delta_{nm}.$$  \hspace{1cm} (2.63)

For linear vector spaces of finite dimensionality, it can be shown that the set $\{|a_{n,i} \rangle\}_{n,i}$ forms a complete orthonormal basis of eigenvectors of a given Hermitian operator $A$. The generalization of this result for the case of arbitrary dimensionality is nontrivial, since generally such a set needs not be
complete. On the other hand, it can be shown that if a given Hermitian operator \( A \) satisfies some conditions (e.g., \( A \) needs to be completely continuous) then completeness is guaranteed. For all Hermitian operators of interest for this course we will assume that all such conditions are satisfied. That is, for any such Hermitian operator \( A \) there exists a set of ket vectors \( \{ |a_{n,i}\rangle \} \), such that:

1. The set is orthonormal, namely
\[
\langle a_{n',i'} | a_{n,i}\rangle = \delta_{nn'} \delta_{ii'},
\]  
(2.64)

2. The ket-vectors \( |a_{n,i}\rangle \) are eigenvectors, namely
\[
A |a_{n,i}\rangle = a_n |a_{n,i}\rangle ,
\]  
(2.65)

where \( a_n \in \mathbb{R} \).

3. The set is complete, namely closure relation [see also Eq. (2.23)] is satisfied
\[
1 = \sum_n \sum_{i=1}^{g_n} |a_{n,i}\rangle \langle a_{n,i}| = \sum_n P_n ,
\]  
(2.66)

where
\[
P_n = \sum_{i=1}^{g_n} |a_{n,i}\rangle \langle a_{n,i}|
\]  
(2.67)

is the projector onto eigen subspace \( \mathcal{F}_n \) with the corresponding eigenvalue \( a_n \).

The closure relation (2.66) can be used to express the operator \( A \) in terms of the projectors \( P_n \)
\[
A = A1 = \sum_n \sum_{i=1}^{g_n} A |a_{n,i}\rangle \langle a_{n,i}| = \sum_n a_n \sum_{i=1}^{g_n} |a_{n,i}\rangle \langle a_{n,i}| ,
\]  
(2.68)

that is
\[
A = \sum_n a_n P_n .
\]  
(2.69)

The last result is very useful when dealing with a function \( f(A) \) of the operator \( A \). The meaning of a function of an operator can be understood in terms of the Taylor expansion of the function
\[
f(x) = \sum_m f_m x^m ,
\]  
(2.70)
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where

\[ f_m = \frac{1}{m!} \frac{\text{d}^m f}{\text{d}x^m}. \]  

(2.71)

With the help of Eqs. (2.63) and (2.69) one finds that

\[
 f(A) = \sum_m f_m A^m \\
 = \sum_m f_m \left( \sum_n a_n P_n \right)^m \\
 = \sum_m f_m \sum_n a_n^m P_n \\
 = \sum_n \sum_m f_m a_n^m P_n, \\
\]

(2.72)

thus

\[
 f(A) = \sum_n f(a_n) P_n. 
\]

(2.73)

**Exercise 2.6.1.** Express the projector \( P_n \) in terms of the operator \( A \) and its set of eigenvalues.

**Solution 2.6.1.** We seek a function \( f \) such that \( f(A) = P_n \). Multiplying from the right by a basis ket-vector \( |a_{m,i}\rangle \) yields

\[
 f(A) |a_{m,i}\rangle = \delta_{mn} |a_{m,i}\rangle. 
\]

(2.74)

On the other hand

\[
 f(A) |a_{m,i}\rangle = f(a_m) |a_{m,i}\rangle. 
\]

(2.75)

Thus we seek a function that satisfy

\[
 f(a_m) = \delta_{mn}. 
\]

(2.76)

The polynomial function

\[
 f(a) = K \prod_{m \neq n} (a - a_m), 
\]

(2.77)

where \( K \) is a constant, satisfies the requirement that \( f(a_m) = 0 \) for every \( m \neq n \). The constant \( K \) is chosen such that \( f(a_n) = 1 \), that is

\[
 f(a) = \prod_{m \neq n} \frac{a - a_m}{a_n - a_m}. 
\]

(2.78)
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Thus, the desired expression is given by

\[ P_n = \prod_{m \neq n} \frac{A - a_m}{a_n - a_m} . \]  

(2.79)

2.7 Quantum Measurement

Consider a measurement of a physical variable denoted as \( A^{(c)} \) performed on a quantum system. The standard textbook description of such a process is described below. The physical variable \( A^{(c)} \) is represented in quantum mechanics by an observable, namely by a Hermitian operator, which is denoted as \( A \). The correspondence between the variable \( A^{(c)} \) and the operator \( A \) will be discussed below in chapter 4. As we have seen above, it is possible to construct a complete orthonormal basis made of eigenvectors of the Hermitian operator \( A \) having the properties given by Eqs. (2.64), (2.65) and (2.66). In that basis, the vector state \( |\alpha_i\rangle \) of the system can be expressed as

\[ |\alpha_i\rangle = \sum_{i=1}^{q_n} \langle a_{n,i} | \alpha \rangle |a_{n,i}\rangle . \]  

(2.80)

Even when the state vector \( |\alpha_i\rangle \) is given, quantum mechanics does not generally provide a deterministic answer to the question: what will be the outcome of the measurement. Instead it predicts that:

1. The possible results of the measurement are the eigenvalues \( \{a_n\} \) of the operator \( A \).
2. The probability \( p_n \) to measure the eigen value \( a_n \) is given by

\[ p_n = \langle \alpha | P_n | \alpha \rangle = \sum_{i=1}^{q_n} |\langle a_{n,i} | \alpha \rangle|^2 . \]  

(2.81)

Note that the state vector \( |\alpha\rangle \) is assumed to be normalized.
3. After a measurement of \( A \) with an outcome \( a_n \), the state vector collapses onto the corresponding eigensubspace and becomes

\[ |\alpha\rangle \rightarrow \frac{P_n |\alpha\rangle}{\sqrt{\langle \alpha | P_n | \alpha \rangle}} . \]  

(2.82)

It is easy to show that the probability to measure something is unity provided that \( |\alpha\rangle \) is normalized:

\[ \sum_n p_n = \sum_n \langle \alpha | P_n | \alpha \rangle = \langle \alpha | \left( \sum_n P_n \right) |\alpha\rangle = 1 . \]  

(2.83)
We also note that a direct consequence of the collapse postulate is that two subsequent measurements of the same observable performed one immediately after the other will yield the same result. It is also important to note that the above ‘standard textbook description’ of the measurement process is highly controversial, especially, the collapse postulate. However, a thorough discussion of this issue is beyond the scope of this course.

Quantum mechanics cannot generally predict the outcome of a specific measurement of an observable $A$, however it can predict the average, namely the expectation value, which is denoted as $\langle A \rangle$. The expectation value is easily calculated with the help of Eq. (2.69)

$$\langle A \rangle = \sum_n a_n p_n = \sum_n a_n \langle \alpha | P_n | \alpha \rangle = \langle \alpha | A | \alpha \rangle.$$  

(2.84)

2.8 Example - Spin 1/2

Spin is an internal degree of freedom of elementary particles. Electrons, for example, have spin 1/2. This means, as we will see in chapter 6, that the state of a spin 1/2 can be described by a state vector $| \alpha \rangle$ in a vector space of dimensionality 2. In other words, spin 1/2 is said to be a two-level system. The spin was first discovered in 1921 by Stern and Gerlach in an experiment in which the magnetic moment of neutral silver atoms was measured. Silver atoms have 47 electrons, 46 out of which fill closed shells. It can be shown that only the electron in the outer shell contributes to the total magnetic moment of the atom. The force $F$ acting on a magnetic moment $\mu$ moving in a magnetic field $B$ is given by $F = \nabla (\mu \cdot B)$. Thus by applying a nonuniform magnetic field $B$ and by monitoring the atoms’ trajectories one can measure the magnetic moment.

It is important to keep in mind that generally in addition to the spin contribution to the magnetic moment of an electron, also the orbital motion of the electron can contribute. For both cases, the magnetic moment is related to angular momentum by the gyromagnetic ratio. However this ratio takes different values for these two cases. The orbital gyromagnetic ratio can be evaluated by considering a simple example of an electron of charge $e$ moving in a circular orbit or radius $r$ with velocity $v$. The magnetic moment is given by

$$\mu_{\text{orbital}} = \frac{AI}{c},$$

(2.85)

where $A = \pi r^2$ is the area enclosed by the circular orbit and $I = ev/(2\pi r)$ is the electrical current carried by the electron, thus

$$\mu_{\text{orbital}} = \frac{erv}{2c}.$$  

(2.86)
This result can be also written as

$$
\mu_{\text{orbital}} = \frac{\mu_B}{\hbar} L ,
$$

(2.87)

where \( L = m_e v r \) is the orbital angular momentum, and where

$$
\mu_B = \frac{e\hbar}{2m_e c}
$$

(2.88)

is the Bohr’s magneton constant. The proportionality factor \( \mu_B/\hbar \) is the orbital gyromagnetic ratio. In vector form and for a more general case of orbital motion (not necessarily circular) the orbital gyromagnetic relation is given by

$$
\mu_{\text{orbital}} = \frac{\mu_B}{\hbar} L .
$$

(2.89)

On the other hand, as was first shown by Dirac, the gyromagnetic ratio for the case of spin angular momentum takes twice this value

$$
\mu_{\text{spin}} = \frac{2\mu_B}{\hbar} S .
$$

(2.90)

Note that we follow here the convention of using the letter \( L \) for orbital angular momentum and the letter \( S \) for spin angular momentum.

The Stern-Gerlach apparatus allows measuring any component of the magnetic moment vector. Alternatively, in view of relation (2.90), it can be said that any component of the spin angular momentum \( S \) can be measured. The experiment shows that the only two possible results of such a measurement are \(+h/2\) and \(-h/2\). As we have seen above, one can construct a complete orthonormal basis to the vector space made of eigenvectors of any given observable. Choosing the observable \( S_z = S \cdot \hat{z} \) for this purpose we construct a basis made of two vectors \{\(|+;\hat{z}\rangle , |−;\hat{z}\rangle\}\}. Both vectors are eigenvectors of \( S_z \)

$$
S_z |+;\hat{z}\rangle = \frac{\hbar}{2} |+;\hat{z}\rangle ,
$$

(2.91)

$$
S_z |−;\hat{z}\rangle = -\frac{\hbar}{2} |−;\hat{z}\rangle .
$$

(2.92)

In what follow we will use the more compact notation

$$
|+\rangle = |+;\hat{z}\rangle ,
$$

(2.93)

$$
|−\rangle = |−;\hat{z}\rangle .
$$

(2.94)

The orthonormality property implied that

$$
\langle + |+\rangle = \langle − |−\rangle = 1 ,
$$

(2.95)

$$
\langle − |+\rangle = 0 .
$$

(2.96)

The closure relation in the present case is expressed as
2.8. Example - Spin 1/2

\[ |+\rangle \langle +| + |-\rangle \langle -| = 1. \]  
(2.97)

In this basis any ket-vector \(|\alpha\rangle\) can be written as

\[ |\alpha\rangle = |+\rangle \langle +| |\alpha\rangle + |-\rangle \langle -| |\alpha\rangle. \]  
(2.98)

The closure relation (2.97) and Eqs. (2.91) and (2.92) yield

\[ S_z = \hbar \left( |+\rangle \langle +| - |-\rangle \langle -| \right) \]  
(2.99)

It is useful to define also the operators \(S_+\) and \(S_-\)

\[ S_+ = \hbar |+\rangle \langle -|, \]  
(2.100)

\[ S_- = \hbar |-\rangle \langle +|. \]  
(2.101)

In chapter 6 we will see that the \(x\) and \(y\) components of \(S\) are given by

\[ S_x = \frac{\hbar}{2} \left( |+\rangle \langle -| + |-\rangle \langle +| \right), \]  
(2.102)

\[ S_y = \frac{\hbar}{2} \left( -i |+\rangle \langle -| + i |-\rangle \langle +| \right). \]  
(2.103)

All these ket-vectors and operators have matrix representation, which for the basis \(|+; \hat{z}\rangle, |-; \hat{z}\rangle\) is given by

\[ |+\rangle \doteq \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \]  
(2.104)

\[ |-\rangle \doteq \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \]  
(2.105)

\[ S_x \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]  
(2.106)

\[ S_y \doteq \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \]  
(2.107)

\[ S_z \doteq \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \]  
(2.108)

\[ S_+ \doteq \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \]  
(2.109)

\[ S_- \doteq \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \]  
(2.110)

**Exercise 2.8.1.** Given that the state vector of a spin 1/2 is \(|+; \hat{z}\rangle\) calculate

(a) the expectation values \(\langle S_x \rangle\) and \(\langle S_z \rangle\)

(b) the probability to obtain a value of \(+\hbar/2\) in a measurement of \(S_x\).

**Solution 2.8.1.** (a) Using the matrix representation one has
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\[ \langle S_x \rangle = \langle + | S_x | + \rangle = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 , \quad (2.111) \]

\[ \langle S_z \rangle = \langle + | S_z | + \rangle = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2} . \quad (2.112) \]

(b) First, the eigenvectors of the operator \( S_x \) are found by solving the equation \( S_x |\alpha\rangle = \lambda |\alpha\rangle \), which is done by diagonalization of the matrix representation of \( S_x \). The relation \( S_x |\alpha\rangle = \lambda |\alpha\rangle \) for the two eigenvectors is written in a matrix form as

\[ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ \sqrt{2} & \sqrt{2} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix} , \quad (2.113) \]

\[ \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ \sqrt{2} & -\sqrt{2} \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix} . \quad (2.114) \]

That is, in ket notation

\[ S_x |\pm\rangle = \pm \frac{\hbar}{\sqrt{2}} |\pm\rangle , \quad (2.115) \]

where the eigenvectors of \( S_x \) are given by

\[ |\pm\rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle) . \quad (2.116) \]

Using this result the probability \( p_+ \) is easily calculated

\[ p_+ = |\langle + | \pm \rangle|^2 = \left| \langle + | \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) \right|^2 = \frac{1}{2} . \quad (2.117) \]

2.9 Unitary Operators

Unitary operators are useful for transforming from one orthonormal basis to another.

Definition 2.9.1. An operator \( U \) is said to be unitary if \( U^\dagger = U^{-1} \), namely if \( UU^\dagger = U^\dagger U = 1 \).

Consider two observables \( A \) and \( B \), and two corresponding complete and orthonormal bases of eigenvectors

\[ A |a_n\rangle = a_n |a_n\rangle , \quad \langle a_m | a_n \rangle = \delta_{nm} , \quad \sum_n |a_n\rangle \langle a_n| = 1 , \quad (2.118) \]

\[ B |b_n\rangle = b_n |b_n\rangle , \quad \langle b_m | b_n \rangle = \delta_{mn} , \quad \sum_n |b_n\rangle \langle b_n| = 1 . \quad (2.119) \]

The operator \( U \), which is given by
2.10. Trace

\[ U = \sum_n |b_n \rangle \langle a_n| , \]  
\[ (2.120) \]
transforms each of the basis vector \(|a_n\rangle\) to the corresponding basis vector \(|b_n\rangle\)

\[ U |a_n\rangle = |b_n\rangle . \]  
\[ (2.121) \]

It is easy to show that the operator \(U\) is unitary

\[ U^\dagger U = \sum_{n,m} |a_n\rangle \langle b_m| |b_n\rangle \langle a_m| = \sum_n |a_n\rangle \langle a_n| = 1 . \]  
\[ (2.122) \]

The matrix elements of \(U\) in the basis \(|a_n\rangle\) are given by

\[ \langle a_n| U |a_m\rangle = \langle a_n| b_m\rangle , \]  
\[ (2.123) \]
and those of \(U^\dagger\) by

\[ \langle a_n| U^\dagger |a_m\rangle = \langle b_n| a_m\rangle . \]

Consider a ket vector

\[ |\alpha\rangle = \sum_n |a_n\rangle \langle a_n| \alpha\rangle , \]  
\[ (2.124) \]
which can be represented as a column vector in the basis \(|a_n\rangle\). The \(n\)th element of such a column vector is \(\langle a_n| \alpha\rangle\). The operator \(U\) can be employed for finding the corresponding column vector representation of the same ket-vector \(|\alpha\rangle\) in the other basis \(|b_n\rangle\)

\[ \langle b_n| \alpha\rangle = \sum_m \langle b_n| a_m\rangle \langle a_m| \alpha\rangle = \sum_m \langle a_n| U^\dagger |a_m\rangle \langle a_m| \alpha\rangle . \]  
\[ (2.125) \]

Similarly, Given an operator \(X\) the relation between the matrix elements \(\langle a_n| X |a_m\rangle\) in the basis \(|a_n\rangle\) to the matrix elements \(\langle b_n| X |b_m\rangle\) in the basis \(|b_n\rangle\) is given by

\[ \langle b_n| X |b_m\rangle = \sum_{k,l} \langle b_n| a_k\rangle \langle a_k| X |a_l\rangle \langle a_l| b_m\rangle \\
= \sum_{k,l} \langle a_n| U^\dagger |a_k\rangle \langle a_k| X |a_l\rangle \langle a_l| U |a_m\rangle . \]  
\[ (2.126) \]

2.10 Trace

Given an operator \(X\) and an orthonormal and complete basis \(|a_n\rangle\), the trace of \(X\) is given by
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\[ \text{Tr} (X) = \sum_n \langle a_n | X | a_n \rangle . \]  

(2.127)

It is easy to show that \( \text{Tr} (X) \) is independent on basis, as is shown below:

\[ \text{Tr} (X) = \sum_n \langle a_n | X | a_n \rangle \\
= \sum_{n,k,l} \langle a_n | b_k \rangle \langle b_k | X | b_l \rangle \langle b_l | a_n \rangle \\
= \sum_{n,k,l} \langle b_l | a_n \rangle \langle a_n | b_k \rangle \langle b_k | X | b_l \rangle \\
= \sum_{k,l} \langle b_k | X | b_l \rangle \delta_{kl} \\
= \sum_k \langle b_k | X | b_k \rangle . \]  

(2.128)

The proof of the following two relations

\[ \text{Tr} (XY) = \text{Tr} (YX) , \]  

(2.129)

\[ \text{Tr} (U^\dagger XU) = \text{Tr} (X) , \]  

(2.130)

is left as an exercise.

2.11 Commutation Relation

The commutation relation of the operators \( A \) and \( B \) is defined as

\[ [A, B] = AB - BA . \]  

(2.131)

As an example, the components \( S_x, S_y \) and \( S_z \) of the spin angular momentum operator, satisfy the following commutation relations

\[ [S_i, S_j] = i\hbar \varepsilon_{ijk} S_k , \]  

(2.132)

where

\[ \varepsilon_{ijk} = \begin{cases} 
0 & \text{if } i, j, k \text{ are not all different} \\
1 & \text{if } i, j, k \text{ is an even permutation of } x, y, z \\
-1 & \text{if } i, j, k \text{ is an odd permutation of } x, y, z 
\end{cases} \]  

(2.133)

is the Levi-Civita symbol. Equation (2.132) employs the Einstein’s convention, according to which if an index symbol appears twice in an expression, it is to be summed over all its allowed values. Namely, the repeated index \( k \) should be summed over the values \( x, y \) and \( z \).
2.12. Simultaneous Diagonalization of Commuting Operators

\[ \varepsilon_{ijk} S_k = \varepsilon_{ijx} S_x + \varepsilon_{ijy} S_y + \varepsilon_{ijz} S_z. \] 

(2.134)

Moreover, the following relations hold

\[ S_x^2 = S_y^2 = S_z^2 = \frac{1}{4} \hbar^2, \] 

(2.135)

\[ \mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3}{4} \hbar^2. \] 

(2.136)

The relations below, which are easy to prove using the above definition, are very useful for evaluating commutation relations

\[ [F,G] = -[G,F], \] 

(2.137)

\[ [F,F] = 0, \] 

(2.138)

\[ [E + F,G] = [E,G] + [F,G], \] 

(2.139)

\[ [E,FG] = [E,F]G + F[E,G]. \] 

(2.140)

2.12 Simultaneous Diagonalization of Commuting Operators

Consider an observable \( A \) having a set of eigenvalues \( \{a_n\} \). Let \( g_n \) be the degree of degeneracy of eigenvalue \( a_n \), namely \( g_n \) is the dimension of the corresponding eigensubspace, which is denoted by \( \mathcal{F}_n \). Thus the following holds

\[ A |a_{n,i}⟩ = a_n |a_{n,i}⟩, \] 

(2.141)

where \( i = 1, 2, \cdots, g_n \), and

\[ \langle a_{n',i'} | a_{n,i}⟩ = \delta_{n,n'} \delta_{i,i'}. \] 

(2.142)

The set of vectors \( \{|a_{n,1}\rangle, |a_{n,2}\rangle, \cdots, |a_{n,g_n}\rangle\} \) forms an orthonormal basis for the eigensubspace \( \mathcal{F}_n \). The closure relation can be written as

\[ 1 = \sum_n \sum_{i=1}^{g_n} |a_{n,i}⟩ \langle a_{n,i}| = \sum_n P_n, \] 

(2.143)

where

\[ P_n = \sum_{i=1}^{g_n} |a_{n,i}⟩ \langle a_{n,i}|. \] 

(2.144)

Now consider another observable \( B \), which is assumed to commute with \( A \), namely \( [A,B] = 0 \).

Claim. The operator \( B \) has a block diagonal matrix in the basis \( \{|a_{n,i}\rangle\} \), namely \( \langle a_{m,j} | B |a_{n,i}\rangle = 0 \) for \( n \neq m \).

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Proof. Multiplying Eq. (2.141) from the left by \( \langle a_{m,j} | B \rangle \) yields

\[
\langle a_{m,j} | B | a_{n,i} \rangle = a_n \langle a_{m,j} | B | a_{n,i} \rangle .
\] (2.145)

On the other hand, since \([A, B] = 0\) one has

\[
\langle a_{m,j} | B | a_{n,i} \rangle = \langle a_{m,j} | AB | a_{n,i} \rangle = a_m \langle a_{m,j} | B | a_{n,i} \rangle ,
\] (2.146)

thus

\[
(a_n - a_m) \langle a_{m,j} | B | a_{n,i} \rangle = 0 .
\] (2.147)

For a given \( n \), the \( g_n \times g_n \) matrix \( \langle a_{n,i'} | B | a_{n,i} \rangle \) is Hermitian, namely \( \langle a_{n,i'} | B | a_{n,i} \rangle = \langle a_{n,i} | B | a_{n,i'} \rangle^* \). Thus, there exists a unitary transformation \( U_n \), which maps \( F_n \) onto \( F_n \), and which diagonalizes the block of \( B \) in the subspace \( F_n \). Since \( F_n \) is an eigensubspace of \( A \), the block matrix of \( A \) in the new basis remains diagonal (with the eigenvalue \( a_n \)). Thus, we conclude that a complete and orthonormal basis of common eigenvectors of both operators \( A \) and \( B \) exists. For such a basis, which is denoted as \( \{ | n, m \rangle \} \), the following holds

\[
A | n, m \rangle = a_n | n, m \rangle ,
\] (2.148)

\[
B | n, m \rangle = b_m | n, m \rangle .
\] (2.149)

2.13 Uncertainty Principle

Consider a quantum system in a state \( | n, m \rangle \), which is a common eigenvector of the commuting observables \( A \) and \( B \). The outcome of a measurement of the observable \( A \) is expected to be \( a_n \) with unity probability, and similarly, the outcome of a measurement of the observable \( B \) is expected to be \( b_m \) with unity probability. In this case it is said that there is no uncertainty corresponding to both of these measurements.

Definition 2.13.1. The variance in a measurement of a given observable \( A \) of a quantum system in a state \( | \alpha \rangle \) is given by \( \langle (\Delta A)^2 \rangle \), where \( \Delta A = A - \langle A \rangle \), namely

\[
\langle (\Delta A)^2 \rangle = \langle A^2 \rangle - 2 \langle A \rangle \langle A \rangle + \langle A \rangle^2 ,
\] (2.150)

where

\[
\langle A \rangle = \langle \alpha | A | \alpha \rangle ,
\] (2.151)

\[
\langle A^2 \rangle = \langle \alpha | A^2 | \alpha \rangle .
\] (2.152)
2.13. Uncertainty Principle

Example 2.13.1. Consider a spin 1/2 system in a state \( |\alpha_i\rangle = |+; \hat{z}\rangle \). Using Eqs. (2.99), (2.102) and (2.135) one finds that

\[
\langle (\Delta S_z)^2 \rangle = \langle S_z^2 \rangle - \langle S_z \rangle^2 = 0 ,
\]

(2.153)

\[
\langle (\Delta S_x)^2 \rangle = \langle S_x^2 \rangle - \langle S_x \rangle^2 = \frac{1}{4} \hbar^2 .
\]

(2.154)

The last example raises the question: can one find a state \( |\alpha_i\rangle \) for which the variance in the measurements of both \( S_z \) and \( S_x \) vanishes? According to the uncertainty principle the answer is no.

**Theorem 2.13.1.** The uncertainty principle - Let \( A \) and \( B \) be two observables. For any ket-vector \( |\alpha_i\rangle \) the following holds

\[
\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B]\rangle| \] .

(2.155)

**Proof.** Applying the Schwartz inequality [see Eq. (2.167)], which is given by

\[
|\langle u | v \rangle| \leq \sqrt{\langle u | u \rangle \langle v | v \rangle} ,
\]

(2.156)

for the ket-vectors

\[
|u\rangle = \Delta_A |\alpha\rangle ,
\]

(2.157)

\[
|v\rangle = \Delta_B |\alpha\rangle ,
\]

(2.158)

and exploiting the fact that \((\Delta A)\dagger = \Delta A\) and \((\Delta B)\dagger = \Delta B\) yield

\[
\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq |\langle \Delta A\Delta B\rangle| \] .

(2.159)

The term \( \Delta A\Delta B \) can be written as

\[
\Delta A\Delta B = \frac{1}{2} [\Delta A, \Delta B] + \frac{1}{2} [\Delta A, \Delta B]_+ ,
\]

(2.160)

where

\[
[\Delta A, \Delta B] = \Delta A\Delta B - \Delta B\Delta A ,
\]

(2.161)

\[
[\Delta A, \Delta B]_+ = \Delta A\Delta B + \Delta B\Delta A .
\]

(2.162)

While the term \( [\Delta A, \Delta B] \) is anti-Hermitian, whereas the term \( [\Delta A, \Delta B]_+ \) is Hermitian, namely

\[
([\Delta A, \Delta B])\dagger = ([\Delta A\Delta B - \Delta B\Delta A])\dagger = \Delta B\Delta A - \Delta A\Delta B = - [\Delta A, \Delta B] ,
\]

\[
([\Delta A, \Delta B]_+)\dagger = (\Delta A\Delta B + \Delta B\Delta A)\dagger = \Delta B\Delta A + \Delta A\Delta B = [\Delta A, \Delta B]_+ .
\]

In general, the following holds

\[
\langle \alpha | X | \alpha \rangle = \langle \alpha | X^\dagger | \alpha \rangle^* = \begin{cases} 
\langle \alpha | X | \alpha \rangle^* & \text{if } X \text{ is Hermitian} \\
-\langle \alpha | X | \alpha \rangle^* & \text{if } X \text{ is anti-Hermitian}
\end{cases} ,
\]

(2.163)
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thus
\[ \langle \Delta A \Delta B \rangle = \frac{1}{2} \langle [\Delta A, \Delta B] \rangle + \frac{1}{2} \langle [\Delta A, \Delta B]_+ \rangle, \]  
(2.164)

and consequently
\[ |\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4} \left| \langle [\Delta A, \Delta B] \rangle \right|^2 + \frac{1}{4} \left| \langle [\Delta A, \Delta B]_+ \rangle \right|^2. \]  
(2.165)

Finally, with the help of the identity \([\Delta A, \Delta B] = [A, B]\), one finds that
\[ \langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} \left| \langle [A, B] \rangle \right|^2. \]  
(2.166)

2.14 Problems

1. Derive the Schwartz inequality
\[ |\langle u | v \rangle| \leq \sqrt{\langle u | u \rangle} \sqrt{\langle v | v \rangle}, \]  
(2.167)

where \(|u\rangle\) and \(|v\rangle\) are any two vectors of a vector space \(\mathcal{F}\).

2. Derive the triangle inequality:
\[ \sqrt{(\langle u \rangle + \langle v \rangle) \langle \langle u \rangle + \langle v \rangle \rangle} \leq \sqrt{\langle u \rangle u} + \sqrt{\langle v \rangle v}. \]  
(2.168)

3. Show that if a unitary operator \(U\) can be written in the form \(U = 1 + iF\), where \(\epsilon\) is a real infinitesimally small number, then the operator \(F\) is Hermitian.

4. A Hermitian operator \(A\) is said to be positive-definite if, for any vector \(|u\rangle\), \(\langle u | A | u \rangle \geq 0\). Show that the operator \(A = |a\rangle \langle a|\) is Hermitian and positive-definite.

5. Show that if \(A\) is a Hermitian positive-definite operator then the following hold
\[ |\langle u | A | v \rangle| \leq \sqrt{\langle u | A | u \rangle} \sqrt{\langle v | A | v \rangle}. \]  
(2.169)

6. Find the expansion of the operator \((A - \lambda B)^{-1}\) in a power series in \(\lambda\), assuming that the inverse \(A^{-1}\) of \(A\) exists.

7. The derivative of an operator \(A(\lambda)\) which depends explicitly on a parameter \(\lambda\) is defined to be
\[ \frac{dA(\lambda)}{d\lambda} = \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) - A(\lambda)}{\epsilon}. \]  
(2.170)

Show that
\[ \frac{d}{d\lambda} (AB) = \frac{dA}{d\lambda} B + A \frac{dB}{d\lambda}. \]  
(2.171)
8. Show that
\[
\frac{d}{d\lambda} (A^{-1}) = -A^{-1} \frac{dA}{d\lambda} A^{-1}.
\] (2.172)

9. Let \(|u\rangle\) and \(|v\rangle\) be two vectors of finite norm. Show that
\[
\text{Tr} (|u\rangle \langle v|) = \langle v | u\rangle.
\] (2.173)

10. If \(A\) is any linear operator, show that \(A^\dagger A\) is a positive-definite Hermitian operator whose trace is equal to the sum of the square moduli of the matrix elements of \(A\) in any arbitrary representation. Deduce that
\[
\text{Tr} (A^\dagger A) = 0 \text{ is true if and only if } A = 0.
\]

11. Show that if \(A\) and \(B\) are two positive-definite observables, then \(\text{Tr} (AB) \geq 0\).

12. Show that for any two operators \(A\) and \(L\)
\[
e^L A e^{-L} = A + [L, A] + \frac{1}{2!} [L, [L, A]] + \frac{1}{3!} [L, [L, [L, A]]] + \cdots.
\] (2.174)

13. Show that if \(A\) and \(B\) are two operators satisfying the relation \([[A, B], A] = 0\), then the relation
\[
[A^m, B] = mA^{m-1} [A, B]
\] (2.175)
holds for all positive integers \(m\).

14. Show that
\[
e^A e^B = e^{A+B} e^{(1/2)[A,B]},
\] (2.176)
provided that \([[A, B], A] = 0\) and \([[A, B], B] = 0\).

15. Proof Kondo’s identity
\[
[A, e^{-\beta H}] = e^{-\beta H} \int_0^\beta e^{\lambda H} [H, A] e^{-\lambda H} d\lambda,
\] (2.177)
where \(A\) and \(H\) are any two operators and \(\beta\) is real.

16. Show that \(\text{Tr} (XY) = \text{Tr} (YX)\).

17. Consider the two normalized spin 1/2 states \(|\alpha\rangle\) and \(|\beta\rangle\). The operator \(A\) is defined as
\[
A = |\alpha\rangle \langle \alpha| - |\beta\rangle \langle \beta|.
\] (2.178)
Find the eigenvalues of the operator \(A\).

18. A molecule is composed of six identical atoms \(A_1, A_2, \ldots, A_6\) which form a regular hexagon. Consider an electron, which can be localized on each of the atoms. Let \(|\varphi_n\rangle\) be the state in which it is localized on the \(n\)th atom \((n = 1, 2, \ldots, 6)\). The electron states will be confined to the
space spanned by the states $|\varphi_n\rangle$, which is assumed to be orthonormal. The Hamiltonian of the system is given by

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{W}. \quad (2.179)$$

The eigenstates of $\mathcal{H}_0$ are the six states $|\varphi_n\rangle$, with the same eigenvalue $E_0$. The operator $\mathcal{W}$ is described by

$$\mathcal{W} |\varphi_1\rangle = -a |\varphi_2\rangle - a |\varphi_6\rangle,$$

$$\mathcal{W} |\varphi_2\rangle = -a |\varphi_3\rangle - a |\varphi_1\rangle,$$

$$\vdots$$

$$\mathcal{W} |\varphi_6\rangle = -a |\varphi_1\rangle - a |\varphi_5\rangle. \quad (2.180)$$

Find the eigenvalues and eigen vectors of $\mathcal{H}$. Clue: Consider a solution of the form

$$|k\rangle = \sum_{n=1}^{6} e^{ikn} |\varphi_n\rangle. \quad (2.181)$$

### 2.15 Solutions

1. Let

$$|\gamma\rangle = |u\rangle + \lambda |v\rangle, \quad (2.182)$$

where $\lambda \in \mathbb{C}$. The requirement $\langle \gamma | \gamma \rangle \geq 0$ leads to

$$\langle u | u \rangle + \lambda \langle u | v \rangle + \lambda^* \langle v | u \rangle + |\lambda|^2 \langle v | v \rangle \geq 0. \quad (2.183)$$

By choosing

$$\lambda = -\frac{\langle v | u \rangle}{\langle v | v \rangle}, \quad (2.184)$$

one has

$$\langle u | u \rangle - \frac{\langle v | u \rangle}{\langle v | v \rangle} \langle u | v \rangle - \frac{\langle u | v \rangle}{\langle v | v \rangle} \langle v | u \rangle + \left| \frac{\langle v | u \rangle}{\langle v | v \rangle} \right|^2 \langle v | v \rangle \geq 0, \quad (2.185)$$

thus

$$|\langle u | v \rangle| \leq \sqrt{\langle u | u \rangle} \sqrt{\langle v | v \rangle}. \quad (2.186)$$
2. The following holds

\[
(\langle u | + \langle v |)(|u⟩ + |v⟩) = \langle u | u⟩ + \langle v | v⟩ + 2 \Re \langle u | v⟩ \\
\leq \langle u | u⟩ + \langle v | v⟩ + 2 |\langle u | v⟩|.
\]

Thus, using Schwartz inequality one has

\[
(\langle u | + \langle v |)(|u⟩ + |v⟩) \leq \langle u | u⟩ + \langle v | v⟩ + 2\sqrt{\langle u | u⟩ \langle v | v⟩} \\
= \left( \sqrt{\langle u | u⟩} + \sqrt{\langle v | v⟩} \right)^2.
\]

(2.187)

3. Since

\[
1 = U^\dagger U = (1 - i \varepsilon F^\dagger)(1 + i \varepsilon F) = 1 + i \varepsilon (F - F^\dagger) + O(\varepsilon^2),
\]

one has \(F = F^\dagger\).

4. In general, \(\langle \beta | \langle \alpha | = | \alpha ⟩ \langle \beta |\), thus clearly the operator \(A\) is Hermitian. Moreover it is positive-definite since for every \(|u⟩\) the following holds

\[
\langle u | A | u⟩ = \langle u | A | u⟩ = |\langle a | u⟩|^2 \geq 0.
\]

(2.190)

5. Let

\[
|γ⟩ = |u⟩ - \frac{\langle v | A | u⟩}{\langle v | A | v⟩} |v⟩.
\]

Since \(A\) is Hermitian and positive-definite the following holds

\[
0 \leq \langle γ | A | γ⟩ \\
= \langle u | - \frac{\langle u | A | v⟩}{\langle v | A | v⟩} |v⟩ |\langle u | A | u⟩ - \frac{\langle v | A | u⟩}{\langle v | A | v⟩} |v⟩ \rangle \\
= \langle u | A | u⟩ - \frac{|\langle u | A | v⟩|^2}{\langle v | A | v⟩} - \frac{|\langle u | A | u⟩|^2}{\langle v | A | v⟩} + \frac{|\langle u | A | v⟩|^2}{\langle v | A | v⟩},
\]

thus

\[
|\langle u | A | v⟩| \leq \sqrt{\langle u | A | u⟩} \sqrt{\langle v | A | v⟩}.
\]

(2.192)

Note that this result allows easy proof of the following: Under the same conditions (namely, \(A\) is a Hermitian positive-definite operator) \(\text{Tr} (A) = 0\) if and only if \(A = 0\).

6. The expansion is given by

\[
(A - \lambda B)^{-1} = (A (1 - \lambda A^{-1} B))^{-1} \\
= (1 - \lambda A^{-1} B)^{-1} A^{-1} \\
= \left( 1 + \lambda A^{-1} B + (\lambda A^{-1} B)^2 + (\lambda A^{-1} B)^3 + \cdots \right) A^{-1}.
\]

(2.193)
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7. By definition:
\[
\frac{d}{d\lambda} (AB) = \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) B(\lambda + \epsilon) - A(\lambda) B(\lambda)}{\epsilon}
\]
\[
= \lim_{\epsilon \to 0} \frac{(A(\lambda + \epsilon) - A(\lambda)) B(\lambda)}{\epsilon} + \lim_{\epsilon \to 0} \frac{A(\lambda + \epsilon) (B(\lambda + \epsilon) - B(\lambda))}{\epsilon}
\]
\[
= \frac{dA}{d\lambda} B + A \frac{dB}{d\lambda}.
\]
(2.194)

8. Taking the derivative of both sides of the identity $1 = AA^{-1}$ on has
\[
0 = \frac{dA}{d\lambda} A^{-1} + A \frac{dA^{-1}}{d\lambda},
\]
(2.195)

thus
\[
\frac{d}{d\lambda} (A^{-1}) = -A^{-1} \frac{dA}{d\lambda} A^{-1}.
\]
(2.196)

9. Let $\{|n\rangle\}$ be a complete orthonormal basis, namely
\[
\sum_n |n\rangle \langle n| = 1.
\]
(2.197)

In this basis
\[
\text{Tr} (|u\rangle \langle v|) = \sum_n \langle n| u \rangle \langle v| n\rangle = \langle v| \left( \sum_n |n\rangle \langle n| \right) |u\rangle = \langle v| u \rangle.
\]
(2.198)

10. The operator $A^\dagger A$ is Hermitian since $(A^\dagger A)^\dagger = A^\dagger A$, and positive-definite since the norm of $A |u\rangle$ is nonnegative for every $|u\rangle$, thus one has $\langle u| A^\dagger A |u\rangle \geq 0$. Moreover, using a complete orthonormal basis $\{|n\rangle\}$ one has
\[
\text{Tr} (A^\dagger A) = \sum_n \langle n| A^\dagger A |n\rangle
\]
\[
= \sum_{n,m} \langle n| A^\dagger |m\rangle \langle m| A |n\rangle
\]
\[
= \sum_{n,m} |\langle m| A |n\rangle|^2.
\]
(2.199)

11. Let $\{|b'\rangle\}$ be a complete orthonormal basis made of eigenvectors of $B$ (i.e., $B |b'\rangle = b' |b'\rangle$). Using this basis for evaluating the trace one has
\[
\text{Tr} (AB) = \sum_{b'} \langle b'| AB |b'\rangle = \sum_{b', b''} b'_b' \langle b'| A |b''\rangle \geq 0.
\]
(2.200)
12. Let \( f(s) = e^{sL}Ae^{-sL} \), where \( s \) is real. Using Taylor expansion one has
\[
f(1) = f(0) + \frac{1}{1!} \frac{df}{ds} \bigg|_{s=0} + \frac{1}{2!} \frac{d^2f}{ds^2} \bigg|_{s=0} + \cdots ,
\]
thus
\[
e^{sL}Ae^{-sL} = A + \frac{1}{1!} \frac{df}{ds} \bigg|_{s=0} + \frac{1}{2!} \frac{d^2f}{ds^2} \bigg|_{s=0} + \cdots ,
\]
where
\[
\frac{df}{ds} = Le^{sL}Ae^{-sL} - e^{sL}Ae^{-sL}L = [L, f(s)] ,
\]
\[
\frac{d^2f}{ds^2} = \left[ L, \frac{df}{ds} \right] = [L, [L, f(s)]] ,
\]
therefore
\[
e^{sL}Ae^{-sL} = A + [L, A] + \frac{1}{2!} [L, [L, A]] + \frac{1}{3!} [L, [L, [L, A]]] + \cdots .
\]

13. The identity clearly holds for the case \( m = 1 \). Moreover, assuming it holds for \( m \), namely assuming that
\[
[A^m, B] = mA^{m-1} [A, B] ,
\]
one has
\[
[A^{m+1}, B] = A [A^m, B] + [A, B] A^m
= mA^m [A, B] + [A, B] A^m .
\]
It is easy to show that if \([ [A, B], A] = 0 \) then \([ [A, B], A^m] = 0 \), thus one concludes that
\[
[A^{m+1}, B] = (m + 1) A^m [A, B] .
\]

14. Define the function \( f(s) = e^{sA}e^{sB} \), where \( s \) is real. The following holds
\[
\frac{df}{ds} = Ae^{sA}e^{sB} + e^{sA}Be^{sB}
= (A + e^{sA}Be^{-sA}) e^{sA}e^{sB}
\]
Using Eq. (2.175) one has
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\[ e^{sA}B = \sum_{m=0}^{\infty} \frac{(sA)^m}{m!}B \]
\[ = \sum_{m=0}^{\infty} \frac{s^m(BA^m + [A^m, B])}{m!} \]
\[ = \sum_{m=0}^{\infty} \frac{s^m(BA^m + mA^{m-1}[A, B])}{m!} \]
\[ = Be^{sA} + s \sum_{m=1}^{\infty} \frac{(sA)^{m-1}}{(m-1)!}[A, B] \]
\[ = Be^{sA} + se^{sA}[A, B] \], \quad (2.209)

thus
\[ \frac{df}{ds} = Ae^{sA}e^{sB} + Be^{sA}e^{sB} + se^{sA}[A, B]e^{sB} \]
\[ = (A + B + [A, B])se^{sB} \] \quad (2.210)

The above differential equation can be easily integrated since \([[A, B], A] = 0\) and \([[A, B], B] = 0\). Thus
\[ f(s) = e^{(A+B)s}e^{[A,B]\frac{s^2}{2}} \]. \quad (2.211)

For \(s = 1\) one gets
\[ e^{Ae^{B}} = e^{A+B}e^{(1/2)[A,B]} \]. \quad (2.212)

15. Define
\[ f(\beta) \equiv [A, e^{-\beta H}] \], \quad (2.213)
\[ g(\beta) \equiv e^{-\beta H} \int_{0}^{\beta} e^{\lambda H}[H, A]e^{-\lambda H}d\lambda \]. \quad (2.214)

Clearly, \(f(0) = g(0) = 0\). Moreover, the following holds
\[ \frac{df}{d\beta} = -AHe^{-\beta H} + He^{-\beta H}A = -Hf + [H, A]e^{-\beta H} \], \quad (2.215)
\[ \frac{dg}{d\beta} = -Hg + [H, A]e^{-\beta H} \], \quad (2.216)

namely, both functions satisfy the same differential equation. Therefore \(f = g\).

16. Using a complete orthonormal basis \(\{|n\}\) one has
\[ \text{Tr} (XY) = \sum_n \langle n | XY | n \rangle \]
\[ = \sum_{n,m} \langle n | X | m \rangle \langle m | Y | n \rangle \]
\[ = \sum_{n,m} \langle m | Y | n \rangle \langle n | X | m \rangle \]
\[ = \sum_m \langle m | YX | m \rangle \]
\[ = \text{Tr} (YX). \quad (2.217) \]

Note that using this result it is easy to show that \( \text{Tr} (U^*XU) = \text{Tr} (X) \), where \( U \) is a unitary operator.

17. Clearly \( A \) is Hermitian, namely \( A^\dagger = A \), thus the two eigenvalues \( \lambda_1 \) and \( \lambda_2 \) are expected to be real. Since the trace of an operator is basis independent, the following must hold

\[ \text{Tr} (A) = \lambda_1 + \lambda_2, \quad (2.218) \]

and

\[ \text{Tr} (A^2) = \lambda_1^2 + \lambda_2^2. \quad (2.219) \]

One the other hand, with the help of Eq. (2.173) one finds that

\[ \text{Tr} (A) = \text{Tr} (|\alpha\rangle \langle \alpha|) - \text{Tr} (|\beta\rangle \langle \beta|) = 0, \quad (2.220) \]

and

\[
\text{Tr} (A^2) = \text{Tr} (|\alpha\rangle \langle \alpha| |\alpha\rangle \langle \alpha|) + \text{Tr} (|\beta\rangle \langle \beta| |\beta\rangle \langle \beta|) - \text{Tr} (|\alpha\rangle \langle \alpha| |\beta\rangle \langle \beta|) - \text{Tr} (|\beta\rangle \langle \beta| |\alpha\rangle \langle \alpha|) \\
= 2 - \langle \alpha | \beta \rangle \text{Tr} (|\alpha\rangle \langle \beta|) - \langle \beta | \alpha \rangle \text{Tr} (|\beta\rangle \langle \alpha|) \\
= 2 \left( 1 - |\langle \alpha | \beta \rangle|^2 \right), \quad (2.221)
\]

thus

\[ \lambda_{\pm} = \pm \sqrt{1 - |\langle \alpha | \beta \rangle|^2}. \quad (2.222) \]

Alternatively, this problem can also be solved as follows. In general, the state \(|\beta\rangle\) can be decomposed into a parallel to and a perpendicular to \(|\alpha\rangle\) terms, namely

\[ |\beta\rangle = a |\alpha\rangle + c |\gamma\rangle, \quad (2.223) \]

where \(a, c \in \mathbb{C}\), the vector \(|\gamma\rangle\) is orthogonal to \(|\alpha\rangle\), namely \(\langle \gamma | \alpha \rangle = 0\), and in addition \(|\gamma\rangle\) is assumed to be normalized, namely \(\langle \gamma | \gamma \rangle = 1\). Since \(|\beta\rangle\)
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is normalized one has \(|a|^2 + |c|^2 = 1\). The matrix representation of \(A\) in the orthonormal basis \(\{|\alpha\rangle, |\gamma\rangle\}\) is given by

\[
A\hat{=} \left( \begin{array}{cc}
|a|^2 & -ac^* \\
|c|^2 & -a^*c - |a|^2
\end{array} \right) \equiv \hat{A} \quad (2.224)
\]

Thus,

\[
\text{Tr} (\hat{A}) = 0 \quad (2.225)
\]

and

\[
\text{Det} (\hat{A}) = - |c|^2 \left( |c|^2 + |a|^2 \right) = - \left( 1 - |\langle \alpha | \beta \rangle|^2 \right) \quad (2.226)
\]

due to the eigenvalues are

\[
\lambda_{\pm} = \pm \sqrt{1 - |\langle \alpha | \beta \rangle|^2} \quad (2.227)
\]

18. Following the clue, we seek a solution to the eigenvalue equation

\[
\mathcal{H} |k\rangle = E_m |k\rangle \quad (2.228)
\]

where

\[
|k\rangle = \sum_{n=1}^{6} e^{ikn} |\varphi_n\rangle \quad (2.229)
\]

thus

\[
\mathcal{H} |k\rangle = E_0 |k\rangle - a \sum_{n=1}^{6} e^{ikn} \left( |\varphi_{(n-1)'}\rangle + |\varphi_{(n+1)'}\rangle \right) = E |k\rangle \quad (2.230)
\]

where \(n'\) is the modulus of \(n\) divided by 6 (e.g., \(1' = 1, 0' = 6, 7' = 1\)). A solution is obtained if

\[
e^{i6k} = 1 \quad (2.231)
\]

or

\[
k_m = \frac{m\pi}{3} \quad (2.232)
\]

where \(m = 1, 2, \cdots, 6\). The corresponding eigen vectors are denoted as

\[
|k_m\rangle = \sum_{n=1}^{6} e^{ik_m n} |\varphi_n\rangle \quad (2.233)
\]

and the following holds

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\[ \mathcal{H} |k_m\rangle = E_0 |k_m\rangle - ae^{ik_m} \sum_{n=1}^{6} e^{ik_m(n-1)} |\varphi_{(n-1)'}\rangle - ae^{-ik_m} \sum_{n=1}^{6} e^{ik_m(n+1)} |\varphi_{(n+1)'}\rangle \]
\[ = (E_0 - 2a \cos k_m) |k_m\rangle , \]

\hspace{1cm} (2.234)

thus
\[ \mathcal{H} |k_m\rangle = E_m |k\rangle , \]

\hspace{1cm} (2.235)

where
\[ E_m = E_0 - 2a \cos k_m . \]

\hspace{1cm} (2.236)
3. The Position and Momentum Observables

Consider a point particle moving in a 3 dimensional space. We first treat the system classically. The position of the particle is described using the Cartesian coordinates $q_x$, $q_y$ and $q_z$. Let

$$p_j = \frac{\partial L}{\partial \dot{q}_j}$$

(3.1)

be the canonically conjugate variable to the coordinate $q_j$, where $j \in \{x, y, z\}$ and where $L$ is the Lagrangian. As we have seen in exercise 4 of set 1, the following Poisson’s brackets relations hold

$$\{q_j, q_k\} = 0,$$

(3.2)

$$\{p_j, p_k\} = 0,$$

(3.3)

$$\{q_j, p_k\} = \delta_{jk}.$$  

(3.4)

In quantum mechanics, each of the 6 variables $q_x$, $q_y$, $q_z$, $p_x$, $p_y$ and $p_z$ is represented by an Hermitian operator, namely by an observable. It is postulated that the commutation relations between each pair of these observables is related to the corresponding Poisson’s brackets according to the rule

$$\{\cdot, \cdot \} \rightarrow \frac{1}{i\hbar} [\cdot, \cdot].$$

(3.5)

Namely the following is postulated to hold

$$[q_j, q_k] = 0,$$

(3.6)

$$[p_j, p_k] = 0,$$

(3.7)

$$[q_j, p_k] = i\hbar \delta_{jk}.$$  

(3.8)

Note that here we use the same notation for a classical variable and its quantum observable counterpart. In this chapter we will derive some results that are solely based on Eqs. (3.6), (3.7) and (3.8).

3.1 The One Dimensional Case

In this section, which deals with the relatively simple case of a one dimensional motion of a point particle, we employ the less cumbersome notation
Chapter 3. The Position and Momentum Observables

$x$ and $p$ for the observables $q_x$ and $p_x$. The commutation relation between these operators is given by [see Eq. (3.8)]

$$[x, p] = i\hbar .$$

(3.9)

The uncertainty principle (2.155) employed for $x$ and $p$ yields

$$\left(\langle \Delta x \rangle^2\right) \left(\langle \Delta p_x \rangle^2\right) \geq \frac{\hbar^2}{4} .$$

(3.10)

3.1.1 Position Representation

Let $x'$ be an eigenvalue of the observable $x$, and let $|x'\rangle$ be the corresponding eigenvector, namely

$$x \ |x'\rangle = x' \ |x'\rangle .$$

(3.11)

Note that $x' \in \mathbb{R}$ since $x$ is Hermitian. As we will see below transformation between different eigenvectors $|x'\rangle$ can be performed using the translation operator $J(\Delta_x)$.

Definition 3.1.1. The translation operator is given by

$$J(\Delta_x) = \exp \left(- \frac{i \Delta_x p}{\hbar} \right) ,$$

(3.12)

where $\Delta_x \in \mathbb{R}$.

Recall that in general the meaning of a function of an operator can be understood in terms of the Taylor expansion of the function, that is, for the present case

$$J(\Delta_x) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(- \frac{i \Delta_x p}{\hbar} \right)^n .$$

(3.13)

It is easy to show that $J(\Delta_x)$ is unitary

$$J^\dagger(\Delta_x) = J(-\Delta_x) = J^{-1}(\Delta_x) .$$

(3.14)

Moreover, the following composition property holds

$$J(\Delta_{x1}) J(\Delta_{x2}) = J(\Delta_{x1} + \Delta_{x2}) .$$

(3.15)

Theorem 3.1.1. Let $x'$ be an eigenvalue of the observable $x$, and let $|x'\rangle$ be the corresponding eigenvector. Then the ket-vector $J(\Delta_x) |x'\rangle$ is a normalized eigenvector of $x$ with an eigenvalue $x' + \Delta_x$.

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Proof. With the help of Eq. (3.76), which is given by
\[ [x, B(p)] = i\hbar \frac{dB}{dp}, \] (3.16)
and which is proven in exercise 1 of set 3, one finds that
\[ [x, J(\Delta x)] = i\hbar \frac{\Delta x}{\hbar} J(\Delta x). \] (3.17)
Using this result one has
\[ xJ(\Delta x)|x'\rangle = (x + \Delta x)J(\Delta x)|x'\rangle, \] (3.18)
thus the ket-vector \( J(\Delta x)|x'\rangle \) is an eigenvector of \( x \) with an eigenvalue \( x + \Delta x \). Moreover, \( J(\Delta x)|x'\rangle \) is normalized since \( J \) is unitary.

In view of the above theorem we will in what follows employ the notation
\[ J(\Delta x)|x'\rangle = |x' + \Delta x\rangle. \] (3.19)
An important consequence of the last result is that the spectrum of eigenvalues of the operator \( x \) is continuous and contains all real numbers. This point will be further discussed below.

The position wavefunction \( \psi_\alpha(x'0) \) of a state vector \( |\alpha\rangle \) is defined as:
\[ \psi_\alpha(x'0) = \langle x'0 | \alpha \rangle. \] (3.20)
Given the wavefunction \( \psi_\alpha(x'0) \) of state vector \( |\alpha\rangle \), what is the wavefunction of the state \( O|\alpha\rangle \), where \( O \) is an operator? We will answer this question below for some cases:

1. The operator \( O = x \). In this case
\[ \langle x'0 | x\rangle = x'(x'0 | \alpha\rangle = x'\psi_\alpha(x'), \] (3.21)
namely, the desired wavefunction is obtained by multiplying \( \psi_\alpha(x') \) by \( x' \).

2. The operator \( O \) is a function \( A(x) \) of the operator \( x \). Let
\[ A(x) = \sum_n a_n x^n. \] (3.22)
be the Taylor expansion of \( A(x) \). Exploiting the fact that \( x \) is Hermitian one finds that
\[ \langle x'0 | A(x) | \alpha\rangle = \sum_n a_n \langle x'0 | x^n | \alpha\rangle = \sum_n a_n x'^n \langle x'0 | \alpha\rangle = A(x') \psi_\alpha(x'). \] (3.23)
3. The operator $O = J(\Delta_x)$. In this case
\begin{equation}
\langle x' | J(\Delta_x) | \alpha \rangle = \langle x' | J^\dagger(-\Delta_x) | \alpha \rangle = \langle x' - \Delta_x | \alpha \rangle = \psi_\alpha (x' - \Delta_x) .
\end{equation}
(3.24)

4. The operator $O = p$. In view of Eq. (3.12), the following holds
\begin{equation}
J(-\Delta_x) = \exp \left( \frac{i p \Delta_x}{\hbar} \right) = 1 + \frac{i \Delta_x}{\hbar} p + O \left( (\Delta_x)^2 \right) ,
\end{equation}
(3.25)
thus
\begin{equation}
\langle x' | J(-\Delta_x) | \alpha \rangle = \psi_\alpha (x') + \frac{i \Delta_x}{\hbar} \langle x' | p | \alpha \rangle + O \left( (\Delta_x)^2 \right) .
\end{equation}
(3.26)
On the other hand, according to Eq. (3.24) also the following holds
\begin{equation}
\langle x' | J(-\Delta_x) | \alpha \rangle = \psi_\alpha (x' + \Delta_x) .
\end{equation}
(3.27)
Equating the above two expressions for $\langle x' | J(-\Delta_x) | \alpha \rangle$ yields
\begin{equation}
\langle x' | p | \alpha \rangle = -i \hbar \frac{\psi_\alpha (x' + \Delta_x) - \psi_\alpha (x')}{\Delta_x} + O (\Delta_x) .
\end{equation}
(3.28)
Thus, in the limit $\Delta_x \to 0$ one has
\begin{equation}
\langle x' | p | \alpha \rangle = -i \hbar \frac{d \psi_\alpha}{dx} .
\end{equation}
(3.29)

To mathematically understand the last result, consider the differential operator
\begin{equation}
\tilde{J}(-\Delta_x) = \exp \left( \Delta_x \frac{d}{dx} \right) = 1 + \Delta_x \frac{d}{dx} + \frac{1}{2!} \left( \Delta_x \frac{d}{dx} \right)^2 + \cdots .
\end{equation}
(3.30)
In view of the Taylor expansion of an arbitrary function $f(x)$
\begin{equation}
f(x_0 + \Delta_x) = f(x_0) + \Delta_x \frac{df}{dx} + \frac{(\Delta_x)^2}{2!} \frac{d^2f}{dx^2} + \cdots \\
= \exp \left( \Delta_x \frac{d}{dx} \right) f \bigg|_{x=x_0} \\
= \tilde{J}(-\Delta_x) f \bigg|_{x=x_0} ,
\end{equation}
(3.31)
one can argue that the operator $\tilde{J}(-\Delta_x)$ generates translation.
As we have pointed out above, the spectrum (i.e., the set of all eigenvalues) of $x$ is continuous. On the other hand, in the discussion in chapter 2 only the case of an observable having discrete spectrum has been considered. Rigorous mathematical treatment of the case of continuous spectrum is nontrivial mainly because typically the eigenvectors in such a case cannot be normalized. However, under some conditions one can generalize some of the results given in chapter 2 for the case of an observable having a continuous spectrum. These generalization is demonstrated below for the case of the position operator $x$:

1. The closure relation (2.23) is written in terms of the eigen vectors $|x'|$ as

$$\int_{-\infty}^{\infty} dx' |x'| (x') = 1 , \quad (3.32)$$

namely, the discrete sum is replaced by an integral.

2. With the help of Eq. (3.32) an arbitrary ket-vector can be written as

$$|\alpha\rangle = \int_{-\infty}^{\infty} dx' |x'| (x') |\alpha\rangle = \int_{-\infty}^{\infty} dx' \psi_x (x') |\alpha\rangle , \quad (3.33)$$

and the inner product between a ket-vector $|\alpha\rangle$ and a bra-vector $\langle \beta |$ as

$$\langle \beta | \alpha \rangle = \int_{-\infty}^{\infty} dx' \langle \beta |x'| (x') \langle x'| \alpha \rangle = \int_{-\infty}^{\infty} dx' \psi^*_x (x') \psi_x (x') . \quad (3.34)$$

3. The normalization condition reads

$$1 = \langle \alpha | \alpha \rangle = \int_{-\infty}^{\infty} dx' |\psi_x (x')|^2 . \quad (3.35)$$

4. The orthonormality relation (2.64) is written in the present case as

$$\langle x'' |x'| = \delta (x' - x'') . \quad (3.36)$$

5. In a measurement of the observable $x$, the quantity

$$f (x') = |\langle x' | \alpha \rangle|^2 = |\psi_x (x')|^2 \quad (3.37)$$

represents the probability density to find the particle at the point $x = x'$.

6. That is, the probability to find the particle in the interval $(x_1, x_2)$ is given by

$$p_{(x_1, x_2)} = \int_{x_1}^{x_2} dx' f (x') . \quad (3.38)$$
Chapter 3. The Position and Momentum Observables

This can be rewritten as

\[ p_{(x_1,x_2)} = \langle \alpha | P_{(x_1,x_2)} | \alpha \rangle , \]  

(3.39)

where the projection operator \( P_{(x_1,x_2)} \) is given by

\[ P_{(x_1,x_2)} = \int_{x_1}^{x_2} dx' |x'\rangle \langle x'| . \]  

(3.40)

The operator \( P_{(x_1,x_2)} \) is considered to be a projection operator since for every \( x_0 \in (x_1,x_2) \) the following holds

\[ P_{(x_1,x_2)} | x_0 \rangle = \int_{x_1}^{x_2} dx' |x'\rangle \langle x' | x_0 \rangle = | x_0 \rangle . \]  

(3.41)

7. Any realistic measurement of a continuous variable such as position is subjected to finite resolution. Assuming that a particle has been measured to be located in the interval \((x' - \delta_x/2, x' + \delta_x/2)\), where \( \delta_x \) is the resolution of the measuring device, the collapse postulate implies that the state of the system undergoes the following transformation

\[ | \alpha \rangle \rightarrow \frac{P_{(x_0-\delta_x/2,x_0+\delta_x/2)}}{\sqrt{\langle \alpha | P_{(x_0-\delta_x/2,x_0+\delta_x/2)} | \alpha \rangle}} | \alpha \rangle . \]  

(3.42)

8. Some observables have a mixed spectrum containing both a discrete and continuous subsets. An example of such a mixed spectrum is the set of eigenvalues of the Hamiltonian operator of a potential well of finite depth.

3.1.2 Momentum Representation

Let \( p' \) be an eigenvalue of the observable \( p \), and let \( |p'\rangle \) be the corresponding eigenvector, namely

\[ p |p'\rangle = p' |p\rangle . \]  

(3.43)

Note that \( p' \in \mathcal{R} \) since \( p \) is Hermitian. Similarly to the case of the position observable, the closure relation is written as

\[ \int dp' |p'\rangle \langle p'| = 1 , \]  

(3.44)

and the orthonormality relation as

\[ \langle p'' | p' \rangle = \delta (p' - p'') . \]  

(3.45)

The momentum wavefunction \( \phi_\alpha (p') \) of a given state \( | \alpha \rangle \) is defined as
3.2 Transformation Function

The probability density to measure a momentum value of \( p = p' \) is

\[ |\phi_\alpha (p')|^2 = |\langle p' | \alpha \rangle|^2 . \]  (3.47)

Any ket-vector can be decomposed into momentum eigenstates as

\[ |\alpha \rangle = \int_{-\infty}^{\infty} dp' |p'\rangle \langle p' | \alpha \rangle = \int_{-\infty}^{\infty} dp' h_{p'\alpha} (p') |p'\rangle . \]  (3.48)

The inner product between a ket-vector \( |\alpha \rangle \) and a bra-vector \( \langle \beta | \) can be expressed as

\[ \langle \beta | \alpha \rangle = \int_{-\infty}^{\infty} dp' \langle \beta | p' \rangle \langle p' | \alpha \rangle = \int_{-\infty}^{\infty} dp' \phi_\beta^* (p') \phi_\alpha (p') . \]  (3.49)

The normalization condition reads

\[ 1 = \langle \alpha | \alpha \rangle = \int_{-\infty}^{\infty} dp' |\phi_\alpha (p')|^2 . \]  (3.50)

3.2 Transformation Function

What is the relation between the position wavefunction \( \psi_\alpha (x') \) and its momentum counterpart \( \phi_\alpha (p') \)?

Claim. The transformation function \( \langle x' | p' \rangle \) is given by

\[ \langle x' | p' \rangle = \frac{1}{\sqrt{2\pi \hbar}} \exp \left( \frac{-ip'x'}{\hbar} \right) . \]  (3.51)

Proof. On one hand, according to Eq. (3.32)

\[ \langle x' | p | p' \rangle = p' \langle x' | p' \rangle , \]  (3.52)

and on the other hand, according to Eq. (3.29)

\[ \langle x' | p | p' \rangle = -i\hbar \frac{\partial}{\partial x'} \langle x' | p' \rangle , \]  (3.53)

thus

\[ p' \langle x' | p' \rangle = -i\hbar \frac{\partial}{\partial x'} \langle x' | p' \rangle . \]  (3.54)
The general solution of this differential equation is

\[ \langle x' \mid p' \rangle = N \exp \left( \frac{i p' x'}{\hbar} \right), \quad (3.55) \]

where \( N \) is a normalization constant. To determine the constant \( N \) we employ Eqs. (3.36) and (3.44):

\[
\begin{align*}
\delta (x' - x'') &= \langle x' \mid x'' \rangle \\
&= \int dp' \langle x' \mid p' \rangle \langle p' \mid x'' \rangle \\
&= \int dp' |N|^2 \exp \left( \frac{i p' (x' - x'')}{\hbar} \right) \\
&= \hbar |N|^2 \int \frac{dke^{ik(x'-x')}}{2\pi \delta(x'-x'')} \, . \\
& \quad (3.56)
\end{align*}
\]

Thus, by choosing \( N \) to be real one finds that

\[ \langle x' \mid p' \rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp \left( \frac{i p' x'}{\hbar} \right). \quad (3.57) \]

The last result together with Eqs. (3.32) and (3.44) yield

\[
\begin{align*}
\psi_{\alpha} (x') &= \langle x' \mid \alpha \rangle = \int_{-\infty}^{\infty} dp' \langle x' \mid p' \rangle \langle p' \mid \alpha \rangle = \frac{\int_{-\infty}^{\infty} dp' e^{i\frac{p' x'}{\hbar}} \phi_{\alpha} (p')}{\sqrt{2\pi\hbar}}, \quad (3.58) \\
\phi_{\alpha} (p') &= \langle p' \mid \alpha \rangle = \int_{-\infty}^{\infty} dx' \langle p' \mid x' \rangle \langle x' \mid \alpha \rangle = \frac{\int_{-\infty}^{\infty} dx' e^{-i\frac{p' x'}{\hbar}} \psi_{\alpha} (x')}{\sqrt{2\pi\hbar}}. \quad (3.59)
\end{align*}
\]

That is, transformations relating \( \psi_{\alpha} (x') \) and \( \phi_{\alpha} (p') \) are the direct and inverse Fourier transformations.

### 3.3 Generalization for 3D

According to Eq. (3.6) the observables \( q_x, q_y \) and \( q_z \) commute with each other, hence, a simultaneous diagonalization is possible. Denoting the common eigenvectors as
3.3. Generalization for 3D

\[ |r'\rangle = |q'_x, q'_y, q'_z \rangle \]  

one has

\[ q_x |r'\rangle = q'_x |q'_x, q'_y, q'_z \rangle \]  
\[ q_y |r'\rangle = q'_y |q'_x, q'_y, q'_z \rangle \]  
\[ q_z |r'\rangle = q'_z |q'_x, q'_y, q'_z \rangle \]  

The closure relation is written as

\[ 1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx' dy' dz' |r'\rangle \langle r'| , \]

and the orthonormality relation as

\[ \langle r' | r'' \rangle = \delta (r' - r'') . \]

Similarly, according to Eq. (3.7) the observables \( p_x, p_y, p_z \) commute with each other, hence, a simultaneous diagonalization is possible. Denoting the common eigenvectors as

\[ |p'\rangle = |p'_x, p'_y, p'_z \rangle \]  

one has

\[ p_x |p'\rangle = p'_x |p'_x, p'_y, p'_z \rangle \]  
\[ p_y |p'\rangle = p'_y |p'_x, p'_y, p'_z \rangle \]  
\[ p_z |p'\rangle = p'_z |p'_x, p'_y, p'_z \rangle \]  

The closure relation is written as

\[ 1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dp'_x dp'_y dp'_z |p'\rangle \langle p'| , \]

and the orthonormality relation as

\[ \langle p' | p'' \rangle = \delta (p' - p'') . \]

The translation operator in three dimensions can be expressed as

\[ J (\Delta) = \exp \left( - \frac{i \Delta \cdot \mathbf{p}}{\hbar} \right) , \]

where \( \Delta = (\Delta_x, \Delta_y, \Delta_z) \in \mathbb{R}^3 \), and where

\[ J (\Delta) |r'\rangle = |r' + \Delta \rangle . \]

The generalization of Eq. (3.51) for three dimensions is

\[ \langle r' | p' \rangle = \frac{1}{(2 \pi \hbar)^{3/2}} \exp \left( \frac{ip' \cdot r'}{\hbar} \right) . \]
3.4 Problems

1. Show that

\[ [p, A(x)] = -i\hbar \frac{dA}{dx}, \tag{3.75} \]

\[ [x, B(p)] = i\hbar \frac{dB}{dp}, \tag{3.76} \]

where \( A(x) \) is a differentiable function of \( x \) and \( B(p) \) is a differentiable function of \( p \).

2. Show that the mean value of \( x \) in a state described by the wavefunction \( \psi(x) \), namely

\[ \langle x \rangle = \int_{-\infty}^{+\infty} dx \psi^*(x) x \psi(x), \tag{3.77} \]

is equal to the value of \( a \) for which the expression

\[ F(a) \equiv \int_{-\infty}^{+\infty} dx \psi^*(x + a) x^2 \psi(x + a) \tag{3.78} \]

obtains a minimum, and that this minimum has the value

\[ F_{\text{min}} = (\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2. \tag{3.79} \]

3. Consider a Gaussian wave packet, whose \( x \)-space wavefunction is given by

\[ \psi_\alpha(x') = \frac{1}{\pi^{1/4}d} \exp\left( i k x' - \frac{x'^2}{2d^2} \right). \tag{3.80} \]

Calculate

a) \( \langle \Delta x^2 \rangle \), \( \langle \Delta p^2 \rangle \)

b) \( \langle p' | \alpha \rangle \)

4. Show that the state \( |\alpha\rangle \) with wave function

\[ \langle x' | \alpha \rangle = \begin{cases} 1/\sqrt{2\alpha} & \text{for } |x| \leq \alpha \\ 0 & \text{for } |x| > \alpha \end{cases} \tag{3.81} \]

the uncertainty in momentum is infinity.

5. Show that

\[ \frac{1}{(2\pi\hbar)^3} \int d^3p' \exp\left( \frac{i \mathbf{p}' \cdot (\mathbf{r}' - \mathbf{r}'')}{\hbar} \right) = \delta (\mathbf{r}' - \mathbf{r}''). \tag{3.82} \]
3.5 Solutions

1. The commutator \([x, p] = i\hbar\) is a constant, thus the relation (2.175) can be employed

\[
[x, p^m] = i\hbar \frac{d p^m}{dp}.
\]  

(3.84)

This holds for any \(m\), thus, for any differentiable function \(A(x)\) of \(x\) and for any differentiable function \(B(p)\) of \(p\) one has

\[
[p, A(x)] = -i\hbar \frac{dA}{dx},
\]

(3.85)

\[
[x, B(p)] = i\hbar \frac{dB}{dp}.
\]

(3.86)

2. The following holds

\[
F(a) = \int_{-\infty}^{+\infty} dx \psi^* (x + a) x^2 \psi (x + a)
\]

\[
= \int_{-\infty}^{+\infty} dx' \psi^* (x') (x' - a)^2 \psi (x')
\]

\[
= \langle (x - a)^2 \rangle
\]

\[
= \langle x^2 \rangle - 2a \langle x \rangle + a^2.
\]

(3.87)

The requirement

\[
\frac{dF}{da} = 0
\]

(3.88)

leads to \(-2 \langle x \rangle + 2a = 0\), or \(a = \langle x \rangle\). At that point one has

\[
F_{\min} = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2.
\]

(3.89)

3. The following hold

\[
\langle x \rangle = \int_{-\infty}^{+\infty} dx' \psi_*^* (x') x' \psi (x')
\]

\[
= \frac{1}{\pi^{1/2} d} \int_{-\infty}^{+\infty} dx' \exp \left( -\frac{x'^2}{d^2} \right) x'
\]

\[
= 0,
\]

(3.90)
\[ \langle x^2 \rangle = \int_{-\infty}^{+\infty} dx' \psi_{\alpha}^*(x') x'^2 \psi_{\alpha}(x') \]
\[ = \frac{1}{\pi^{1/2} d} \int_{-\infty}^{+\infty} dx' \exp \left( -\frac{x'^2}{d^2} \right) x'^2 \]
\[ = \frac{1}{\pi^{1/2} d} \frac{d^3 \pi^{1/2}}{2} \]
\[ = \frac{d^2}{2}, \tag{3.91} \]

\[ \langle p \rangle = -i\hbar \int_{-\infty}^{+\infty} dx' \psi_{\alpha}^*(x') \frac{d\psi_{\alpha}}{dx'} \]
\[ = -\frac{i\hbar}{\pi^{1/2} d} \int_{-\infty}^{+\infty} dx' \exp \left( -\frac{x'^2}{d^2} \right) \left( ik - \frac{x'}{d^2} \right) \]
\[ = -\frac{i\hbar}{\pi^{1/2} d} ik \pi^{1/2} \]
\[ = \hbar k, \tag{3.92} \]

\[ \langle p^2 \rangle = (-i\hbar)^2 \int_{-\infty}^{+\infty} dx' \psi_{\alpha}^*(x') \frac{d^2\psi_{\alpha}}{dx'^2} \]
\[ = (-i\hbar)^2 \frac{1}{\pi^{1/2} d} \int_{-\infty}^{+\infty} dx' \exp \left( -\frac{x'^2}{d^2} \right) \left( \left( ik - \frac{x'}{d^2} \right)^2 - \frac{1}{d^2} \right) \]
\[ = (-i\hbar)^2 \frac{1}{\pi^{1/2} d} \left( -\frac{1}{2} \right) d \sqrt{\pi} \frac{2d^4 k^2 + d^2}{d^4} \]
\[ = (\hbar^2)^2 \left( 1 + \frac{1}{2(\hbar k)^2} \right), \tag{3.93} \]

a) thus

\[ \langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \frac{d^2}{2} \left( (\hbar k)^2 \left( 1 + \frac{1}{2(\hbar k)^2} \right) - (\hbar k)^2 \right) = \frac{\hbar^2}{4}. \tag{3.94} \]
3.5. Solutions

b) Using Eq. (3.59) one has

\[ \langle p' | \alpha \rangle = \frac{1}{\sqrt{2\pi \hbar}} \int dx' \exp \left( -\frac{i p' x'}{\hbar} \right) \psi_\alpha (x') \]

\[ = \frac{1}{\sqrt{2\pi \hbar} \pi^{1/4} \sqrt{d}} \int dx' \exp \left( ik - \frac{i p'}{\hbar} x' - \frac{x'^2}{2d} \right) \]

\[ = \frac{\sqrt{d}}{\pi^{1/4} \sqrt{\hbar}} \exp \left( -\frac{(hk - p')^2 d^2}{2\hbar} \right) . \]

(3.95)

4. The momentum wavefunction is found using Eq. (3.59)

\[ \phi_\alpha (p') = \frac{1}{\sqrt{2\pi \hbar}} \int_{-\infty}^{\infty} dx' \exp \left( -\frac{i p' x'}{\hbar} \right) \langle x' | \alpha \rangle \]

\[ = \frac{1}{\sqrt{4\pi \hbar} a} \int_{-a}^{a} dx' \exp \left( -\frac{i p' x'}{\hbar} \right) \]

\[ = \sqrt{\frac{a}{\pi \hbar}} \sin \left( \frac{ap'}{\hbar} \right) . \]

(3.96)

The momentum wavefunction \( \phi_\alpha (p') \) is normalizable, however, the integrals for evaluating both \( \langle p \rangle \) and \( \langle p^2 \rangle \) do not converge.

5. With the help of Eqs. (3.65), (3.70) and (3.74) one finds that

\[ \delta (r' - r'') = \langle r' | r'' \rangle \]

\[ = \int d^3 p' \langle r' | p' \rangle \langle p' | r'' \rangle \]

\[ = \frac{1}{(2\pi \hbar)^3} \int d^3 p' \exp \left( i \frac{p' \cdot (r' - r'')}{\hbar} \right) . \]

(3.97)
4. Quantum Dynamics

The time evolution of a state vector $|\alpha\rangle$ is postulated to be given by the Schrödinger equation

$$i\hbar \frac{d|\alpha\rangle}{dt} = \mathcal{H}|\alpha\rangle,$$  \hspace{1cm} (4.1)

where the Hermitian operator $\mathcal{H} = \mathcal{H}^\dagger$ is the Hamiltonian of the system. The Hamiltonian operator is the observable corresponding to the classical Hamiltonian function that we have studied in chapter 1. The time evolution produced by Eq. (4.1) is unitary, as is shown below:

Claim. The norm $\langle \alpha |\alpha\rangle$ is time independent.

Proof. Since $\mathcal{H} = \mathcal{H}^\dagger$, the dual of the Schrödinger equation (4.1) is given by

$$-i\hbar \frac{d\langle \alpha |}{dt} = \langle \alpha |\mathcal{H}.$$  \hspace{1cm} (4.2)

Using this one has

$$\frac{d\langle \alpha |\alpha\rangle}{dt} = \left(\frac{d\langle \alpha |}{dt}\right)\langle \alpha | + \langle \alpha |\frac{d|\alpha\rangle}{dt} = \frac{1}{i\hbar}(-\langle \alpha |\mathcal{H}|\alpha\rangle + \langle \alpha |\mathcal{H}|\alpha\rangle) = 0.$$  \hspace{1cm} (4.3)

4.1 Time Evolution Operator

The time evolution operator $u(t, t_0)$ relates the state vector at time $|\alpha(t_0)\rangle$ with its value $|\alpha(t)\rangle$ at time $t$:

$$|\alpha(t)\rangle = u(t, t_0)|\alpha(t_0)\rangle.$$ \hspace{1cm} (4.4)

Claim. The time evolution operator satisfies the Schrödinger equation (4.1).

Proof. Expressing the Schrödinger equation (4.1) in terms of Eq. (4.4)

$$i\hbar \frac{d}{dt}u(t, t_0)|\alpha(t_0)\rangle = \mathcal{H}u(t, t_0)|\alpha(t_0)\rangle,$$ \hspace{1cm} (4.5)

and noting that $|\alpha(t_0)\rangle$ is $t$ independent yield
Chapter 4. Quantum Dynamics

\[ i\hbar \left( \frac{d}{dt} u(t, t_0) \right) |\alpha(t_0)\rangle = \mathcal{H}u(t, t_0) |\alpha(t_0)\rangle. \]  

(4.6)

Since this holds for any \( |\alpha(t_0)\rangle \) one concludes that

\[ i\hbar \frac{du(t, t_0)}{dt} = \mathcal{H}u(t, t_0). \]  

(4.7)

This results leads to the following conclusion:

Claim. The time evolution operator is unitary.

Proof. Using Eq. (4.7) one finds that

\[
\frac{d}{dt} (u^\dagger u) = u^\dagger \frac{du}{dt} + \frac{du^\dagger}{dt} u \\
= \frac{1}{i\hbar} (u^\dagger \mathcal{H} u - u^\dagger \mathcal{H} u) \\
= 0. 
\]  

(4.8)

Furthermore, for \( t = t_0 \) clearly \( u(t_0, t_0) = u^\dagger (t_0, t_0) = 1 \). Thus, one concludes that \( u^\dagger u = 1 \) for any time, namely \( u \) is unitary.

4.2 Time Independent Hamiltonian

A special case of interest is when the Hamiltonian is time independent. In this case the solution of Eq. (4.7) is given by

\[ u(t, t_0) = \exp \left( -\frac{i\mathcal{H}(t - t_0)}{\hbar} \right). \]  

(4.9)

The operator \( u(t, t_0) \) takes a relatively simple form in the basis of eigenvectors of the Hamiltonian \( \mathcal{H} \). Denoting these eigenvectors as \( |a_{n,i}\rangle \), where the index \( i \) is added to account for possible degeneracy, and denoting the corresponding eigenenergies as \( E_n \) one has

\[ \mathcal{H} |a_{n,i}\rangle = E_n |a_{n,i}\rangle, \]  

(4.10)

where

\[ \langle a_{n',i'} | a_{n,i} \rangle = \delta_{n'n} \delta_{ii'} . \]  

(4.11)

By using the closure relation, which is given by

\[ 1 = \sum_{n} \sum_{i=1}^{g_n} |a_{n,i}\rangle \langle a_{n,i}|. \]  

(4.12)
4.3 Example - Spin 1/2

and Eq. (4.9) one finds that
\[ u(t, t_0) = \exp \left( -\frac{i\mathcal{H}(t-t_0)}{\hbar} \right) \]
\[ = \sum_n \sum_{i=1}^{g_n} \exp \left( -\frac{i\mathcal{H}(t-t_0)}{\hbar} \right) |a_{n,i}\rangle \langle a_{n,i}| \]
\[ = \sum_n \sum_{i=1}^{g_n} \exp \left( -\frac{iE_n(t-t_0)}{\hbar} \right) |a_{n,i}\rangle \langle a_{n,i}| . \]  

(4.13)

Using this results the state vector \(|\alpha(t)\rangle\) can be written as
\[ |\alpha(t)\rangle = u(t, t_0) |\alpha(t_0)\rangle \]
\[ = \sum_n \sum_{i=1}^{g_n} \exp \left( -\frac{iE_n(t-t_0)}{\hbar} \right) |a_{n,i}\rangle \langle a_{n,i}| |\alpha(t_0)\rangle \]  

(4.14)

Note that if the system is initially in an eigenvector of the Hamiltonian with eigenenergy \(E_n\), then according to Eq. (4.14)
\[ |\alpha(t)\rangle = \exp \left( -\frac{iE_n(t-t_0)}{\hbar} \right) |\alpha(t_0)\rangle . \]  

(4.15)

However, the phase factor multiplying \(|\alpha(t_0)\rangle\) has no effect on any measurable physical quantity of the system, that is, the system’s properties are time independent. This is why the eigenvectors of the Hamiltonian are called stationary states.

4.3 Example - Spin 1/2

In classical mechanics, the potential energy \(U\) of a magnetic moment \(\mu\) in a magnetic field \(B\) is given by
\[ U = -\mu \cdot B . \]  

(4.16)

The magnetic moment of a spin 1/2 is given by [see Eq. (2.90)]
\[ \mu_{\text{spin}} = \frac{2\mu_B}{h} \mathbf{S} , \]  

(4.17)

where \(\mathbf{S}\) is the spin angular momentum vector and where
\[ \mu_B = \frac{e\hbar}{2mec} \]  

(4.18)
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is the Bohr’s magneton (note that the electron charge is taken to be negative \( e < 0 \)). Based on these relations we hypothesize that the Hamiltonian of a spin \( 1/2 \) in a magnetic field \( B \) is given by

\[
\mathcal{H} = -\frac{e}{mc} \mathbf{S} \cdot \mathbf{B} .
\] (4.19)

Assume the case where

\[
\mathbf{B} = B\hat{z} ,
\] (4.20)

where \( B \) is a constant. For this case the Hamiltonian is given by

\[
\mathcal{H} = \omega \mathbf{S}_z ,
\] (4.21)

where

\[
\omega = \frac{|e| B}{mc} \] (4.22)

is the so-called Larmor frequency. In terms of the eigenvectors of the operator \( \mathbf{S}_z \)

\[
\mathbf{S}_z |\pm\rangle = \pm \frac{h}{2} |\pm\rangle ,
\] (4.23)

where the compact notation \(|\pm\rangle\) stands for the states \(|\pm;\hat{z}\rangle\), one has

\[
\mathcal{H} |\pm\rangle = \pm \frac{\hbar \omega}{2} |\pm\rangle ,
\] (4.24)

namely the states \(|\pm\rangle\) are eigenstates of the Hamiltonian. Equation (4.13) for the present case reads

\[
u(t, 0) = e^{-\frac{i\omega t}{2}} |+\rangle \langle +| + e^{i\frac{\omega t}{2}} |\rangle \langle -| .
\] (4.25)

Exercise 4.3.1. Consider spin \( 1/2 \) in magnetic field given by \( \mathbf{B} = B\hat{z} \), where \( B \) is a constant. Given that \( |\alpha(0)\rangle = |+;\hat{x}\rangle \) at time \( t = 0 \) calculate (a) the probability \( p_\pm(t) \) to measure \( \mathbf{S}_z = \pm h/2 \) at time \( t \); (b) the expectation value \( \langle \mathbf{S}_x \rangle(t) \) at time \( t \).

Solution 4.3.1. Recall that [see Eq. (2.102)]

\[
|\pm;\hat{x}\rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm |-\rangle)
\] (4.26)

(a) Using Eq. (4.25) one finds

\[
p_\pm(t) = |\langle |\pm;\hat{x}| \nu(t, 0) |\alpha(0)\rangle|^2
\]
\[
= \frac{1}{2} \left( \langle + | \pm |-\rangle \left( e^{-\frac{i\omega t}{2}} |+\rangle \langle +| + e^{i\frac{\omega t}{2}} |-\rangle \langle -| \right) (|+\rangle + |-\rangle) \right)^2
\]
\[
= \frac{1}{2} \left( e^{-i\omega t} \pm e^{i\omega t} \right)^2 ,
\] (4.27)
4.4. Connection to Classical Dynamics

thus

\[ p_+ (t) = \cos^2 \left( \frac{\omega t}{2} \right), \]  
\[ p_- (t) = \sin^2 \left( \frac{\omega t}{2} \right). \]  

(b) Using the results for \( p_+ \) and \( p_- \) one has

\[ \langle S_x \rangle = \frac{\hbar}{2} (p_+ - p_-) \]
\[ = \frac{\hbar}{2} \left( \cos^2 \left( \frac{\omega t}{2} \right) - \sin^2 \left( \frac{\omega t}{2} \right) \right) \]
\[ = \frac{\hbar}{2} \cos \omega t. \]  

(4.30)

4.4 Connection to Classical Dynamics

In chapter 1 we have found that in classical physics, the dynamics of a variable \( A^{(c)} \) is governed by Eq. (1.38), which is given by

\[
\frac{dA^{(c)}}{dt} = \left\{ A^{(c)}, \mathcal{H}^{(c)} \right\} + \frac{\partial A^{(c)}}{\partial t}.
\]  

(4.31)

We seek a quantum analogy to this equation. To that end, we derive an equation of motion for the expectation value \( \langle A \rangle \) of the observable \( A \) that corresponds to the classical variable \( A^{(c)} \). In general, the expectation value can be expressed as

\[
\langle A \rangle = \langle \alpha (t) | A | \alpha (t) \rangle = \langle \alpha (t_0) | u^\dagger (t, t_0) A u (t, t_0) | \alpha (t_0) \rangle = \langle \alpha (t_0) | A^{(H)} | \alpha (t_0) \rangle,
\]  

(4.32)

where \( u \) is the time evolution operator and

\[
A^{(H)} = u^\dagger (t, t_0) A u (t, t_0).
\]  

(4.33)

The operator \( A^{(H)} \) is called the Heisenberg representation of \( A \). We first derive an equation of motion for the operator \( A^{(H)} \). By using Eq. (4.7) one finds that the following holds

\[
\frac{du}{dt} = \frac{1}{i\hbar} \mathcal{H} u, \quad (4.34)
\]
\[
\frac{du^\dagger}{dt} = -\frac{1}{i\hbar} u^\dagger \mathcal{H}, \quad (4.35)
\]

therefore
\[
\frac{dA^{(H)}}{dt} = \frac{du^\dagger}{dt}Au + u^\dagger A\frac{du}{dt} + u^\dagger \frac{\partial A}{\partial t}u
\]

\[
= \frac{1}{\hbar} \left( -u^\dagger HAu + u^\dagger A\mathcal{H}u \right) + u^\dagger \frac{\partial A}{\partial t}u
\]

\[
= \frac{1}{\hbar} \left( -\mathcal{H}^{(H)}A^{(H)} + A^{(H)}\mathcal{H}^{(H)} \right) + \frac{\partial A^{(H)}}{\partial t}.
\]

(4.36)

Thus, we have found that

\[
\frac{dA^{(H)}}{dt} = \frac{1}{\hbar} \left[ A^{(H)}, \mathcal{H}^{(H)} \right] + \frac{\partial A^{(H)}}{\partial t}.
\]

(4.37)

Furthermore, the desired equation of motion for \( \langle A \rangle \) is found using Eqs. (4.32) and (4.37)

\[
\frac{d\langle A \rangle}{dt} = \frac{1}{\hbar} \langle [A, \mathcal{H}] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle .
\]

(4.38)

We see that the Poisson’s brackets in the classical equation of motion (4.31) for the classical variable \( A^{(c)} \) are replaced by a commutation relation in the quantum counterpart equation of motion (4.38) for the expectation value \( \langle A \rangle \)

\[
\{, \} \rightarrow \frac{1}{\hbar} [ , ] .
\]

(4.39)

Note that for the case where the Hamiltonian is time independent, namely for the case where the time evolution operator is given by Eq. (4.9), \( u \) commutes with \( \mathcal{H} \), namely \([u, \mathcal{H}] = 0\), and consequently

\[
\mathcal{H}^{(H)} = u^\dagger \mathcal{H}u = \mathcal{H}.
\]

(4.40)

### 4.5 Symmetric Ordering

What is in general the correspondence between a classical variable and its quantum operator counterpart? Consider for example the system of a point particle moving in one dimension. Let \( x^{(c)} \) be the classical coordinate and let \( p^{(c)} \) be the canonically conjugate momentum. As we have done in chapter 3, the quantum observables corresponding to \( x^{(c)} \) and \( p^{(c)} \) are the Hermitian operators \( x \) and \( p \). The commutation relation \([x, p]\) is derived from the corresponding Poisson’s brackets \( \{x^{(c)}, p^{(c)}\} \) according to the rule

\[
\{, \} \rightarrow \frac{1}{\hbar} [ , ] .
\]

(4.41)
4.5. Symmetric Ordering

\[ \{ x^{(c)}, p^{(c)} \} = 1 \rightarrow [x, p] = i\hbar . \]  

However, what is the quantum operator corresponding to a general function \( A(x^{(c)}, p^{(c)}) \)? This question raises the issue of ordering. As an example, let \( A(x^{(c)}, p^{(c)}) = x^{(c)} p^{(c)} \). Classical variables obviously commute, therefore \( x^{(c)} p^{(c)} = p^{(c)} x^{(c)} \). However, this is not true for quantum operators \( xp \neq px \). Moreover, it is clear that both operators \( xp \) and \( px \) cannot be considered as observables since they are not Hermitian.

\[ (xp)^\dagger = px \neq xp, \quad (px)^\dagger = xp \neq px. \]  

A better candidate to serve as the quantum operator corresponding to the classical variables \( x^{(c)} p^{(c)} \) is the operator \( (xp + px)/2 \), which is obtained from \( x^{(c)} p^{(c)} \) by a procedure called symmetric ordering. A general transformation that produces a symmetric ordered observable \( A(x, p) \) that corresponds to a given general function \( A(x^{(c)}, p^{(c)}) \) of the classical variable \( x^{(c)} \) and its canonical conjugate \( p^{(c)} \) is given below

\[ A(x, p) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A(x^{(c)}, p^{(c)}) \Upsilon dx^{(c)} dp^{(c)}, \]  

where

\[ \Upsilon = \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\frac{\eta(x^{(c)} - x)}{\hbar} + i\frac{\xi(p^{(c)} - p)}{\hbar}} d\eta d\xi. \]  

This transformation is called the Weyl transformation. The identity

\[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dke^{ik(x' - x'')} = 2\pi \delta (x' - x''), \]  

implies that

\[ \frac{1}{2\pi\hbar} \int e^{i\frac{\eta(x^{(c)} - x)}{\hbar}} d\eta = \delta (x^{(c)} - x), \]  

\[ \frac{1}{2\pi\hbar} \int e^{i\frac{\xi(p^{(c)} - p)}{\hbar}} d\xi = \delta (p^{(c)} - p). \]  

At first glance these relations may lead to the (wrong) conclusion that the term \( \Upsilon \) equals to \( \delta (x^{(c)} - x) \) \( \delta (p^{(c)} - p) \), however, this is incorrect since \( x \) and \( p \) are non-commuting operators.
4.6 Problems

1. Consider spin $\frac{1}{2}$ in magnetic field given by $\mathbf{B} = B \hat{z}$, where $B$ is a constant. At time $t = 0$ the system is in the state $|+; \mathbf{x}\rangle$. Calculate $\langle S_y \rangle$ and $\langle S_z \rangle$ as a function of time $t$.

2. Consider the Hamiltonian operator

$$\hat{H} = \frac{p^2}{2m} + V(\mathbf{r}) , \quad \text{(4.50)}$$

where $\mathbf{r} = (x, y, z)$ is the vector of position operators, $\mathbf{p} = (p_x, p_y, p_z)$ is the vector of canonical conjugate operators, and the mass $m$ is a constant. Let $|\psi_n\rangle$ be a normalizable eigenvector of the Hamiltonian $\hat{H}$ with eigenvalue $E_n$. Show that

$$\langle \psi_n | \mathbf{p} | \psi_n \rangle = 0 . \quad \text{(4.51)}$$

3. Show that in the $p$ representation the Schrödinger equation

$$i \hbar \frac{d |\alpha\rangle}{dt} = \hat{H} |\alpha\rangle , \quad \text{(4.52)}$$

where $\hat{H}$ is the Hamiltonian

$$\hat{H} = \frac{p^2}{2m} + V(\mathbf{r}) , \quad \text{(4.53)}$$

can be transformed into the integro-differential equation

$$i \hbar \frac{d \phi_\alpha}{dt} = \frac{p^2}{2m} \phi_\alpha + \int d\mathbf{p}' U(\mathbf{p} - \mathbf{p}') \phi_\alpha , \quad \text{(4.54)}$$

where $\phi_\alpha = \phi_\alpha(\mathbf{p}', t) = \langle \mathbf{p}' | \alpha \rangle$ is the momentum wave function and where

$$U(\mathbf{p}) = (2\pi \hbar)^{-3} \int d\mathbf{r} V(\mathbf{r}) \exp \left( -\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{r} \right) . \quad \text{(4.55)}$$

4. Consider a particle of mass $m$ in a scalar potential energy $V(\mathbf{r})$. Prove Ehrenfest’s theorem

$$m \frac{d^2}{dt^2} (\mathbf{r}) = -\langle \nabla V(\mathbf{r}) \rangle . \quad \text{(4.56)}$$

5. Show that if the potential energy $V(\mathbf{r})$ can be written as a sum of functions of a single coordinate, $V(\mathbf{r}) = V_1(x_1) + V_2(x_2) + V_3(x_3)$, then the time-independent Schrödinger equation can be decomposed into a set of one-dimensional equations of the form

$$\frac{d^2 \psi_i(x_i)}{dx_i^2} + \frac{2m}{\hbar^2} [E_i - V_i(x_i)] \psi_i(x_i) = 0 , \quad \text{(4.57)}$$

where $i \in \{1, 2, 3\}$, with $\psi(\mathbf{r}) = \psi_1(x_1) \psi_2(x_2) \psi_3(x_3)$ and $E = E_1 + E_2 + E_3$. 

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6. Show that, in one-dimensional problems, the energy spectrum of the bound states is always non-degenerate.

7. Let \( \psi_n(x) \) \((n = 1, 2, 3, \cdots)\) be the eigen-wave-functions of a one-dimensional Schrödinger equation with eigen-energies \( E_n \) placed in order of increasing magnitude \( (E_1 < E_2 < \cdots)\). Show that between any two consecutive zeros of \( \psi_n(x) \), \( \psi_{n+1}(x) \) has at least one zero.

8. What conclusions can be drawn about the parity of the eigen-functions of the one-dimensional Schrödinger equation

\[
\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0
\]

if the potential energy is an even function of \( x \), namely \( V(x) = V(-x) \).

9. Show that the first derivative of the time-independent wavefunction is continuous even at points where \( V(x) \) has a finite discontinuity.

10. A particle having mass \( m \) is confined by a one dimensional potential given by

\[
V_s(x) = \begin{cases} 
-W \text{ if } |x| \leq a \\
0 \text{ if } |x| > a 
\end{cases}
\]

where \( a > 0 \) and \( W > 0 \) are real constants. Show that the particle has at least one bound state (i.e., a state having energy \( E < 0 \)).

11. Consider a particle having mass \( m \) confined in a potential well given by

\[
V(x) = \begin{cases} 
0 \text{ if } 0 \leq x \leq a \\
\infty \text{ if } x < 0 \text{ or } x > a 
\end{cases}
\]

The eigen energies are denoted by \( E_n \) and the corresponding eigen states are denoted by \( |\varphi_n\rangle \), where \( n = 1, 2, \cdots \) (as usual, the states are numbered in increasing order with respect to energy). The state of the system at time \( t = 0 \) is given by

\[
|\Psi(0)\rangle = a_1 |\varphi_1\rangle + a_2 |\varphi_2\rangle + a_3 |\varphi_3\rangle.
\]

(a) The energy \( E \) of the system is measured at time \( t = 0 \). What is the probability to measure a value smaller than \( 3\pi^2\hbar^2/(ma^2) \)? (b) Calculate the standard deviation \( \Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} \) at time \( t = 0 \). (c) The same as (b), however for any time \( t > 0 \). (d) The energy was measured at time \( t \) and the value of \( 2\pi^2\hbar^2/(ma^2) \) was found. The energy is measured again at later time \( t_0 > t \). Calculate \( \langle E \rangle \) and \( \langle \Delta E \rangle \) at time \( t_0 \).

12. Consider a point particle having mass \( m \) in a one dimensional potential given by

\[
V(x) = \begin{cases} 
-\alpha \delta(x) \text{ if } |x| < a \\
\infty \text{ if } |x| \geq a 
\end{cases}
\]

where \( \delta(x) \) is the delta function and \( \alpha \) is a constant. Let \( E_0 \) be the energy of the ground state. Under what conditions \( E_0 < 0 \)?
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13. **Thomas-Reiche-Kuhn sum rule** - Let

\[
H = \frac{p^2}{2m} + V(r)
\]  

(4.63)

be the Hamiltonian of a particle of mass \( m \) moving in a potential \( V(r) \). Show that

\[
\sum_k (E_k - E_l) |\langle k | x | l \rangle|^2 = \frac{\hbar^2}{2m},
\]  

(4.64)

where the sum is taken over all energy eigen-states of the particle (where \( \mathcal{H} |k \rangle = E_k |k \rangle \)), and \( x \) is the \( x \) component of the position vector operator \( r \) (the Thomas-Reiche-Kuhn sum rule).

14. A particle having mass \( m \) is confined in a one dimensional potential well given by

\[
V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{else} \end{cases}
\]

(a) At time \( t = 0 \) the position was measured and the result was \( x = a/2 \). The resolution of the position measurement is \( \Delta x \), where \( \Delta x << a \). After time \( \tau_1 \) the energy was measured. Calculate the probability \( p_n \) to measure that the energy of the system is \( E_n \), where \( E_n \) are the eigenenergies of the particle in the well, and where \( n = 1, 2, \cdots \). (b) Assume that the result of the measurement in the previous section was \( E_2 \). At a later time \( \tau_2 > \tau_1 \) the momentum \( p \) of the particle was measured. Calculate the expectation value \( \langle p \rangle \).

15. A particle having mass \( m \) is in the ground state of an infinite potential well of width \( a \), which is given by

\[
V_1(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{else} \end{cases}
\]  

(4.65)

At time \( t = 0 \) the potential suddenly changes and becomes

\[
V_2(x) = \begin{cases} 0 & 0 < x < 2a \\ \infty & \text{else} \end{cases}
\]  

(4.66)

namely the width suddenly becomes \( 2a \). (a) Find the probability \( p \) to find the particle in the ground state of the new well. (b) Calculate the expectation value of the energy \( \langle \mathcal{H} \rangle \) before and after the change in the potential.

16. **The continuity equation** - Consider a point particle having mass \( m \) and charge \( q \) placed in an electromagnetic field. Show that

\[
\frac{d\rho}{dt} + \nabla J = 0,
\]  

(4.67)
4.7 Solutions

where

\[ \rho = \psi \psi^* \]  

(4.68)

is the probability density, \( \psi(x') \) is the wavefunction,

\[ J = \frac{\hbar}{m} \text{Im} (\psi^* \nabla \psi) - \frac{q}{mc} (\rho A) \]  

(4.69)

is the current density, and \( A \) is the electromagnetic vector potential.

17. Calculate the Weyl transformation \( A(x, p) \) of the classical variable \( A^{(c)} \),

18. Invert Eq. (4.45), i.e. express the variable \( A^{(c)} \) as a function of the operator \( A(x, p) \).

4.7 Solutions

1. The operators \( S_x, S_y \) and \( S_z \) are given by Eqs. (2.102), (2.103) and (2.99) respectively. The Hamiltonian is given by Eq. (4.21). Using Eqs. (4.38) and (2.132) one has

\[
\frac{d}{dt} \langle S_x \rangle = \frac{\omega}{\hbar} \langle [S_x, S_z] \rangle = -\omega \langle S_y \rangle ,
\]

(4.70)

\[
\frac{d}{dt} \langle S_y \rangle = \frac{\omega}{\hbar} \langle [S_y, S_z] \rangle = \omega \langle S_x \rangle ,
\]

(4.71)

\[
\frac{d}{dt} \langle S_z \rangle = \frac{\omega}{\hbar} \langle [S_z, S_z] \rangle = 0 ,
\]

(4.72)

where

\[
\omega = \frac{|e| B}{mc} .
\]

(4.73)

At time \( t = 0 \) the system is in state

\[
|\pm; \hat{x}\rangle = \frac{1}{\sqrt{2}} (|\pm\rangle + |\pm\rangle) ,
\]

(4.74)

thus

\[
\langle S_x \rangle (t = 0) = \frac{\hbar}{4} (|+\rangle + |-\rangle) (|+\rangle - |\pm\rangle) (|\pm\rangle + |-\rangle) = \frac{\hbar}{2} .
\]

(4.75)

\[
\langle S_y \rangle (t = 0) = \frac{\hbar}{4} (|+\rangle + |-\rangle) (-i|+\rangle - i|\pm\rangle) (|\pm\rangle + |-\rangle) = 0 .
\]

(4.76)

\[
\langle S_z \rangle (t = 0) = \frac{\hbar}{4} (|+\rangle + |-\rangle) (|+\rangle - |\pm\rangle) (|\pm\rangle + |-\rangle) = 0 .
\]

(4.77)

The solution is easily found to be given by
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\[ \langle S_x \rangle (t) = \left( \frac{\hbar}{2} \right) \cos (\omega t), \quad (4.75) \]

\[ \langle S_y \rangle (t) = \left( \frac{\hbar}{2} \right) \sin (\omega t), \quad (4.76) \]

\[ \langle S_z \rangle (t) = 0. \quad (4.77) \]

2. Using \([x, p_x] = [y, p_y] = [z, p_z] = i \hbar\) one finds that

\[
[\mathcal{H}, \mathbf{r}] = \left[ \begin{array}{c} \mathbf{p}^2 \cdot \mathbf{r} \\ \frac{1}{2m} \end{array} \right] \\
= \frac{1}{2m} (p_x^2, x, p_y^2, y, p_z^2, z) \\
= \frac{\hbar}{im} (p_x, p_y, p_z) \\
= \frac{\hbar}{im} \mathbf{p}. \quad (4.78)
\]

Thus

\[
\langle \psi_n | \mathbf{p} | \psi_n \rangle = \frac{im}{\hbar} \langle \psi_n | [\mathcal{H}, \mathbf{r}] | \psi_n \rangle \\
= \frac{im}{\hbar} \langle \psi_n | (\mathcal{H} \mathbf{r} - \mathbf{r} \mathcal{H}) | \psi_n \rangle \\
= \frac{imE_n}{\hbar} \langle \psi_n | (\mathbf{r} - \mathbf{r}) | \psi_n \rangle \\
= 0. \quad (4.79)
\]

3. Multiplying Eq. (4.52) from the left by the bra \( \langle \mathbf{p}' \rangle \) and inserting the closure relation

\[
1 = \int d\mathbf{p}'' \langle \mathbf{p}' | \mathbf{p}'' \rangle \langle \mathbf{p}'' \rangle 
\]

yields

\[
\frac{i \hbar}{d\alpha} \frac{d\phi_{\alpha} (\mathbf{p}')}{dt} = \int d\mathbf{p}'' \langle \mathbf{p}' | \mathcal{H} | \mathbf{p}'' \rangle \phi_{\alpha} (\mathbf{p}''). \quad (4.81)
\]

The following hold

\[
\langle \mathbf{p}' | \mathbf{p}^2 | \mathbf{p}'' \rangle = \mathbf{p}^2 \delta (\mathbf{p}' - \mathbf{p}''), \quad (4.82)
\]

and
\begin{align*}
\langle p' | V(\mathbf{r}) | p'' \rangle &= \int d\mathbf{r}' \int d\mathbf{r}'' \langle p' | \mathbf{r}' \rangle \langle \mathbf{r}' | V(\mathbf{r}) | \mathbf{r}'' \rangle \langle \mathbf{r}'' | p'' \rangle \\
&= (2\pi\hbar)^{-3} \int d\mathbf{r}' \int d\mathbf{r}'' \exp\left(-\frac{i(p' \cdot \mathbf{r}')}{\hbar}\right) V(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}'') \exp\left(-\frac{i(p'' \cdot \mathbf{r}'')}{\hbar}\right) \\
&= (2\pi\hbar)^{-3} \int d\mathbf{r}' \exp\left(-\frac{i(p' - p'') \cdot \mathbf{r}'}{\hbar}\right) V(\mathbf{r}') \\
&= U(p' - p''),
\end{align*}

thus the momentum wave function \( \phi_\alpha(p') \) satisfies the following equation

\begin{equation}
\frac{i\hbar}{m} \frac{d\phi_\alpha}{dt} = \frac{p'^2}{2m} \phi_\alpha + \int dp'' U(p' - p'') \phi_\alpha.
\end{equation}

4. The Hamiltonian is given by

\begin{equation}
\mathcal{H} = \frac{p^2}{2m} + V(\mathbf{r}).
\end{equation}

Using Eq. (4.38) one has

\begin{equation}
\frac{d}{dt} \langle x \rangle = \frac{1}{i\hbar} \langle [x, \mathcal{H}] \rangle = \frac{1}{i\hbar 2m} \langle [x, p_2^2] \rangle = \frac{\langle p_x \rangle}{m},
\end{equation}

and

\begin{equation}
\frac{d}{dt} \langle p_x \rangle = \frac{1}{i\hbar} \langle [p_x, V(\mathbf{r})] \rangle,
\end{equation}

or with the help of Eq. (3.75)

\begin{equation}
\frac{d}{dt} \langle p_x \rangle = -\left(\frac{\partial V}{\partial x}\right).
\end{equation}

This together with Eq. (4.86) yield

\begin{equation}
m \frac{d^2}{dt^2} \langle x \rangle = -\left(\frac{\partial V}{\partial x}\right).
\end{equation}

Similar equations are obtained for \( \langle y \rangle \) and \( \langle z \rangle \), which together yield Eq. (4.56).

5. Substituting a solution having the form

\begin{equation}
\psi(\mathbf{r}) = \psi_1(x_1) \psi_2(x_2) \psi_3(x_3)
\end{equation}

into the time-independent Schrödinger equation, which is given by

\begin{equation}
\nabla^2 \psi(\mathbf{r}) + \frac{2m}{\hbar^2} [E - V(\mathbf{r})] \psi(\mathbf{r}) = 0,
\end{equation}

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and dividing by $\psi_1 (r)$ yield

$$\sum_{i=1}^{3} \left( \frac{1}{\psi_1 (x_i)} \frac{d^2 \psi_i (x_i)}{dx_i^2} - \frac{2m}{\hbar^2} V_i (x_i) \right) = - \frac{2m}{\hbar^2} E . \tag{4.92}$$

In the sum, the $i$th term ($i \in \{1,2,3\}$) depends only on $x_i$, thus each term must be a constant

$$\frac{1}{\psi_i (x_i)} \frac{d^2 \psi_i (x_i)}{dx_i^2} - \frac{2m}{\hbar^2} V_i (x_i) = - \frac{2m}{\hbar^2} E_i , \tag{4.93}$$

where $E_1 + E_2 + E_3 = E$.

6. Consider two eigen-wave-functions $\psi_1 (x)$ and $\psi_2 (x)$ having the same eigenenergy $E$. The following holds

$$\frac{d^2 \psi_1}{dx_1^2} + \frac{2m}{\hbar^2} (E - V (x)) \psi_1 = 0 , \tag{4.94}$$

$$\frac{d^2 \psi_2}{dx_2^2} + \frac{2m}{\hbar^2} (E - V (x)) \psi_2 = 0 , \tag{4.95}$$

thus

$$\frac{1}{\psi_1} \frac{d^2 \psi_1}{dx_1^2} = \frac{1}{\psi_2} \frac{d^2 \psi_2}{dx_2^2} , \tag{4.96}$$

or

$$\psi_2 \frac{d^2 \psi_1}{dx_1^2} - \psi_1 \frac{d^2 \psi_2}{dx_2^2} = \frac{d}{dx} \left( \psi_2 \frac{d \psi_1}{dx} - \psi_1 \frac{d \psi_2}{dx} \right) = 0 , \tag{4.97}$$

therefore

$$\psi_2 \frac{d \psi_1}{dx} - \psi_1 \frac{d \psi_2}{dx} = C , \tag{4.98}$$

where $C$ is a constant. However, for bound states

$$\lim_{x \to \pm \infty} \psi (x) = 0 , \tag{4.99}$$

thus $C = 0$, and consequently

$$\frac{1}{\psi_1} \frac{d \psi_1}{dx} = \frac{1}{\psi_2} \frac{d \psi_2}{dx} . \tag{4.100}$$

Integrating the above equation yields

$$\log \psi_1 = \log \psi_2 + \alpha , \tag{4.101}$$

where $\alpha$ is a constant. Therefore

$$\psi_1 = e^\alpha \psi_2 , \tag{4.102}$$

and therefore $\psi_2$ is just proportional to $\psi_1$ (both represent the same physical state).
7. Consider two eigen-wave-functions $\psi_n(x)$ and $\psi_{n+1}(x)$ with $E_n < E_{n+1}$. As we saw in the previous exercise, the spectrum is non-degenerate. Moreover, the Schrödinger equation
\[
\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi = 0 ,
\]
which the eigen-wave-functions satisfy, is real. Therefore given that $\psi(x)$ is a solution with a given eigenenergy $E_n$, then also $\psi^*(x)$ is a solution with the same $E$. Therefore, all eigen-wave-functions can be chosen to be real (i.e., by the transformation $\psi(x) \rightarrow (\psi(x) + \psi^*(x))/2$). We have
\[
\frac{d^2\psi_n}{dx^2} + \frac{2m}{\hbar^2} (E_n - V(x)) \psi_n = 0 ,
\]
and
\[
\frac{d^2\psi_{n+1}}{dx^2} + \frac{2m}{\hbar^2} (E_{n+1} - V(x)) \psi_{n+1} = 0 .
\]
By multiplying the first Eq. by $\psi_{n+1}$, the second one by $\psi_n$, and subtracting one has
\[
\frac{d^2\psi_{n+1}}{dx^2} - \psi_n \frac{d^2\psi_n}{dx^2} + \frac{2m}{\hbar^2} (E_n - E_{n+1}) \psi_n \psi_{n+1} = 0 ,
\]
or
\[
\frac{d}{dx} \left( \psi_{n+1} \frac{d\psi_n}{dx} - \psi_n \frac{d\psi_{n+1}}{dx} \right) + \frac{2m}{\hbar^2} [E_n - E_{n+1}] \psi_n \psi_{n+1} = 0 .
\]
Let $x_1$ and $x_2$ be two consecutive zeros of $\psi_n(x)$ (i.e., $\psi_n(x_1) = \psi_n(x_2) = 0$). Integrating from $x_1$ to $x_2$ yields
\[
\left( \psi_{n+1} \frac{d\psi_n}{dx} - \psi_n \frac{d\psi_{n+1}}{dx} \right)_{x_1}^{x_2} = \frac{2m}{\hbar^2} (E_{n+1} - E_n) \int_{x_1}^{x_2} dx \psi_n \psi_{n+1} .
\]
Without loss of generality, assume that $\psi_n(x) > 0$ in the range $(x_1, x_2)$. Since $\psi_n(x)$ is expected to be continuous, the following must hold
\[
\frac{d\psi_n}{dx} \bigg|_{x=x_1} > 0 ,
\]
and
\[
\frac{d\psi_n}{dx} \bigg|_{x=x_2} < 0 .
\]
As can be clearly seen from Eq. (4.108), the assumption that $\psi_{n+1}(x) > 0$ in the entire range $(x_1, x_2)$ leads to contradiction. Similarly, the possibility that $\psi_{n+1}(x) < 0$ in the entire range $(x_1, x_2)$ is excluded. Therefore, $\psi_{n+1}$ must have at least one zero in this range.
8. Clearly if $\psi(x)$ is an eigen function with energy $E$, also $\psi(-x)$ is an eigen function with the same energy. Consider two cases: (i) The level $E$ is non-degenerate. In this case $\psi(x) = c\psi(-x)$, where $c$ is a constant. Normalization requires that $|c|^2 = 1$. Moreover, since the wavefunctions can be chosen to be real, the following holds: $\psi(x) = \pm\psi(-x)$. (ii) The level $E$ is degenerate. In this case every superposition of $\psi(x)$ and $\psi(-x)$ can be written as a superposition of an odd eigen function $\psi_{\text{odd}}(x)$ and an even one $\psi_{\text{even}}(x)$, which are defined by

$$
\begin{align*}
\psi_{\text{odd}}(x) &= \psi(x) - \psi(-x), \\
\psi_{\text{even}}(x) &= \psi(x) + \psi(-x).
\end{align*}
$$

9. The time-independent Schrödinger equation reads

$$
\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0.
$$

Assume $V(x)$ has a finite discontinuity at $x = x_0$. Integrating the Schrödinger equation in the interval $(x_0 - \epsilon, x_0 + \epsilon)$ yields

$$
\left. \frac{d\psi(x)}{dx} \right|_{x_0 - \epsilon}^{x_0 + \epsilon} = \frac{2m}{\hbar^2} \int_{x_0 - \epsilon}^{x_0 + \epsilon} (V(x) - E)\psi(x) = 0.
$$

In the limit $\epsilon \to 0$ the right hand side vanishes (assuming $\psi(x)$ is bounded). Therefore $d\psi(x)/dx$ is continuous at $x = x_0$. 

10. Since $V_s(-x) = V_s(x)$ the ground state wavefunction is expected to be an even function of $x$. Consider a solution having an energy $E$ and a wavefunction of the form

$$
\psi(x) = \begin{cases} 
A e^{-\gamma x} & \text{if } x > a \\
B \cos(kx) & \text{if } -a \leq x \leq a \\
A e^{\gamma x} & \text{if } x < -a
\end{cases},
$$

where

$$
\gamma = \sqrt{-2mE}/\hbar,
$$

and

$$
k = \sqrt{2m(W + E)}/\hbar.
$$

Requiring that both $\psi(x)$ and $d\psi(x)/dx$ are continuous at $x = a$ yields

$$
A e^{-\gamma a} = B \cos(ka),
$$

and
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\[-\gamma Ae^{-\gamma a} = -kB \sin (ka) , \tag{4.119}\]

or in a matrix form

\[C \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} , \tag{4.120}\]

where

\[C = \begin{pmatrix} e^{-\gamma a} - \cos (ka) \\ -\gamma e^{-\gamma a} k \sin (ka) \end{pmatrix} . \tag{4.121}\]

A nontrivial solution exists iff \( \text{Det} \ (C) = 0 \), namely iff

\[\frac{\gamma}{k} = \tan (ka) . \tag{4.122}\]

This condition can be rewritten using Eqs. (4.116) and (4.117) and the dimensionless parameters

\[K = ka , \tag{4.123}\]

\[K_0 = \sqrt{\frac{2mW}{\hbar^2}} - a , \tag{4.124}\]

as

\[\cos^2 K = \frac{1}{1 + \tan^2 K} = \frac{1}{1 + \left( \frac{\gamma}{k} \right)^2} = \left( \frac{K}{K_0} \right)^2 . \tag{4.125}\]

Note, however, that according to Eq. (4.122) \( \tan K > 0 \). Thus, Eq. (4.122) is equivalent to the set of equations

\[|\cos K| = \frac{K}{K_0} , \tag{4.126}\]

\[\tan K > 0 . \tag{4.127}\]

This set has at least one solution (this can be seen by plotting the functions \( |\cos K| \) and \( K/K_0 \)).

11. Final answers: (a) \( |a_1|^2 + |a_2|^2 \). (b)

\[\Delta E = \frac{\pi^2 \hbar^2}{2ma^2} \left[ \sum_{n=1}^{3} |a_n|^2 n^4 - \left( \sum_{n=1}^{3} |a_n|^2 \right)^2 \right] . \tag{4.128}\]

(c) The same as at \( t = 0 \). (d) \( \langle E \rangle = 2\pi^2 \hbar^2 / (ma^2) \), \( \langle \Delta E \rangle = 0 \).

12. The Schrödinger equation for the wavefunction \( \psi(x) \) is given by

\[\frac{d^2}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi(x) = 0 . \tag{4.129}\]

The boundary conditions imposed upon \( \psi(x) \) by the potential are
\[
\psi(\pm a) = 0, \quad (4.130)
\]
\[
\psi(0^+) = \psi(0^-), \quad (4.131)
\]
\[
\frac{d\psi(0^+)}{dx} - \frac{d\psi(0^-)}{dx} = -\frac{2}{a_0} \psi(0), \quad (4.132)
\]

where
\[
a_0 = \frac{\hbar^2}{ma}. \quad (4.133)
\]

Due to symmetry \( V(x) = V(-x) \) the solutions are expected to have definite symmetry (even \( \psi(x) = \psi(-x) \) or odd \( \psi(x) = -\psi(-x) \)). For the ground state, which is expected to have even symmetry, we consider a wavefunction having the form
\[
\psi(x) = \begin{cases} 
A \sinh(\kappa(x-a)) & x > 0 \\
-A \sinh(\kappa(x+a)) & x < 0 
\end{cases}, \quad (4.134)
\]

where \( A \) is a normalization constants and where
\[
\kappa = \sqrt{-2mE_0}/\hbar. \quad (4.135)
\]

The parameter \( \kappa \) is real for \( E_0 < 0 \). This even wavefunction satisfies Eq. (4.129) for \( x \neq 0 \) and the boundary conditions (4.130) and (4.131). The condition (4.132) reads
\[
\kappa a_0 = \tanh(\kappa a). \quad (4.136)
\]

Nontrivial \( (\kappa \neq 0) \) real solution exists only when \( a > a_0 \), thus \( E_0 < 0 \) iff
\[
a > a_0 = \frac{\hbar^2}{ma}. \quad (4.137)
\]

13. Using Eq. (4.37) one has
\[
\frac{dx^{(H)}}{dt} = \frac{1}{i\hbar} \left[ x^{(H)}, \mathcal{H} \right], \quad (4.138)
\]

therefore
\[
\langle k | \frac{dx^{(H)}}{dt} | l \rangle = \frac{1}{i\hbar} \langle k | x^{(H)} \mathcal{H} - \mathcal{H} x^{(H)} | l \rangle = \frac{i(E_k - E_l)}{\hbar} \langle k | x^{(H)} | l \rangle. \quad (4.139)
\]

Integrating yields
\[
\langle k | x^{(H)}(t) | l \rangle = \langle k | x^{(H)}(t = 0) | l \rangle \exp \left( \frac{i(E_k - E_l)t}{\hbar} \right). \quad (4.140)
\]
Using this result one has

\[
\sum_k (E_k - E_l) \left| \langle k | x | l \rangle \right|^2 = \sum_k (E_k - E_l) \left| \langle k | x^{(H)} | l \rangle \right|^2
\]

\[
= \sum_k (E_k - E_l) \langle k | x^{(H)} | l \rangle \langle k | x^{(H)} | l \rangle
\]

\[
= \frac{\hbar}{2i} \sum_k \left( \langle k | \frac{dx^{(H)}}{dt} | k \rangle \langle l | x^{(H)} | l \rangle - \langle k | x^{(H)} | l \rangle \langle l | \frac{dx^{(H)}}{dt} | k \rangle \right)
\]

\[
= \frac{\hbar}{2i} \sum_k \left( \langle l | x^{(H)} | k \rangle \langle k | \frac{dx^{(H)}}{dt} | l \rangle - \langle l | x^{(H)} | l \rangle \langle k | \frac{dx^{(H)}}{dt} | k \rangle \right)
\]

\[
= \frac{\hbar}{2i} \langle l | x^{(H)} | \frac{dx^{(H)}}{dt} \rangle - \frac{\hbar}{2i} \langle k | x^{(H)} | \frac{dx^{(H)}}{dt} \rangle.
\]

(4.141)

Using again Eq. (4.37) one has

\[
\frac{dx^{(H)}}{dt} = \frac{1}{i\hbar} \left[ x^{(H)}, \mathcal{H} \right] = \frac{p_x^{(H)}}{m},
\]

(4.142)

therefore

\[
\sum_k (E_k - E_l) \left| \langle k | x | l \rangle \right|^2 = \frac{\hbar}{2im} \langle l | \left[ x^{(H)}, p_x^{(H)} \right] | l \rangle
\]

\[
= \frac{\hbar}{2im} \frac{\hbar}{\hbar} = \frac{\hbar}{2m}.
\]

(4.143)

14. The wavefunctions of the normalized eigenstates are given by

\[
\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a},
\]

(4.144)

and the corresponding eigenenergies are

\[
E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}.
\]

(4.145)

(a) The wavefunction after the measurement is a normalized wavepacket centered at \( x = a/2 \) and having a width \( \Delta x \)

\[
\psi(x) = \begin{cases} \sqrt{\frac{2}{\Delta x}} & |x - \frac{a}{2}| \leq \frac{\Delta x}{2} \\ 0 & \text{else} \end{cases}.
\]

(4.146)

Thus in the limit \( \Delta x \ll a \)
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\[ p_n = \left| \int_0^a dx \psi_n^*(x) \psi(x) \right|^2 \approx \frac{2 \Delta x}{a} \sin^2 \frac{n\pi}{2}. \]  

(4.147)

Namely, \( p_n = 0 \) for all even \( n \), and the probability of all energies with odd \( n \) is equal. (b) Generally, for every bound state in one dimension \( \langle \hat{p} \rangle = 0 \) [see Eq. (4.51)].

15. For a well of width \( a \) the wavefunctions of the normalized eigenstates are given by

\[ \psi_n^{(a)}(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \]  

(4.148)

and the corresponding eigenenergies are

\[ E_n^{(a)} = \frac{\hbar^2 n^2}{2ma^2}. \]  

(4.149)

(a) The probability is given by

\[ p = \left| \int_0^a dx \psi_1^{(a)}(x) \psi_1^{(2a)}(x) \right|^2 = \frac{32}{9\pi^2}. \]  

(4.150)

(b) For times \( t < 0 \) it is given that \( \langle \hat{H} \rangle = E_1^{(a)} \). Immediately after the change \( (t = 0^+) \) the wavefunction remains unchanged. A direct evaluation of \( \langle \hat{H} \rangle \) using the new Hamiltonian yields the same result \( \langle \hat{H} \rangle = E_1^{(a)} \) as for \( t < 0 \). At later times \( t > 0 \) the expectation value \( \langle \hat{H} \rangle \) remains unchanged due to energy conservation.

16. The Schrödinger equation is given by

\[ i\hbar \frac{d|\alpha\rangle}{dt} = \hat{H}|\alpha\rangle, \]  

(4.151)

where the Hamiltonian is given by [see Eq. (1.62)]

\[ \hat{H} = \frac{(\hat{p}-2\hat{A})^2}{2m} + q\varphi. \]  

(4.152)

Multiplying from the left by \( \langle x' | \) yields

\[ i\hbar \frac{d\psi}{dt} = \frac{1}{2m} \left( -i\hbar \nabla - \frac{q}{c} \hat{A} \right)^2 \psi + q\varphi \psi, \]  

(4.153)

where

\[ \psi = \psi(x') = \langle x' | \alpha \rangle. \]  

(4.154)

Multiplying Eq. (4.153) by \( \psi^* \), and subtracting the complex conjugate of Eq. (4.153) multiplied by \( \psi \) yields
\[ i\hbar \frac{d\rho}{dt} = \frac{1}{2m} \left[ \psi^* \left( -i\hbar \nabla - \frac{q}{c} A \right)^2 \psi - \psi \left( i\hbar \nabla - \frac{q}{c} A \right)^2 \psi^* \right] \]  
\tag{4.155}

where

\[ \rho = \psi \psi^* \]  
\tag{4.156}

is the probability density. Moreover, the following holds

\[
\psi^* \left( -i\hbar \nabla - \frac{q}{c} A \right)^2 \psi - \psi \left( i\hbar \nabla - \frac{q}{c} A \right)^2 \psi^* \\
= \psi^* \left( -\frac{h^2}{c^2} \nabla^2 + \left( \frac{q}{c} \right)^2 A^2 + \frac{i\hbar q}{c} \nabla A + \frac{i\hbar q}{c} A \nabla \right) \psi - \psi \left( -\frac{h^2}{c^2} \nabla^2 + \left( \frac{q}{c} \right)^2 A^2 - \frac{i\hbar q}{c} \nabla A - \frac{i\hbar q}{c} A \nabla \right) \psi^*
\]

\[
= -\frac{h^2}{c^2} \left( \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right) + \frac{i\hbar q}{c} \left( \psi^* \nabla A \psi + \psi^* A \nabla \psi + \psi A \nabla \psi^* + \psi^* A \nabla \psi^* \right)
\]

\[
= -\frac{h^2}{c^2} \nabla \left( \psi^* \nabla \psi - \psi \nabla \psi^* \right) + \frac{i\hbar q}{c} \nabla \left( \psi^* A \psi + \psi A \psi^* \right).
\]  
\tag{4.157}

Thus, Eq. (4.155) can be written as

\[ \frac{d\rho}{dt} + \nabla J = 0 \]  
\tag{4.158}

where

\[ J = \frac{\hbar}{m} \text{Im} \left( \psi^* \nabla \psi \right) - \frac{q}{mc} (\rho A) \]  
\tag{4.159}

17. Using Eq. (4.45) one has

\[
A(x,p) = \frac{1}{(2\pi \hbar)^2} \int \int \int p^{(c)} x^{(c)} e^{\frac{i}{\hbar}[\eta(x^{(c)}-x)+\xi(p^{(c)}-p)]} dp^d x^d \]  
\tag{4.160}

With the help of Eq. (2.176), which is given by

\[
e^{A^{(1/2)}B} = e^{A^{1/2}} e^{B^{1/2}} ,
\]  
\tag{4.161}

one has

\[
e^{-\frac{i}{\hbar} \eta x - \frac{i}{\hbar} \xi p} = e^{-\frac{i}{\hbar} \left( \eta x + \xi p \right) - \frac{i}{\hbar} \eta x} e^{-\frac{i}{\hbar} \xi p} \]  
\tag{4.162}

thus

\[
A(x,p) = \frac{1}{(2\pi \hbar)^2} \int \int \int p^{(c)} x^{(c)} e^{\frac{i}{\hbar} \left( \eta x^{(c)} + \xi p^{(c)} \right) - \frac{i}{\hbar} \eta x} e^{-\frac{i}{\hbar} \xi p} dp^d x^d p^{(c)}
\]

\[
= \frac{1}{(2\pi \hbar)^2} \int \int \int p^{(c)} x^{(c)} e^{\frac{i}{\hbar} \left[ \eta \left( x^{(c)} + \frac{\xi}{\hbar} p^{(c)} \right) + \xi p^{(c)} \right]} e^{-\frac{i}{\hbar} \eta x} e^{-\frac{i}{\hbar} \xi p} dp^d x^d p^{(c)}.
\]  
\tag{4.163}
Chapter 4. Quantum Dynamics

Changing the integration variable

\[ x^{(c)} = x^{(c)'} - \frac{\xi}{2}, \]  

one has

\[
A(x, p) = \frac{1}{(2\pi \hbar)^{2}} \int \int \int p^{(c)} \left( x^{(c)'} - \frac{\xi}{2} \right) e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, dx^{(c)} \, dp^{(c)} \, d\xi d\eta dx^{(c)'} dp^{(c)} = \frac{1}{(2\pi \hbar)^{2}} \int \int \int p^{(c)} \left( x^{(c)'} - \frac{\xi}{2} \right) e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, dx^{(c)} \, dp^{(c)} \, d\xi d\eta dx^{(c)'} dp^{(c)} .
\]

(4.165)

Using the identity

\[
\int_{-\infty}^{\infty} \, dke^{ik(x'-x')} = 2\pi \delta(x' - x''),
\]

one finds that

\[
\frac{1}{2\pi \hbar} \int e^{i\hbar \eta (x^{(c)'} - x)} \, d\eta = \delta \left( x^{(c)'} - x \right), \tag{4.166}
\]

\[
\frac{1}{2\pi \hbar} \int e^{i\hbar \xi (p^{(c)} - p)} \, d\xi = \delta \left( p^{(c)} - p \right), \tag{4.167}
\]

thus

\[
A(x, p) = \frac{1}{2\pi \hbar} \int \int \int p^{(c)} \left( x^{(c)'} - \frac{\xi}{2} \right) e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, dx^{(c)} \, dp^{(c)} \, d\xi d\eta dx^{(c)'} dp^{(c)} = \frac{1}{2\pi \hbar} \int \int \int p^{(c)} \left( x^{(c)'} - \frac{\xi}{2} \right) e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, dx^{(c)} \, dp^{(c)} \, d\xi d\eta dx^{(c)'} dp^{(c)}
\]

\[
= \frac{1}{2\pi \hbar} \int \int \int p^{(c)} \left( x - \frac{\xi}{2} \right) e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, dx^{(c)} \, dp^{(c)} \, d\xi d\eta dx^{(c)'} dp^{(c)}
\]

\[
= \frac{1}{2\pi \hbar} \int \int \int p^{(c)} x \, dp^{(c)} \frac{1}{2\pi \hbar} \int e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, d\xi - \frac{1}{2\pi \hbar} \int \int p^{(c)} \frac{\xi}{2} e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, d\xi dp^{(c)}
\]

\[
= px - \frac{1}{2\pi \hbar} \int \int \int p^{(c)} x dp^{(c)} \frac{1}{2\pi \hbar} \int e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, d\xi dp^{(c)}
\]

\[
= px - \frac{1}{2\pi \hbar} \int \int \int p^{(c)} \frac{\partial}{\partial p^{(c)}} e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} \, d\xi dp^{(c)}
\]

\[
= px - \frac{h}{2i} \int dp^{(c)} p^{(c)} \frac{\partial}{\partial p^{(c)}} \frac{1}{2\pi \hbar} \int d\xi e^{i\frac{\hbar}{2} \xi (p^{(c)} - p)} .
\]

(4.169)

Integration by parts yields
4.7. Solutions

\[ A(x, p) = px - \frac{h}{2i} \int \left( \frac{\partial p(c)}{\partial x} \right) \delta \left( p(c) - p \right) \, dp(c) \]

\[ = px - \frac{h}{2i} \]

\[ = px + \frac{[x, p]}{2} \]

\[ = \frac{xp + px}{2}. \]

(4.170)

18. Below we derive an expression for the variable \( A(x', p) \) in terms of the matrix elements of the operator \( A(x, p) \) in the basis of position eigenvectors \(|x\rangle\). To that end we begin by evaluating the matrix element

\[ \langle x' - \frac{x''}{2} | A(x, p) | x' + \frac{x''}{2} \rangle \]

using Eqs. (4.163), (3.19) and (4.167)

\[ = \frac{1}{(2\pi \hbar)^2} \int \int \int A(x', p) e^{i\left(\xi(x' + \frac{x''}{2}) + \eta p\right)} \, dp \, dx \, d\eta \]

\[ \times \langle x' - \frac{x''}{2} \left| e^{-i\xi x} e^{-i\eta p} \right| x' + \frac{x''}{2} \rangle \]

\[ = \frac{1}{(2\pi \hbar)^2} \int \int \int A(x', p) e^{i\left(\xi(x' + \frac{x''}{2}) + \eta p\right)} e^{-i\xi x} e^{-i\eta p} \, dp \, dx \, d\eta \]

\[ \times \langle x' - \frac{x''}{2} \left| e^{-i\xi x} e^{-i\eta p} \right| x' + \frac{x''}{2} + \xi \rangle \]

\[ = \frac{1}{(2\pi \hbar)^2} \int \int A(x', p) e^{-i\xi x''} dx'' dp \]

\[ \times \int e^{i\xi x'} dx' \]

\[ = \frac{1}{2\pi \hbar} \int A(x', p) e^{-i\xi x''} dp \]

\[ \delta \left( x' - x \right) \]

\[ = \frac{1}{2\pi \hbar} \int A(x', p) dp \left( e^{i\xi (p - p')} dx'' \right). \]

Applying the inverse Fourier transform, i.e. multiplying by \( e^{i\xi x''} p' \) and integrating over \( x'' \) yields

\[ \int \langle x' - \frac{x''}{2} | A(x, p) | x' + \frac{x''}{2} \rangle \, dx'' \]

\[ = \frac{1}{2\pi \hbar} \int A(x', p) \, dp \left( e^{i\xi (p - p')} dx'' \right). \]

(4.171)

thus with the help of Eq. (4.168) one finds the desired inversion of Eq. (4.45) is given by
Chapter 4. Quantum Dynamics

\[ A(x', p') = \int \left( x' - \frac{x''}{2} \right) A(x, p) \left( x' + \frac{x''}{2} \right) e^{i x'' p'} dx'' . \] (4.172)

A useful relations can be obtained by integrating \( A(x', p') \) over \( p' \). With the help of Eq. (4.167) one finds that

\[
\int A(x', p') \, dp' = \int dx'' \left( x' - \frac{x''}{2} \right) A(x, p) \left( x' + \frac{x''}{2} \right) e^{i x'' p'} dp'
= 2\pi \hbar \langle x' | A(x, p) | x' \rangle .
\] (4.173)

Another useful relations can be obtained by integrating \( A(x', p') \) over \( x' \). With the help of Eqs. (3.51) and (4.168) one finds that

\[
\int A(x', p') \, dx' = \int \int \left( x' - \frac{x''}{2} \right) A(x, p) \left( x' + \frac{x''}{2} \right) e^{i x'' p'} dx'' dx'
= \frac{1}{2\pi \hbar} \int \int \int \int e^{i x'(p'' - p''')} e^{i \frac{1}{2\hbar}(p'' - p''')} \langle p'' | A(x, p) | p''' \rangle e^{i x'' p'} dx'' dp'' dx'' dp''
= \int \int \delta(p'' - p''') e^{i \frac{1}{2\hbar}(p'' - p''')} \langle p''' | A(x, p) | p''' \rangle e^{i x'' p'} dx'' dp''
= \int \int \langle p''' | A(x, p) | p''' \rangle e^{i \frac{1}{2\hbar}(p'' - p''')} \delta(p' - p''') \, dp''
= 2\pi \hbar \int \langle p''' | A(x, p) | p''' \rangle \delta(p' - p''') \, dp''
= 2\pi \hbar \langle p' | A(x, p) | p' \rangle .
\] (4.174)
5. The Harmonic Oscillator

Consider a particle of mass $m$ in a parabolic potential well

$$U(x) = \frac{1}{2}m\omega^2x^2,$$

where the angular frequency $\omega$ is a constant. The classical equation of motion for the coordinate $x$ is given by [see Eq. (1.19)]

$$m\ddot{x} = -\frac{\partial U}{\partial x} = -m\omega^2x.$$  \hfill (5.1)

It is convenient to introduce the complex variable $\alpha$, which is given by

$$\alpha = \frac{1}{x_0} \left( x + \frac{i}{\omega} \dot{x} \right),$$  \hfill (5.2)

where $x_0$ is a constant having dimension of length. Using Eq. (5.1) one finds that

$$\dot{\alpha} = \frac{1}{x_0} \left( \dot{x} + \frac{i}{\omega} \ddot{x} \right) = \frac{1}{x_0} \left( \dot{x} - \frac{i}{\omega} \omega^2 x \right) = -i\omega \alpha.$$  \hfill (5.3)

The solution is given by

$$\alpha = \alpha_0 e^{-i\omega t},$$  \hfill (5.4)

where $\alpha_0 = \alpha (t = 0)$. Thus, $x$ and $\dot{x}$ oscillate in time according to

$$x = x_0 \text{Re} \left( \alpha_0 e^{-i\omega t} \right),$$  \hfill (5.5)

$$\dot{x} = x_0 \omega \text{Im} \left( \alpha_0 e^{-i\omega t} \right).$$  \hfill (5.6)

The Hamiltonian is given by [see Eq. (1.34)]

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2x^2}{2}.$$  \hfill (5.7)

In quantum mechanics the variables $x$ and $p$ are regarded as operators satisfying the following commutation relations [see Eq. (3.9)]

$$[x, p] = xp - px = i\hbar.$$  \hfill (5.8)
5.1 Eigenstates

The annihilation and creation operators are defined as

\[ a = \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{ip}{m\omega} \right), \quad (5.9) \]

\[ a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( x - \frac{ip}{m\omega} \right). \quad (5.10) \]

The inverse transformation is given by

\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad (5.11) \]

\[ p = i \sqrt{\frac{m\hbar\omega}{2}} (-a + a^\dagger). \quad (5.12) \]

The following holds

\[ [a, a^\dagger] = \frac{i}{2\hbar} ([p, x] - [x, p]) = 1, \quad (5.13) \]

The number operator, which is defined as

\[ N = a^\dagger a, \quad (5.14) \]

can be expressed in terms of the Hamiltonian

\[ N = a^\dagger a \]
\[ = \frac{m\omega}{2\hbar} \left( x - \frac{ip}{m\omega} \right) \left( x + \frac{ip}{m\omega} \right) \]
\[ = \frac{m\omega}{2\hbar} \left( \frac{p^2}{m^2\omega^2} + x^2 + i [x, p] \frac{m^2\omega^2}{m\omega} \right) \]
\[ = \frac{1}{\hbar\omega} \left( \frac{p^2}{2m} + \frac{m^2\omega^2x^2}{2} \right) - \frac{1}{2} \]
\[ = \frac{\mathcal{H}}{\hbar\omega} - \frac{1}{2}. \quad (5.15) \]

Thus, the Hamiltonian can be written as

\[ \mathcal{H} = \hbar\omega \left( N + \frac{1}{2} \right). \quad (5.16) \]

The operator \( N \) is Hermitian, i.e. \( N = N^\dagger \), therefore its eigenvalues are expected to be real. Let \( \{|n\rangle\} \) be the set of eigenvectors of \( N \) and let \( \{n\} \) be the corresponding set of eigenvalues.
5.1. Eigenstates

\[ N \ket{n} = n \ket{n} \]  

(5.17)

According to Eq. (5.16) the eigenvectors of \( N \) are also eigenvectors of \( \mathcal{H} \)

\[ \mathcal{H} \ket{n} = E_n \ket{n} \]  

(5.18)

where the eigenenergies \( E_n \) are given by

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right) . \]  

(5.19)

**Theorem 5.1.1.** Let \( \ket{n} \) be a normalized eigenvector of the operator \( N \) with eigenvalue \( n \). Then (i) the vector

\[ \ket{n + 1} = (n + 1)^{-1/2} a^\dagger \ket{n} \]  

(5.20)

is a normalized eigenvector of the operator \( N \) with eigenvalue \( n + 1 \); (ii) the vector

\[ \ket{n - 1} = n^{-1/2} a \ket{n} \]  

(5.21)

is a normalized eigenvector of the operator \( N \) with eigenvalue \( n - 1 \).

**Proof.** Using the commutation relations

\[ [N, a^\dagger] = a^\dagger [a, a^\dagger] = a^\dagger , \]  

(5.22)

\[ [N, a] = [a^\dagger, a] = -a , \]  

(5.23)

one finds that

\[ Na^\dagger \ket{n} = \left( [N, a^\dagger] + a^\dagger N \right) \ket{n} = (n + 1) a^\dagger \ket{n} , \]  

(5.24)

and

\[ Na \ket{n} = (\left[ N, a \right] + a N) \ket{n} = (n - 1) a \ket{n} . \]  

(5.25)

Thus, the vector \( a^\dagger \ket{n} \), which is proportional to \( \ket{n + 1} \), is an eigenvector of the operator \( N \) with eigenvalue \( n + 1 \) and the vector \( a \ket{n} \), which is proportional to \( \ket{n - 1} \), is an eigenvector of the operator \( N \) with eigenvalue \( n - 1 \). Normalization is verified as follows

\[ \langle n + 1 | n + 1 \rangle = (n + 1)^{-1} \langle n | a a^\dagger | n \rangle = (n + 1)^{-1} \langle n | [a, a^\dagger] + a^\dagger a | n \rangle = 1 , \]  

(5.26)

and

\[ \langle n - 1 | n - 1 \rangle = n^{-1} \langle n | a^\dagger a | n \rangle = 1 . \]  

(5.27)
As we have seen from the above theorem the following hold
\[ a |n\rangle = \sqrt{n} |n-1\rangle , \tag{5.28} \]
\[ a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle . \tag{5.29} \]

**Claim.** The spectrum (i.e. the set of eigenvalues) of \( N \) are the nonnegative integers \( \{0,1,2,\cdots\} \).

**Proof.** First, note that since the operator \( N \) is positive-definite the eigenvalues are necessarily non negative
\[ n = (n|a^\dagger a|n) \geq 0 . \tag{5.30} \]

On the other hand, according to Eq. (5.28), if \( n \) is an eigenvalue also \( n-1 \) is an eigenvalue, unless \( n = 0 \). For the later case according to Eq. (5.28) \( a|0\rangle = 0 \). Therefore, \( n \) must be an integer, since otherwise one reaches a contradiction with the requirement that \( n \geq 0 \).

According to exercise 6 of set 4, in one-dimensional problems the energy spectrum of the bound states is always non-degenerate. Therefore, one concludes that all eigenvalues of \( N \) are non-degenerate. Therefore, the closure relation can be written as
\[ 1 = \sum_{n=0}^{\infty} |n\rangle \langle n| . \tag{5.31} \]

Furthermore, using Eq. (5.29) one can express the state \( |n\rangle \) in terms of the ground state \( |0\rangle \) as
\[ |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |0\rangle . \tag{5.32} \]

### 5.2 Coherent States

As can be easily seen from Eqs. (5.11), (5.12), (5.28) and (5.29), all energy eigenstates \( |n\rangle \) have vanishing position and momentum expectation values
\[ \langle n| x |n\rangle = 0 , \tag{5.33} \]
\[ \langle n| p |n\rangle = 0 . \tag{5.34} \]

Clearly these states don’t oscillate in phase space as classical harmonic oscillators do. Can one find quantum states having dynamics that resembles classical harmonic oscillators?
5.2. Coherent States

Definition 5.2.1. Consider an harmonic oscillator having ground state \( |0\rangle \).
A coherent state \( |\alpha\rangle \) with a complex parameter \( \alpha \) is defined by

\[
|\alpha\rangle = D (\alpha) |0\rangle ,
\]

where

\[
D (\alpha) = \exp \left( \alpha a^\dagger - \alpha^* a \right),
\]

is the displacement operator.

In the set of problems at the end of this chapter the following results are obtained:

- The displacement operator is unitary \( D^\dagger (\alpha) D (\alpha) = D (\alpha) D^\dagger (\alpha) = 1 \).
- The coherent state \( |\alpha\rangle \) is an eigenvector of the operator \( a \) with an eigenvalue \( \alpha \), namely
  \[
a |\alpha\rangle = \alpha |\alpha\rangle .
\]
- For any function \( f \left( a, a^\dagger \right) \) having a power series expansion the following holds
  \[
  D^\dagger (\alpha) f \left( a, a^\dagger \right) D (\alpha) = f \left( a + \alpha, a^\dagger + \alpha^* \right).
  \]
- The displacement operator satisfies the following relations
  \[
  D (\alpha) = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} e^{-\alpha^* a} = e^{\alpha a^\dagger} e^{-\alpha^* a} e^{\alpha a^\dagger},
  \]
  \[
  D (\alpha) = e^{\sqrt{\frac{|\alpha|^2}{2}}} e^{-\frac{\alpha^* a + \alpha a^\dagger}{2}} e^{\alpha a^\dagger} e^{-\alpha^* a} e^{\alpha a^\dagger},
  \]
  \[
  D (\alpha) D (\alpha') = \exp \left( \frac{\alpha \alpha'^* - \alpha^* \alpha'}{2} \right) D (\alpha + \alpha').
  \]
- Coherent state expansion in the basis of number states
  \[
  |\alpha\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle .
  \]
- The following expectation values hold
Chapter 5. The Harmonic Oscillator

\[ \langle \mathcal{H} \rangle_\alpha = \langle \alpha | \mathcal{H} | \alpha \rangle = \hbar \omega \left( |\alpha|^2 + 1/2 \right), \quad (5.43) \]

\[ \langle \alpha | \mathcal{H}^2 | \alpha \rangle = \hbar^2 \omega^2 \left( |\alpha|^4 + 2 |\alpha|^2 + 1/4 \right), \quad (5.44) \]

\[ \Delta \mathcal{H}_\alpha = \sqrt{\langle \alpha | (\Delta \mathcal{H})^2 | \alpha \rangle} = \hbar \omega |\alpha|, \quad (5.45) \]

\[ \langle x \rangle_\alpha = \langle \alpha | x | \alpha \rangle = \sqrt{2 \hbar \omega} \text{Re} \langle \alpha \rangle, \quad (5.46) \]

\[ \langle p \rangle_\alpha = \langle \alpha | p | \alpha \rangle = \sqrt{2 \hbar m \omega} \text{Im} \langle \alpha \rangle, \quad (5.47) \]

\[ \Delta x_\alpha = \sqrt{\langle \alpha | (\Delta x)^2 | \alpha \rangle} = \sqrt{\frac{\hbar}{2 m \omega}}, \quad (5.48) \]

\[ \Delta p_\alpha = \sqrt{\langle \alpha | (\Delta p)^2 | \alpha \rangle} = \sqrt{\frac{\hbar m \omega}{2}}, \quad (5.49) \]

\[ \Delta x_\alpha \Delta p_\alpha = \frac{\hbar}{2}. \quad (5.50) \]

- The wave function of a coherent state is given by

\[ \psi_\alpha (x') = \langle x' | \alpha \rangle = \exp \left( \frac{\alpha^2 - x'^2}{4} \right) \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \exp \left[ - \left( \frac{x' - \langle x \rangle_\alpha}{2 \Delta x_\alpha} \right)^2 + i \langle p \rangle_\alpha \frac{x'}{\hbar} \right]. \quad (5.51) \]

- The following closure relation holds

\[ 1 = \frac{1}{\pi} \int \int |\alpha\rangle \langle \alpha| d^2 \alpha, \quad (5.52) \]

where \( d^2 \alpha \) denotes infinitesimal area in the \( \alpha \) complex plane, namely \( d^2 \alpha = d \{ \text{Re} \alpha \} d \{ \text{Im} \alpha \} \).

Given that at time \( t = 0 \) the oscillator is in a coherent state with parameter \( \alpha_0 \), namely \( |\psi (t = 0)\rangle = |\alpha_0\rangle \), the time evolution can be found with the help of Eqs. (4.14), (5.19) and (5.42)

\[ |\psi (t)\rangle = e^{-i \omega t / 2} \sum_{n=0}^{\infty} \exp \left( -i E_n t \right) \frac{\alpha_0^n}{\sqrt{n!}} |n\rangle 
  = e^{-i \omega t / 2} e^{-i \omega t / 2} \sum_{n=0}^{\infty} \exp \left( -i \omega n t \right) \frac{\alpha_0^n}{\sqrt{n!}} |n\rangle 
  = e^{-i \omega t / 2} e^{-i \omega t / 2} \sum_{n=0}^{\infty} \frac{(\alpha_0 e^{-i \omega t})^n}{\sqrt{n!}} |n\rangle 
  = e^{-i \omega t / 2} | \alpha = \alpha_0 e^{-i \omega t} \rangle. \quad (5.53) \]
5.3 Problems

In view of Eqs. (5.43), (5.45) (5.48) and (5.49), we see from this results that $\langle H \rangle_\alpha$, $\Delta H_\alpha$, $\Delta x_\alpha$ and $\Delta p_\alpha$ are all time independent. On the other hand, as can be seen from Eqs. (5.46) and (5.47) the following holds

$$h^x_\alpha = |x_\alpha| = \sqrt{2\hbar m}\omega \exp (-i\omega t),$$

(5.54)

$$h^p_\alpha = |p_\alpha| = \sqrt{2\hbar m\omega} \exp (-i\omega t).$$

(5.55)

These results show that indeed, $h^x_\alpha$ and $h^p_\alpha$ have oscillatory time dependence identical to the dynamics of the position and momentum of a classical harmonic oscillator [compare with Eqs. (5.5) and (5.6)].

5.3 Problems

1. Calculate the wave functions $\psi_n(x) = \langle x | n \rangle$ of the number states $|n\rangle$ of a harmonic oscillator.

2. Show that

$$\exp (2Xt - t^2) = \sum_{n=0}^{\infty} H_n(X) \frac{t^n}{n!},$$

(5.56)

where $H_n(X)$ is the Hermite polynomial of order $n$, which is defined by

$$H_n(X) = \exp \left( \frac{X^2}{2} \right) \left( X - \frac{d}{dX} \right)^n \exp \left( -\frac{X^2}{2} \right).$$

(5.57)

3. Show that for the state $|n\rangle$ of a harmonic oscillator

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \left( n + \frac{1}{2} \right)^2 \hbar^2.$$

(5.58)

4. Consider a free particle in one dimension having mass $m$. Express the Heisenberg operator $x^{(H)}(t)$ in terms $x^{(H)}(0)$ and $p^{(H)}(0)$.

5. Consider a harmonic oscillator of angular frequency $\omega$ and mass $m$.

a) Express the Heisenberg picture $x^{(H)}(t)$ and $p^{(H)}(t)$ in terms $x^{(H)}(0)$ and $p^{(H)}(0)$.

b) Calculate the following commutators $[p^{(H)}(t_1), x^{(H)}(t_2)]$, $[p^{(H)}(t_1), p^{(H)}(t_2)]$ and $[x^{(H)}(t_1), x^{(H)}(t_2)]$.

6. Consider an harmonic oscillator having angular resonance frequency $\omega$ and mass $m$. The oscillator at time $t = 0$ is in its ground state. Calculate the correlation function $G(t) = \langle x^{(H)}(t) x^{(H)}(0) \rangle$, where $x^{(H)}(t)$ is the Heisenberg representation of the position operator.
7. Consider a particle having mass $m$ confined by a one dimensional potential $V(x)$, which is given by

$$V(x) = \begin{cases} \frac{m\omega^2}{2} x^2 & x > 0 \\ \infty & x \leq 0 \end{cases}.$$ \hfill (5.59)

where $\omega$ is a constant.

a) Calculate the eigenenergies of the system.

b) Calculate the expectation values $\langle x^2 \rangle$ of all energy eigenstates of the particle.

8. Calculate the possible energy values of a particle in the potential given by

$$V(x) = \frac{m\omega^2}{2} x^2 + \alpha x.$$ \hfill (5.60)

9. A particle is in the ground state of harmonic oscillator with potential energy

$$V(x) = \frac{m\omega^2}{2} x^2.$$ \hfill (5.61)

Find the probability $p$ to find the particle in the classically forbidden region.

10. Consider an harmonic oscillator having angular resonance frequency $\omega_0$. At time $t = 0$ the system’s state is given by

$$|\alpha(t = 0)\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle),$$ \hfill (5.62)

where the states $|0\rangle$ and $|1\rangle$ are the ground and first excited states, respectively, of the oscillator. Calculate as a function of time $t$ the following quantities:

a) $\langle x \rangle$

b) $\langle p \rangle$

c) $\langle x^2 \rangle$

d) $\Delta x \Delta p$

11. Harmonic oscillator having angular resonance frequency $\omega$ is in state

$$|\psi(t = 0)\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |n\rangle)$$ \hfill (5.63)

at time $t = 0$, where $|0\rangle$ is the ground state and $|n\rangle$ is the eigenstate with eigenenergy $\hbar\omega (n + 1/2)$ ($n$ is a non zero integer). Calculate the expectation value $\langle x \rangle$ for time $t \geq 0$. 

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12. Consider a harmonic oscillator having mass $m$ and angular resonance frequency $\omega$. At time $t = 0$ the system’s state is given by $|\psi(0)\rangle = c_0 |0\rangle + c_1 |1\rangle$, where $|n\rangle$ are the eigenstates with energies $E_n = \hbar \omega (n + 1/2)$. Given that $\langle \mathcal{H} \rangle = \hbar \omega$, $|\psi(0)\rangle$ is normalized, and $\langle x \rangle (t = 0) = \frac{1}{2} \sqrt{\frac{\hbar}{m \omega}}$, calculate $\langle x \rangle (t)$ at times $t > 0$.

13. Show that

$$ D(\alpha) = e^{-\frac{|\alpha|^2}{2}} e^{\alpha \sigma^1 - \alpha^* \sigma^0} = e^{-\frac{|\alpha|^2}{2}} e^{\sigma^0} e^{\sigma^1} \ . $$

(5.64)

14. Show that the displacement operator $D(\alpha)$ is unitary.

15. Show that

$$ |\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \ . $$

(5.65)

16. Show that the coherent state $|\alpha\rangle$ is an eigenvector of the operator $a$ with an eigenvalue $\alpha$, namely

$$ a |\alpha\rangle = \alpha |\alpha\rangle \ . $$

(5.66)

17. Show that

$$ D(\alpha) = \exp \left( \sqrt{\frac{m \omega}{\hbar}} \alpha - \alpha^* \right) x \times \exp \left( -i \frac{\alpha + \alpha^*}{\sqrt{m \hbar \omega}} p \right) \exp \left( \frac{\alpha^2 - \alpha^2}{4} \right) \ . $$

(5.67)

18. Show that for any function $f(a, a^\dagger)$ having a power series expansion the following holds

$$ D^\dagger(\alpha) f(a, a^\dagger) D(\alpha) = f(a + \alpha, a^\dagger + \alpha^*) \ . $$

(5.68)

19. Show that the following holds for a coherent state $|\alpha\rangle$:

a) $\langle \alpha | \mathcal{H} | \alpha \rangle = \hbar \omega (|\alpha|^2 + 1/2)$.

b) $\langle \alpha | \mathcal{H}^2 | \alpha \rangle = \hbar^2 \omega^2 (|\alpha|^4 + 2 |\alpha|^2 + 1/4)$.

c) $\sqrt{\langle \alpha | (\Delta \mathcal{H})^2 | \alpha \rangle} = \hbar \omega |\alpha|$.

d) $\langle x | \alpha \rangle = \frac{2 \hbar \omega}{\sqrt{2m}} \Re \langle \alpha \rangle$.

e) $\langle p | \alpha \rangle = \frac{2 \hbar \omega}{\sqrt{2m}} \Im \langle \alpha \rangle$.

f) $\Delta x_{\alpha} = \sqrt{\langle \alpha | (\Delta x)^2 | \alpha \rangle} = \sqrt{\frac{\hbar}{2m \omega}}$.

g) $\Delta p_{\alpha} = \sqrt{\langle \alpha | (\Delta p)^2 | \alpha \rangle} = \sqrt{\frac{\hbar \omega}{2}}$. 

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20. Consider a harmonic oscillator of mass $m$ and angular resonance frequency $\omega$. The Hamiltonian is given by

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \quad (5.69)$$

The system at time $t$ is in a normalized state $|\alpha\rangle$, which is an eigenvector of the annihilation operator $a$, thus

$$a|\alpha\rangle = \alpha|\alpha\rangle, \quad (5.70)$$

where the eigenvalue $\alpha$ is a complex number. At time $t > 0$ the energy of the system is measured. What are the possible results $E_n$ and what are the corresponding probabilities $p_n(t)$?

21. Show that the wave function of a coherent state is given by

$$\psi_\alpha(x^\prime) = \langle x^\prime |\alpha \rangle = \exp \left( \frac{\alpha^2 - \alpha^2}{4} \right) \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \exp \left[ -\frac{1}{2} \frac{\langle x^\prime - x\rangle_\alpha^2}{\Delta x_{\alpha}} \right] + i \frac{\langle p\rangle_{\alpha}}{\hbar} x^\prime. \quad (5.71)$$

22. Show that

$$D(\alpha) D(\alpha^\prime) = \exp \left( \frac{\alpha\alpha^* - \alpha^*\alpha^\prime}{2} \right) D(\alpha + \alpha^\prime). \quad (5.72)$$

23. Show that the following closure relation holds

$$1 = \frac{1}{\pi} \int \int |\alpha\rangle \langle \alpha| \, d^2\alpha, \quad (5.73)$$

where $d^2\alpha$ denotes infinitesimal area in the $\alpha$ complex plane, namely $d^2\alpha = d\{\text{Re}\, \alpha\} d\{\text{Im}\, \alpha\}$.

24. Calculate the inner product between two coherent states $|\alpha\rangle$ and $|\beta\rangle$, where $\alpha, \beta \in \mathbb{C}$.

25. A one dimensional potential acting on a particle having mass $m$ is given by

$$V_1(x) = \frac{1}{2}m\omega^2 x^2 + \beta m\omega^2 x. \quad (5.74)$$

a) Calculate the Heisenberg representation of the position operator $x^{(H)}(t)$ and its canonically conjugate operator $p^{(H)}(t)$.

b) Given that the particle at time $t = 0$ is in the state $|0\rangle$, where the state $|0\rangle$ is the ground state of the potential

$$V_1(x) = \frac{1}{2}m\omega^2 x^2. \quad (5.75)$$

Calculate the expectation value $\langle x \rangle$ at later times $t > 0$. 
26. A particle having mass $m$ is in the ground state of the one-dimensional potential well $V_1(x) = (1/2) m\omega^2 (x - \Delta x)^2$ for times $t < 0$. At time $t = 0$ the potential suddenly changes and becomes $V_2(x) = (1/2) m\omega^2 x^2$.

a) Calculate the expectation value $\langle x \rangle$ at times $t > 0$.

b) Calculate the variance $\langle (\Delta x)^2 \rangle$ at times $t > 0$, where $\Delta x = x - \langle x \rangle$.

c) The energy of the particle is measured at time $t > 0$. What are the possible results and what are the probabilities to obtain any of these results.

27. Consider a particle having mass $m$ in the ground state of the potential well $V_a(x) = (1/2) m\omega^2 x^2$ for times $t < 0$. At time $t = 0$ the potential suddenly changes and becomes $V_b(x) = gx$.

a) Calculate the expectation value $\langle x \rangle$ at times $t > 0$.

b) Calculate the variance $\langle (\Delta x)^2 \rangle$ at times $t > 0$, where $\Delta x = x - \langle x \rangle$.

c) The energy of the particle is measured at time $t > 0$. What are the possible results and what are the probabilities to obtain any of these results.

28. Consider a particle of mass $m$ in a potential of a harmonic oscillator having angular frequency $\omega$. The operator $S(r)$ is defined as

$$S(r) = \exp \left[ \frac{r}{2} \left( a^2 - (a^\dagger)^2 \right) \right],$$

(5.76)

where $r$ is a real number, and $a$ and $a^\dagger$ are the annihilation and creation operators respectively. The operator $T$ is defined as

$$T = S(r) a S^\dagger(r).$$

(5.77)

a) Find an expression for the operator $T$ of the form $T = Aa + Ba^\dagger$, where both $A$ and $B$ are constants.

b) The vector state $|r\rangle$ is defined as

$$|r\rangle = S^\dagger(r) |0\rangle,$$

(5.78)

where $|0\rangle$ is the ground state of the harmonic oscillator. Calculate the expectation values $\langle r | x | r \rangle$ of the operator $x$ (displacement) and the expectation value $\langle r | p | r \rangle$ of the operator $p$ (momentum).

c) Calculate the variance $(\Delta x)^2$ of $x$ and the variance $(\Delta p)^2$ of $p$.

29. Consider one dimensional motion of a particle having mass $m$. The Hamiltonian is given by

$$\mathcal{H} = \hbar \omega_0 a^\dagger a + \hbar \omega_1 a^\dagger a^\dagger a a,$$

(5.79)

where

$$a = \sqrt{\frac{m\omega_0}{2\hbar}} \left( x + \frac{ip}{m\omega_0} \right),$$

(5.80)

is the annihilation operator, $x$ is the coordinate and $p$ is its canonical conjugate momentum. The frequencies $\omega_0$ and $\omega_1$ are both positive.
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a) Calculate the eigenenergies of the system.
b) Let \( |0\rangle \) be the ground state of the system. Calculate
   i. \( \langle 0| x |0\rangle \)
   ii. \( \langle 0| p |0\rangle \)
   iii. \( \langle 0| (\Delta x)^2 |0\rangle \)
   iv. \( \langle 0| (\Delta p)^2 |0\rangle \)

30. The Hamiltonian of a system is given by

\[
    \mathcal{H} = \epsilon N , \tag{5.81}
\]

where the real non-negative parameter \( \epsilon \) has units of energy, and where the operator \( N \) is given by

\[
    N = b\dagger b . \tag{5.82}
\]

The following holds

\[
    b\dagger b + bb\dagger = 1 , \tag{5.83}
\]

\[
    b^2 = 0 , \tag{5.84}
\]

\[
    (b\dagger)^2 = 0 . \tag{5.85}
\]

a) Find the eigenvalues of \( \mathcal{H} \). Clue: show first that \( N^2 = N \).
b) Let \( |0\rangle \) be the ground state of the system, which is assumed to be non-degenerate. Define the two states

\[
    |+\rangle = A_+ \left( 1 + b\dagger \right) |0\rangle , \tag{5.86a}
\]

\[
    |-\rangle = A_- \left( 1 - b\dagger \right) |0\rangle , \tag{5.86b}
\]

where the real non-negative numbers \( A_+ \) and \( A_- \) are normalization constants. Calculate \( A_+ \) and \( A_- \). Clue: show first that \( b\dagger |0\rangle \) is an eigenvector of \( N \).
c) At time \( t = 0 \) the system is in the state

\[
    |\alpha (t = 0)\rangle = |+\rangle , \tag{5.87}
\]

Calculate the probability \( p(t) \) to find the system in the state \( |-\rangle \) at time \( t > 0 \).

31. Normal ordering - Let \( X(a, a\dagger) \) be a function of the annihilation \( a \) and creation \( a\dagger \) operators. The normal ordering of \( X(a, a\dagger) \), which is denoted by \( :X(a, a\dagger): \) places the \( a \) operators on the right and the \( a\dagger \) operators on the left. Some examples are given below

\[
    :aa\dagger : = a\dagger a , \tag{5.88}
\]

\[
    :a\dagger a : = a\dagger a , \tag{5.89}
\]

\[
    : (a\dagger a)^n : = (a\dagger)^n a^n . \tag{5.90}
\]
Normal ordering is linear, i.e.: $X + Y := X : + : Y :$. Show that the projection operator $P_n = |n\rangle \langle n|$, where $|n\rangle$ is an eigenvector of the Hamiltonian of a harmonic oscillator, can be expressed as

$$P_n = \frac{1}{n!} (a^\dagger)^n \exp (-a^\dagger a) a^n :.$$ (5.91)

32. Consider a harmonic oscillator of angular frequency $\omega$ and mass $m$. A time dependent force is applied $f(t)$. The function $f(t)$ is assumed to vanish $\lim_{t \to \pm \infty} f(t) \to 0$. Given that the oscillator was initially in its ground state $|0\rangle$ at $t \to -\infty$ calculate the probability $p_n$ to find the oscillator in the number state $|n\rangle$ in the limit $t \to \infty$.

### 5.4 Solutions

1. The Hamiltonian is given by

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$  

Using Eqs. (3.21), (3.29), (5.9) and (5.10) one has

$$\langle x'|a|n\rangle = (2x_0^2)^{-1/2} \left( x' \psi_n(x') + x_0^2 \frac{d\psi_n}{dx'} \right),$$ (5.92)

$$\langle x'|a^\dagger|n\rangle = (2x_0^2)^{-1/2} \left( x' \psi_n(x') - x_0^2 \frac{d\psi_n}{dx'} \right),$$ (5.93)

where

$$x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$ (5.94)

For the ground state $|0\rangle$, according to Eq. (5.28), $a|0\rangle = 0$, thus

$$x' \psi_0(x') + x_0^2 \frac{d\psi_0}{dx'} = 0.$$ (5.95)

The solution is given by

$$\psi_0(x') = A_0 \exp \left( -\frac{1}{2} \left( \frac{x'}{x_0} \right)^2 \right),$$ (5.96)

where the normalization constant $A_0$ is found from the requirement

$$\int_{-\infty}^{\infty} |\psi_0(x')|^2 \, dx = 1,$$ (5.97)

thus
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\[ |A_0|^2 \int_{-\infty}^{\infty} \exp \left( -\left( \frac{x}{x_0} \right)^2 \right) \, dx = 1. \] 

(5.98)

Choosing \( A_0 \) to be real leads to

\[ \psi_0 (x') = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp \left( -\frac{1}{2} \left( \frac{x'}{x_0} \right)^2 \right). \]

(5.99)

All other wavefunctions are found using Eqs. (5.32) and (5.93)

\[ \psi_n (x') = \frac{1}{(2x_0)^{n/2} \sqrt{n!}} \left( x' - x_0^2 \frac{d}{dx'} \right)^n \psi_0 (x') \]

\[ = \frac{1}{\pi^{1/4} \sqrt{2^{n+1} x_0^{n+1/2}}} \left( x' - x_0^2 \frac{d}{dx'} \right)^n \exp \left( -\frac{1}{2} \left( \frac{x'}{x_0} \right)^2 \right). \]

(5.100)

Using the notation

\[ H_n (X) = \exp \left( \frac{X^2}{2} \right) \left( X - \frac{d}{dX} \right)^n \exp \left( -\frac{X^2}{2} \right), \]

(5.101)

the expression for \( \psi_n (x') \) can be rewritten as

\[ \psi_n (x') = \frac{\exp \left( \frac{x'^2}{2} \right) H_n \left( \frac{x'}{x_0} \right)}{\pi^{1/4} x_0^{1/2} \sqrt{2^{n+1} n!}}. \]

(5.102)

The term \( H_n (X) \), which is called the Hermite polynomial of order \( n \), is calculated below for some low values of \( n \)

\[ H_0 (X) = 1, \]

(5.103)

\[ H_1 (X) = 2X, \]

(5.104)

\[ H_2 (X) = 4X^2 - 2, \]

(5.105)

\[ H_3 (X) = 8X^3 - 12X, \]

(5.106)

\[ H_4 (X) = 16X^4 - 48X^2 + 12. \]

(5.107)

2. The relation (5.56), which is a Taylor expansion of the function \( f(t) = \exp (2Xt - t^2) \) around the point \( t = 0 \), implies that

\[ H_n (X) = \frac{d^n}{dt^n} \exp \left( 2Xt - t^2 \right) \bigg|_{t=0}. \]

(5.108)

The identity \( 2Xt - t^2 = X^2 - (X - t)^2 \) yields
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\[ H_n (X) = \exp \left( X^2 \right) \frac{d^n}{dX^n} \exp \left( -(X-t)^2 \right) \bigg|_{t=0}. \]  

(5.109)

Moreover, using the relation

\[ \frac{d}{dt} \exp \left( -(X-t)^2 \right) = -\frac{d}{dX} \exp \left( -(X-t)^2 \right), \]  

(5.110)

one finds that

\[ H_n (X) = \exp \left( X^2 \right) (-1)^n \frac{d^n}{dX^n} \exp \left( -(X-t)^2 \right) \bigg|_{t=0} = \exp \left( X^2 \right) (-1)^n \frac{d^n}{dX^n} \exp \left( -X^2 \right). \]  

(5.111)

Note that for an arbitrary function \( g(X) \) the following holds

\[ -\exp \left( X^2 \right) \frac{d}{dX} \exp \left( -X^2 \right) g = \left( 2X - \frac{d}{dX} \right) g, \]  

(5.112)

and

\[ \exp \left( \frac{X^2}{2} \right) \left( X - \frac{d}{dX} \right) \exp \left( -\frac{X^2}{2} \right) g = \left( 2X - \frac{d}{dX} \right) g, \]  

(5.113)

thus

\[ H_n (X) = \exp \left( \frac{X^2}{2} \right) \left( X - \frac{d}{dX} \right)^n \exp \left( -\frac{X^2}{2} \right). \]  

(5.114)

3. With the help of Eqs. (5.9), (5.10), (5.11), (5.12) and (5.13) one finds

\[ \langle n | x | n \rangle = 0, \]  

(5.115)

\[ \langle n | x^2 | n \rangle = \frac{\hbar}{2m\omega} \langle n | aa^\dagger + a^\dagger a | n \rangle = \frac{\hbar}{2m\omega} (2n + 1), \]  

(5.116)

\[ \langle n | p | n \rangle = 0, \]  

(5.117)

\[ \langle n | p^2 | n \rangle = \frac{m\hbar\omega}{2} \langle n | aa^\dagger + a^\dagger a | n \rangle = \frac{m\hbar\omega}{2} (2n + 1), \]  

(5.118)

thus

\[ \langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle = \left( n + \frac{1}{2} \right)^2 \hbar^2. \]  

4. The Hamiltonian is given by

\[ \mathcal{H} = \frac{p^2}{2m}. \]  

(5.119)

Using Eqs. (4.37) and (5.8) one finds that
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\[
\frac{dx^{(H)}}{dt} = \frac{1}{i\hbar} \left[ x^{(H)}, \mathcal{H}^{(H)} \right] = \frac{p^{(H)}}{im\hbar} \left[ x^{(H)}, p^{(H)} \right] = \frac{p^{(H)}}{m} \tag{5.120}
\]

\[
\frac{dp^{(H)}}{dt} = \frac{1}{i\hbar} \left[ p^{(H)}, \mathcal{H}^{(H)} \right] = 0 \tag{5.121}
\]

The solution is thus

\[
x^{(H)}(t) = x^{(H)}(0) + \frac{1}{m} p^{(H)}(0) t \tag{5.122}
\]

5. The Hamiltonian is given by

\[
\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \tag{5.123}
\]

Using Eqs. (4.37) and (5.8) one finds that

\[
\frac{dx^{(H)}}{dt} = \frac{1}{i\hbar} \left[ x^{(H)}, \mathcal{H}^{(H)} \right] = \frac{p^{(H)}}{m} , \tag{5.124}
\]

and

\[
\frac{dp^{(H)}}{dt} = \frac{1}{i\hbar} \left[ p^{(H)}, \mathcal{H}^{(H)} \right] = -m\omega^2 x^{(H)} . \tag{5.125}
\]

a) The solutions of the above equations are given by

\[
x^{(H)}(t) = x^{(H)}(0) \cos(\omega t) + \frac{\sin(\omega t)}{m\omega} p^{(H)}(0) , \tag{5.126}
\]

and

\[
p^{(H)}(t) = p^{(H)}(0) \cos(\omega t) - m\omega \sin(\omega t) x^{(H)}(0) . \tag{5.127}
\]

b) Using the expressions for \(x^{(H)}(t)\) and \(p^{(H)}(t)\) and Eq. (5.8) one finds that

\[
\left[ p^{(H)}(t_1) , x^{(H)}(t_2) \right] = -(\cos(\omega t_1) \cos(\omega t_2) + \sin(\omega t_1) \sin(\omega t_2)) \left[ x^{(H)}(0) , p^{(H)}(0) \right] = -i\hbar \cos(\omega (t_1 - t_2)) , \tag{5.128}
\]

\[
\left[ p^{(H)}(t_1) , p^{(H)}(t_2) \right] = m\omega(\cos(\omega t_1) \sin(\omega t_2) - \sin(\omega t_1) \cos(\omega t_2)) \left[ x^{(H)}(0) , p^{(H)}(0) \right] = -i\hbar m\omega \sin(\omega (t_1 - t_2)) , \tag{5.129}
\]

and
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\[
\left[ x^{(H)} (t_1), x^{(H)} (t_2) \right] = \frac{i}{\hbar} \left( \cos (\omega t_1) \sin (\omega t_2) - \sin (\omega t_1) \cos (\omega t_2) \right) \left[ x^{(H)} (0), p^{(H)} (0) \right] \\
= -\frac{\hbar}{\omega} \sin (\omega (t_1 - t_2)).
\]

(5.130)

6. The correlation function is defined as

\[
G(t) = \langle x^{(H)} (t) x^{(H)} (0) \rangle.
\]

(5.131)

Using Eq. (5.126), which is given by

\[
x^{(H)} (t) = x^{(H)} (0) \cos (\omega t) + p^{(H)} (0) \frac{\hbar}{2m\omega} \sin (\omega t),
\]

(5.132)

one finds

\[
G(t) = \cos (\omega t) \left( x^{2} (0) \right) + \sin (\omega t) \langle p^{(H)} (0) x^{(H)} (0) \rangle.
\]

(5.133)

Using the relations

\[
x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger),
\]

(5.134)

\[
p = i \sqrt{\frac{\hbar m\omega}{2}} (-a + a^\dagger),
\]

(5.135)

\[
[a, a^\dagger] = 1,
\]

(5.136)

one finds

\[
x^2 = \frac{\hbar}{2m\omega} \left( a^2 + (a^\dagger)^2 + 2a^\dagger a + 1 \right),
\]

(5.137)

\[
px = \frac{\hbar}{2m\omega} \left( -a^2 + (a^\dagger)^2 - 1 \right),
\]

(5.138)

thus for the ground state

\[
G(t) = \frac{\hbar}{2m\omega} \left[ \cos (\omega t) - i \sin (\omega t) \right] = \frac{\hbar}{2m\omega} \exp (-i\omega t).
\]

(5.139)

7. Due to the infinite barrier for \( x \leq 0 \) the wavefunction must vanish at \( x = 0 \). This condition is satisfied by the wavefunction of all number states \( |n \rangle \) with odd value of \( n \) (the states \( |n \rangle \) are eigenstates of the ‘regular’ harmonic oscillator with potential \( V(x) = (m\omega^2/2) x^2 \)). These wavefunctions obviously satisfy the Schrödinger equation for \( x > 0 \).

a) Thus the possible energy values are \( E_k = \hbar \omega (2k + 3/2) \) where \( k = 0, 1, 2, \cdots \).
b) The corresponding normalized wavefunctions are given by

\[ \tilde{\psi}_k(x) = \begin{cases} \sqrt{2} \psi_{2k+1}(x) & x > 0 \\ 0 & x \leq 0 \end{cases} , \]  

(5.140)

where \( \psi_n(x) \) is the wavefunction of the number states \( |n\rangle \). Thus for a given \( k \)

\[
\langle x^2 \rangle_k = \int_0^\infty dx \left| \tilde{\psi}_k(x) \right|^2 x^2 \\
= 2 \int_0^\infty dx \left| \psi_{2k+1}(x) \right|^2 x^2 \\
= \int_{-\infty}^\infty dx \left| \psi_{2k+1}(x) \right|^2 x^2 \\
= (2k+1) |x|^2 |2k+1| ,
\]

(5.141)

thus with the help of Eq. (5.116) one finds that

\[
\langle x^2 \rangle_k = \frac{\hbar}{m\omega} \left( 2k + \frac{3}{2} \right) ,
\]

(5.142)

8. The potential can be written as

\[ V(x) = \frac{m\omega^2}{2} \left( x + \frac{\alpha}{m\omega^2} \right)^2 - \frac{\alpha^2}{2m\omega^2} . \]

(5.143)

This describes a harmonic oscillator centered at \( x_0 = -\alpha/m\omega^2 \) having angular resonance frequency \( \omega \). The last constant term represents energy shift. Thus, the eigenenergies are given by

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right) - \frac{\alpha^2}{2m\omega^2} , \]

(5.144)

where \( n = 0, 1, 2, \ldots \).

9. In the classically forbidden region \( V(x) > E_0 = \hbar \omega/2 \), namely \( |x| > x_0 \) where

\[ x_0 = \sqrt{\frac{\hbar}{m\omega}} . \]

(5.145)

Using Eq. (5.99) one finds
5.4. Solutions

\[ p = 2 \int_{x_0}^{\infty} |\psi(x)|^2 \, dx \]
\[ = \frac{2}{\pi^{1/2} x_0} \int_{x_0}^{\infty} \exp \left( - \left( \frac{x}{x_0} \right)^2 \right) \, dx \]
\[ = 1 - \text{erf} \left( \frac{1}{\sqrt{2}} \right) \]
\[ = 0.157 . \] \hfill (5.146)

10. With the help of Eq. (4.14) one has

\[ |\alpha(t)\rangle = \frac{1}{\sqrt{2}} e^{-i\omega_0 t} (|0\rangle + e^{-i\omega_0 t} |1\rangle) . \] \hfill (5.147)

Moreover, the following hold

\[ x = \sqrt{\frac{\hbar}{2m\omega_0}} (a + a^\dagger) , \] \hfill (5.148)
\[ p = i\sqrt{\frac{m\hbar\omega_0}{2}} (-a + a^\dagger) , \] \hfill (5.149)
\[ a |n\rangle = \sqrt{n} |n - 1\rangle , \] \hfill (5.150)
\[ a^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle , \] \hfill (5.151)
\[ [a, a^\dagger] = 1 , \] \hfill (5.152)

thus

a) \hfill (5.153)

\[ \langle x \rangle = \sqrt{\frac{\hbar}{2m\omega_0}} \langle \alpha(t) | (a + a^\dagger) | \alpha(t) \rangle \]
\[ = \sqrt{\frac{\hbar}{2m\omega_0}} \frac{1}{2} \left( |0\rangle + e^{i\omega_0 t} |1\rangle \right) (a + a^\dagger) \left( |0\rangle + e^{-i\omega_0 t} |1\rangle \right) \]
\[ = \sqrt{\frac{\hbar}{2m\omega_0}} \frac{1}{2} \left( e^{i\omega_0 t} + e^{-i\omega_0 t} \right) \]
\[ = \sqrt{\frac{\hbar}{2m\omega_0}} \cos (\omega_0 t) . \]

b) \hfill (5.154)

\[ \langle p \rangle = i\sqrt{\frac{m\hbar\omega_0}{2}} \langle \alpha(t) | (-a + a^\dagger) | \alpha(t) \rangle \]
\[ = i\sqrt{\frac{m\hbar\omega_0}{2}} \frac{1}{2} \left( |0\rangle + e^{i\omega_0 t} |1\rangle \right) (-a + a^\dagger) \left( |0\rangle + e^{-i\omega_0 t} |1\rangle \right) \]
\[ = -\sqrt{\frac{m\hbar\omega_0}{2}} \sin (\omega_0 t) . \]
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c) \[
\langle x^2 \rangle = \frac{\hbar}{2m\omega_0} (\alpha(t)) (a + a\dagger)^2 |\alpha(t)\rangle \\
= \frac{\hbar}{2m\omega_0} \langle \alpha(t) | \left( a^2 + (a\dagger)^2 + [a, a\dagger] + 2a\dagger a \right) |\alpha(t)\rangle \\
= \frac{\hbar}{2m\omega_0} \left( 1 + 2\frac{1}{2} \right) \\
= \frac{\hbar}{2m\omega_0} .
\]

(5.155)

d) Similarly
\[
\langle p^2 \rangle = -\frac{m\hbar\omega_0}{2} (\alpha(t)) (-a + a\dagger)^2 |\alpha(t)\rangle \\
= -\frac{m\hbar\omega_0}{2} \langle \alpha(t) | \left( a^2 + (a\dagger)^2 - [a, a\dagger] - 2a\dagger a \right) |\alpha(t)\rangle \\
= m\hbar\omega_0 ,
\]

thus
\[
\Delta x \Delta p = \hbar \sqrt{1 - \frac{\cos^2 (\omega_0 t)}{2}} \sqrt{1 - \frac{\sin^2 (\omega_0 t)}{2}} \\
= \frac{\hbar}{2} \sqrt{2 + \frac{1}{4} \sin^2 (2\omega_0 t)} .
\]

(5.156)

11. The state \(|\psi(t)\rangle\) is given by
\[
|\psi(t)\rangle = \frac{1}{\sqrt{2}} \left[ \exp \left( -\frac{iE_0 t}{\hbar} \right) |0\rangle + \exp \left( -\frac{iE_n t}{\hbar} \right) |n\rangle \right] ,
\]

(5.158)

where
\[
E_n = \hbar \omega \left( n + \frac{1}{2} \right) ,
\]

(5.159)

thus, using
\[
x = \sqrt{\frac{\hbar}{2m\omega}} (a + a\dagger) ,
\]

(5.160)

and
\[
a |n\rangle = \sqrt{n} |n - 1\rangle ,
\]

(5.161)

\[
a\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle ,
\]

(5.162)

one finds that \(\langle x \rangle(t) = 0\) if \(n > 1\), and for \(n = 1\)
\[\langle x \rangle (t) = \sqrt{\frac{\hbar}{2m\omega}} (\psi(t) | (a + a^\dagger) | \psi(t)) = \sqrt{\frac{\hbar}{2m\omega}} \cos (\omega t) .\]  

(5.163)

12. Since \( \langle \mathcal{H} \rangle = \hbar \omega \) and \(|\psi(0)\rangle\) is normalized one has

\[|c_0|^2 = |c_1|^2 = \frac{1}{2},\]  

(5.164)

thus \(|\psi(0)\rangle\) can be written as

\[|\psi(0)\rangle = \sqrt{\frac{1}{2}} (|0\rangle + e^{i\theta} |1\rangle),\]  

(5.165)

where \(\theta\) is real. Given that at time \(t = 0\)

\[\langle x \rangle (t = 0) = \frac{1}{2} \sqrt{\frac{\hbar}{m\omega}},\]  

(5.166)

one finds using the identities

\[x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger),\]  

(5.167)

\[a |n\rangle = \sqrt{n} |n - 1\rangle,\]  

(5.168)

\[a^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle,\]  

(5.169)

that

\[\cos \theta = \frac{\sqrt{2}}{2} .\]  

(5.170)

Using this result one can evaluate \(\langle p \rangle (t = 0)\), where

\[p = i \sqrt{\frac{\hbar m\omega}{2}} (-a + a^\dagger),\]  

(5.171)

thus

\[\langle p \rangle (t = 0) = \sqrt{\frac{\hbar m\omega}{2}} \sin \theta = \pm \sqrt{\frac{\hbar m\omega}{2}} \frac{\sqrt{2}}{2} = \pm m\omega \langle x \rangle (t = 0) .\]  

(5.172)

Using these results together with Eq. (5.126) yields

\[\langle x \rangle (t) = \frac{1}{2} \sqrt{\frac{\hbar}{m\omega}} (\cos (\omega t) \pm \sin (\omega t)) = \sqrt{\frac{\hbar}{2m\omega}} \cos (\omega t \mp \frac{\pi}{4}) .\]  

(5.173)
13. According to identity (2.176), which states that
\[ e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} = e^B e^A e^{-\frac{1}{2}[A,B]} \],
(5.174)
provided that
\[ [A, [A, B]] = [B, [A, B]] = 0 \],
(5.175)
one finds with the help of Eq. (5.13) that
\[ D(\alpha) = \exp(\alpha a^\dagger - \alpha^* a) \]
\[ = e^{-\frac{1}{2} |\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} \]
\[ = e^{\frac{1}{2} |\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger} \].
(5.176)

14. Using Eq. (5.176) one has
\[ D(\alpha) = \exp(\alpha a^\dagger - \alpha^* a) \]
\[ = e^{-\frac{1}{2} |\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} \]
\[ = e^{\frac{1}{2} |\alpha|^2} e^{-\alpha^* a} e^{\alpha a^\dagger} \].
(5.177)

15. Using Eqs. (5.35), (5.28) and (5.29) one finds that
\[ |\alpha\rangle = e^{-\frac{1}{2} |\alpha|^2} e^{\alpha a^\dagger} e^{-\alpha^* a} |0\rangle = e^{-\frac{1}{2} |\alpha|^2} e^{\alpha a^\dagger} |0\rangle \]
\[ = e^{-\frac{1}{2} |\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \].
(5.179)

16. Using Eqs. (5.42) and (5.28) one has
\[ a |\alpha\rangle = e^{-\frac{1}{2} |\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \]
\[ = \alpha e^{-\frac{1}{2} |\alpha|^2} \sum_{n=1}^{\infty} \frac{\alpha^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle \]
\[ = \alpha |\alpha\rangle \].
(5.180)

17. Using Eqs. (5.36), (5.9) and (5.10) one has
\[ D(\alpha) = \exp \left[ \frac{1}{2\hbar \omega} (\alpha - \alpha^*) x - i \sqrt{\frac{1}{2\hbar \omega}} (\alpha + \alpha^*) p \right] \],
(5.181)
thus with the help of Eqs. (2.176) and (5.8) the desired result is obtained.
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\[ D(\alpha) = \exp \left( \sqrt{\frac{m\omega}{\hbar}} \alpha - \alpha^* x \right) \times \exp \left( -\frac{i}{\sqrt{\hbar m\omega}} \frac{\alpha + \alpha^*}{\sqrt{2}} p \right) \exp \left( \frac{\alpha^2 - \alpha^2}{4} \right) \].

(i)

18. Using the operator identity (2.174)

\[ e^L A e^{-L} = A + [L, A] + \frac{1}{2!} [L, [L, A]] + \cdots \],

and the definition (5.36)

\[ D(\alpha) = \exp \left( \alpha a^\dagger - \alpha^* a \right) \],

one finds that

\[ D^\dagger (\alpha) a D(\alpha) = a + \alpha \],

\[ D^\dagger (\alpha) a^\dagger D(\alpha) = a^\dagger + \alpha^* \].

Exploiting the unitarity of \( D(\alpha) \)

\[ D(\alpha) D^\dagger (\alpha) = 1 \]

it is straightforward to show that for any function \( f(a, a^\dagger) \) having a power series expansion the following holds

\[ D^\dagger (\alpha) f(a, a^\dagger) D(\alpha) = f(a + \alpha, a^\dagger + \alpha^*) \]

(e.g., \( D^\dagger a^2 D = D^\dagger D a D^\dagger a D = (a + \alpha)^2 \)).

19. Using Eq. (5.68) and the following identities

\[ \mathcal{H} = \hbar \omega \left( a^\dagger a + \frac{1}{2} \right) \],

\[ x = \sqrt{\frac{\hbar}{2m\omega}} \left( a + a^\dagger \right) \],

\[ p = i \sqrt{\frac{\hbar m\omega}{2}} \left( -a + a^\dagger \right) \],

all these relations are easily obtained.

20. Expressing the state \( |\alpha\rangle \) in the basis of eigenvectors of the Hamiltonian \( |n\rangle \)

\[ |\alpha\rangle = \sum_{n=0}^\infty c_n |n\rangle \],

using
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\[ a |\alpha\rangle = \alpha |\alpha\rangle , \]  
\[ (5.192) \]

and

\[ a |n\rangle = \sqrt{n} |n - 1\rangle , \]  
\[ (5.193) \]

one finds

\[ \sum_{n=0}^{\infty} c_n \sqrt{n} |n - 1\rangle = \alpha \sum_{n=0}^{\infty} c_n |n\rangle , \]  
\[ (5.194) \]

thus

\[ c_{n+1} = \frac{\alpha}{\sqrt{n+1}} c_n , \]  
\[ (5.195) \]

therefore

\[ |\alpha\rangle = A \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle . \]  
\[ (5.196) \]

The normalization constant \( A \) is found by

\[ 1 = |A|^2 \sum_{n=0}^{\infty} \frac{(|\alpha|^2)^n}{n!} = |A|^2 e^{\frac{|\alpha|^2}{2}} . \]  
\[ (5.197) \]

Choosing \( A \) to be real yields

\[ A = e^{-\frac{|\alpha|^2}{2}} , \]  
\[ (5.198) \]

thus

\[ c_n = e^{-\frac{|\alpha|^2}{2}} \frac{\alpha^n}{\sqrt{n!}} . \]  
\[ (5.199) \]

Note that this result is identical to Eq. (5.42), thus \( |\alpha\rangle \) is a coherent state. The possible results of the measurement are

\[ E_n = \hbar \omega \left( n + \frac{1}{2} \right) , \]  
\[ (5.200) \]

and the corresponding probabilities, which are time independent, are given by

\[ p_n(t) = |c_n|^2 = e^{-|\alpha|^2} \frac{(|\alpha|^2)^n}{n!} . \]  
\[ (5.201) \]
21. Using the relations
\[ \langle x \rangle_\alpha = \sqrt{\frac{2\hbar}{m\omega}} \text{Re}(\alpha), \quad (5.202) \]
\[ \langle p \rangle_\alpha = \sqrt{2\hbar m\omega} \text{Im}(\alpha), \quad (5.203) \]
Eq. (5.67) can be written as
\[ D(\alpha) = \exp \left( \frac{i\langle p \rangle_\alpha x}{\hbar} \right) \exp \left( -\frac{i\langle x \rangle_\alpha p}{\hbar} \right) \exp \left( \frac{\alpha^* - \alpha^2}{4} \right). \quad (5.204) \]
Using Eqs. (3.12) and (3.19) one finds that
\[ \exp \left( -\frac{i\langle x \rangle_\alpha p}{\hbar} \right) |x'\rangle = |x' + \langle x \rangle_\alpha\rangle, \]
thus
\[ \langle x' | \alpha \rangle = \langle x' | \exp \left( \frac{i\langle p \rangle_\alpha x}{\hbar} \right) \exp \left( -\frac{i\langle x \rangle_\alpha p}{\hbar} \right) \exp \left( \frac{\alpha^* - \alpha^2}{4} \right) |0\rangle = \exp \left( \frac{\alpha^* - \alpha^2}{4} \right) \exp \left( \frac{i\langle p \rangle_\alpha x'}{\hbar} \right) (x' - \langle x \rangle_\alpha) |0\rangle. \quad (5.205) \]
Using Eq. (5.99) the wavefunction of the ground state is given by
\[ \langle x' | 0 \rangle = \frac{1}{(2\pi)^{1/4} \sqrt{\Delta x_\alpha}} \exp \left( -\frac{(x')^2}{2\Delta x_\alpha} \right), \quad (5.206) \]
where
\[ \Delta x_\alpha = \frac{\hbar}{2m\omega}, \quad (5.207) \]
thus
\[ \langle x' | \alpha \rangle = \exp \left( \frac{\alpha^* - \alpha^2}{4} \right) \exp \left( \frac{i\langle p \rangle_\alpha x'}{\hbar} \right) \frac{\exp \left( -\frac{(x' - \langle x \rangle_\alpha)^2}{4 \Delta x_\alpha^2} \right)}{(2\pi)^{1/4} \sqrt{\Delta x_\alpha}} \left[ \exp \left( -\frac{(x - \langle x \rangle_\alpha)^2}{2\Delta x_\alpha^2} \right) + i \langle p \rangle_\alpha \frac{x'}{\hbar} \right]. \quad (5.208) \]
22. Using Eqs. (5.36) and (2.176) this relation is easily obtained.
23. With the help of Eq. (5.42) one has
\[ \frac{1}{\pi} \int \int |\alpha\rangle \langle \alpha| d^2\alpha = \frac{1}{\pi} \sum\limits_{n,m} |n\rangle \langle m| \frac{1}{\sqrt{n!m!}} \int \int e^{-|\alpha|^2} |\alpha^*\rangle^m d^2\alpha. \]
Employing polar coordinates in the complex plane $\alpha = \rho e^{i\theta}$, where $\rho$ is non-negative real and $\theta$ is real, leads to

\[
\frac{1}{\pi} \int \int |\alpha\rangle \langle \alpha| \, d^2\alpha = \frac{1}{\pi} \sum_{n,m} |n\rangle \langle m| \int \int_0^{2\pi} d\rho d\theta e^{i\theta(n-m)} e^{-\rho^2} \frac{1}{\sqrt{n!m!}} e^{-\rho^{n+m+1}} = \sum_{n} |n\rangle \langle n| \frac{1}{n!} \Gamma(n+1) = 1.
\]

24. Using Eqs. (5.35) and (5.41) one finds that

\[
\langle \beta | \alpha \rangle = \langle 0 | D^{\dagger}(\beta) D(\alpha) | 0 \rangle = \langle 0 | D(-\beta) D(\alpha) | 0 \rangle = \exp \left( -\frac{\beta\alpha^* + \beta^*\alpha}{2} \right) \langle 0 | D(-\beta + \alpha) | 0 \rangle = \exp \left( -\frac{\beta\alpha^* + \beta^*\alpha}{2} \right) \langle 0 | \alpha - \beta \rangle.
\]

Thus, with the help of Eq. (5.42) one has

\[
\langle \beta | \alpha \rangle = \exp \left( -\frac{\beta\alpha^* + \beta^*\alpha}{2} \right) e^{-|\alpha - \beta|^2/2} = \exp \left( -\frac{|\beta|^2}{2} - \frac{|\alpha|^2}{2} + \alpha\beta^* \right) = \exp \left( -\frac{|\alpha - \beta|^2}{2} + i \text{Im} (\alpha\beta^*) \right).
\]
5.4. Solutions

\[ V_1 (x) = \frac{1}{2} m \omega^2 (x + \beta)^2 - \frac{1}{2} m \omega^2 \beta^2 \]
\[ = \frac{1}{2} m \omega^2 x'^2 - \frac{1}{2} m \omega^2 \beta^2 , \]

where
\[ x' = x + \beta . \]  

(5.213)

a) Thus, using Eqs. (5.126) and (5.127) together with the relations
\[ x^{(H)} (t) = x^{(H)} (0) + \beta , \]
\[ p^{(H)} (t) = p^{(H)} (0) , \]

one finds
\[ x^{(H)} (t) = \left( x^{(H)} (0) + \beta \right) \cos (\omega t) + \frac{\sin (\omega t)}{m \omega} p^{(H)} (0) - \beta , \]
\[ p^{(H)} (t) = p^{(H)} (0) \cos (\omega t) - m \omega \sin (\omega t) \left( x^{(H)} (0) + \beta \right) . \]

(5.215)

(5.216)

(5.217)

(5.218)

b) For this case at time \( t = 0 \)
\[ \langle x^{(H)} (0) \rangle = 0 , \]
\[ \langle p^{(H)} (0) \rangle = 0 , \]

thus
\[ \langle x^{(H)} (t) \rangle = \beta (\cos (\omega t) - 1) . \]

(5.219)

(5.220)

(5.221)

26. The state of the system at time \( t = 0 \) is given by
\[ |\psi (t = 0) \rangle = \exp \left( - i \Delta x \frac{p}{\hbar} \right) |0 \rangle , \]

where \( |0 \rangle \) is the ground state of the potential \( V_2 \). In general a coherent state with parameter \( \alpha \) can be written as
\[ |\alpha \rangle = \exp \left( \sqrt{\frac{m \omega}{\hbar}} \frac{\alpha - \alpha^* x}{\sqrt{2}} \right) \exp \left( - \frac{i}{\sqrt{m \hbar \omega}} \frac{\alpha + \alpha^*}{\sqrt{2}} p \right) \exp \left( \frac{\alpha^2 - \alpha^* 2}{4} \right) |0 \rangle . \]

(5.222)

(5.223)

a) Thus \( |\psi (t = 0) \rangle = |\alpha_0 \rangle \), where
\[ \alpha_0 = \Delta x \sqrt{\frac{m \omega}{2 \hbar}} . \]

(5.224)

The time evolution of a coherent state is given by
\[ |\psi (t) \rangle = e^{-i \omega t/2} |\alpha = \alpha_0 e^{-i \omega t} \rangle , \]

(5.225)
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and the following holds

\[ \langle x \rangle (t) = \sqrt{\frac{2\hbar}{m\omega}} \text{Re} [\alpha_0 e^{-i\omega t}] = \Delta_x \cos(\omega t) \], \hspace{1cm} (5.226)

b) According to Eq. (5.48)

\[ \langle (\Delta x)^2 \rangle (t) = \frac{\hbar}{2m\omega} \]. \hspace{1cm} (5.227)

c) In general a coherent state can be expanded in the basis of number states \(|n\rangle\)

\[ |\alpha\rangle = e^{-|\alpha|^2/2} \sum_n \frac{\alpha^n}{\sqrt{n!}} |n\rangle \], \hspace{1cm} (5.228)

thus the probability to measure energy \(E_n = \hbar \omega (N + 1/2)\) at time \(t\) is given by

\[ P_n = |\langle n|\psi(t)\rangle|^2 = e^{-|\alpha|^2} \frac{\alpha^2}{n!} = \frac{1}{n!} \exp \left( -\frac{m\omega \Delta x^2}{2\hbar} \right) \left( \frac{m\omega \Delta x^2}{2\hbar} \right)^n \]. \hspace{1cm} (5.229)

27. At time \(t = 0\) the following holds

\[ \langle x \rangle = 0 \], \hspace{1cm} (5.230)

\[ \langle p \rangle = 0 \], \hspace{1cm} (5.231)

\[ \langle (\Delta x)^2 \rangle = \langle x^2 \rangle = \frac{\hbar}{2m\omega} \], \hspace{1cm} (5.232)

\[ \langle (\Delta p)^2 \rangle = \langle p^2 \rangle = \frac{\hbar m\omega}{2} \]. \hspace{1cm} (5.233)

Moreover, to calculate \(\langle xp\rangle\) it is convenient to use

\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) \], \hspace{1cm} (5.234)

\[ p = i\sqrt{\frac{m\hbar \omega}{2}} (-a + a^\dagger) \], \hspace{1cm} (5.235)

\[ [a, a^\dagger] = 1 \], \hspace{1cm} (5.236)

thus at time \(t = 0\)

\[ \langle xp\rangle = i\hbar \langle 0|aa^\dagger - a^\dagger a|0\rangle = i\hbar \frac{\Delta x}{2} \]. \hspace{1cm} (5.237)

The Hamiltonian for times \(t > 0\) is given by

\[ \mathcal{H} = \frac{p^2}{2m} + gx \]. \hspace{1cm} (5.238)
Using the Heisenberg equation of motion for the operators $x$ and $x^2$ one finds

\[
\frac{dx(H)}{dt} = \frac{1}{i\hbar} \left[ x(H), \mathcal{H} \right], \quad (5.239)
\]

\[
\frac{dp(H)}{dt} = \frac{1}{i\hbar} \left[ p(H), \mathcal{H} \right], \quad (5.240)
\]

\[
\frac{dx^2(H)}{dt} = \frac{1}{i\hbar} \left[ x^2(H), \mathcal{H} \right], \quad (5.241)
\]

or using $[x, p] = i\hbar$

\[
\frac{dx(H)}{dt} = \frac{p(H)}{m}, \quad (5.242)
\]

\[
\frac{dp(H)}{dt} = -g, \quad (5.243)
\]

\[
\frac{dx^2(H)}{dt} = \frac{1}{m} (x(H)p(H) + p(H)x(H)) - \frac{1}{m} \left( 2x(H)p(H) - i\hbar \right), \quad (5.244)
\]

thus

\[
p(H)(t) = p(H)(0) - gt, \quad (5.245)
\]

\[
x(H)(t) = x(H)(0) + \frac{p(H)(0) t}{m} - \frac{gt^2}{2m}, \quad (5.246)
\]

\[
x^2(H)(t) = x^2(H)(0) - \frac{iht}{m} + \frac{2}{m} \int_0^t x(H)(t') p(H)(t') \, dt'
\]

\[
= x^2(H)(0) - \frac{iht}{m} + \frac{2}{m} \int_0^t \left( x(H)(0) + \frac{p(H)(0) t'}{m} - \frac{gt'^2}{2m} \right) \left[ p(H)(0) - gt' \right] \, dt'
\]

\[
= x^2(H)(0) - \frac{iht}{m}
\]

\[
+ \frac{2}{m} \int_0^t \left( x(H)(0) p(H)(0) + \frac{p^2(H)(0) t'^2}{2m} - \frac{gt'^2 p(H)(0)}{2m} - x(H)(0) gt' - \frac{p(H)(0) gt'^2}{m} + \frac{g^2 t'^3}{2m} \right) \, dt'
\]

\[
= x^2(H)(0) - \frac{iht}{m}
\]

\[
+ \frac{2}{m} \left( x(H)(0) p(H)(0) t + \frac{p^2(H)(0) t^2}{2m} - \frac{p(H)(0) gt^2}{6m} - \frac{x(H)(0) gt^2}{2} - \frac{p(H)(0) gt^3}{3m} + \frac{g^2 t^4}{8m} \right). \quad (5.247)
\]

Using the initial conditions Eqs. (5.230), (5.231), (5.232), (5.233) and (5.237) one finds

\[
\langle x(t) \rangle = -\frac{gt^2}{2m}, \quad (5.248)
\]
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\[ \langle x(t) \rangle^2 = \frac{\hbar^2 t^4}{4m^2}, \quad (5.249) \]

\[ \langle p(t) \rangle = -gt, \quad (5.250) \]

\[ \langle x^2(t) \rangle = \frac{\hbar}{2m\omega} - \frac{iht}{m} + \frac{2}{m} \left( \frac{iht}{2} + \frac{\hbar\omega t^2}{4} + \frac{\hbar^2 t^4}{8m} \right), \quad (5.251) \]

and

\[ \left\langle (\Delta x)^2(t) \right\rangle = \langle x^2(t) \rangle - \langle x(t) \rangle^2 = \frac{\hbar}{2m\omega} + \frac{\hbar\omega t^2}{2m} = \frac{\hbar}{2m\omega} (1 + \omega^2 t^2). \quad (5.252) \]

28. Using the operator identity (2.174), which is given by

\[ e^L O e^{-L} = O + [L, O] + \frac{1}{2!} [L, [L, O]] + \frac{1}{3!} [L, [L, [L, O]]] + \cdots, \quad (5.253) \]

for the operators

\[ O = a, \quad (5.254) \]

\[ L = r \left( a^2 - (a^\dagger)^2 \right), \quad (5.255) \]

and the relations

\[ [a, a^\dagger] = 1, \quad (5.256) \]

\[ [L, O] = ra^\dagger, \quad (5.257) \]

\[ [L, [L, O]] = r^2 a, \quad (5.258) \]

\[ [L, [L, [L, O]]] = r^3 a^\dagger, \quad (5.259) \]

\[ [L, [L, [L, [L, O]]]] = r^4 a, \quad (5.260) \]

etc., one finds

\[ T = \left( 1 + \frac{r^2}{2!} + \frac{r^4}{4!} + \cdots \right) a + \left( r + \frac{r^3}{3!} + \cdots \right) a^\dagger + \cdots, \quad (5.261) \]

a) Thus

\[ T = Aa + Ba^\dagger, \quad (5.262) \]

where

\[ A = \cosh r, \quad (5.263) \]

\[ B = \sinh r. \quad (5.264) \]

b) Using the relations

\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad (5.265) \]

\[ p = i\sqrt{\frac{\hbar m \omega}{2}} (-a + a^\dagger). \quad (5.266) \]
one finds
\[ \langle r| x | r \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle 0 | S(r)(a + a^\dagger) S^\dagger(r) | 0 \rangle \]
\[ = \sqrt{\frac{\hbar}{2m\omega}} (\langle 0 | T | 0 \rangle + \langle 0 | T^\dagger | 0 \rangle) \]
\[ = 0 , \]
(5.267)

\[ \langle r| p | r \rangle = i \sqrt{\frac{\hbar \omega}{2}} \langle 0 | S(r)(-a + a^\dagger) S^\dagger(r) | 0 \rangle \]
\[ = \sqrt{\frac{\hbar}{2m\omega}} (-\langle 0 | T | 0 \rangle + \langle 0 | T^\dagger | 0 \rangle) \]
\[ = 0 . \]
(5.268)
c) Note that \( S(r) \) is unitary, namely \( S^\dagger(r) S(r) = 1 \), since the operator \( a^2 - (a^\dagger)^2 \) is anti Hermitian. Thus
\[ \langle r| x^2 | r \rangle = \frac{\hbar}{2m\omega} \langle 0 | S(r)(a + a^\dagger)(a + a^\dagger) S^\dagger(r) | 0 \rangle \]
\[ = \frac{\hbar}{2m\omega} \langle 0 | S(r)(a + a^\dagger) S^\dagger(r) S(r)(a + a^\dagger) S^\dagger(r) | 0 \rangle \]
\[ = \frac{\hbar}{2m\omega} \langle 0 | (T + T^\dagger)^2 | 0 \rangle \]
\[ = \frac{\hbar(A + B)^2}{2m\omega} \langle 0 | (a + a^\dagger)^2 | 0 \rangle \]
\[ = \frac{\hbar (\cosh r + \sinh r)^2}{2m\omega} \]
\[ = \frac{\hbar e^{2r}}{2m\omega} , \]
(5.269)
and
\[ \langle r| p^2 | r \rangle = \frac{m\hbar \omega}{2} \langle 0 | S(r)(a - a^\dagger)^2 S^\dagger(r) | 0 \rangle \]
\[ = \frac{m\hbar \omega}{2} \langle 0 | (T - T^\dagger)^2 | 0 \rangle \]
\[ = \frac{m\hbar \omega (A - B)^2}{2} \langle 0 | (a - a^\dagger)^2 | 0 \rangle \]
\[ = \frac{m\hbar \omega (\cosh r - \sinh r)^2}{2} \]
\[ = \frac{m\hbar \omega e^{-2r}}{2} . \]
(5.270)

Thus
Chapter 5. The Harmonic Oscillator

\begin{align}
(\Delta x)^2 &= \frac{\hbar^2}{2m\omega}, \\
(\Delta p)^2 &= \frac{\hbar}{2m\omega^2}, \\
(\Delta x)(\Delta p) &= \frac{\hbar}{2}.
\end{align}

29. Using the commutation relation

\[ [a, a^\dagger] = 1, \]

one finds

\[ \mathcal{H} = \hbar \omega_0 N + \hbar \omega_1 (N^2 - N), \]

where

\[ N = a^\dagger a \]

is the number operator.

a) The eigenvectors of \( N \)

\[ N |n\rangle = n |n\rangle, \]

(where \( n = 0, 1, \cdots \)) are also eigenvectors of \( \mathcal{H} \) and the following holds

\[ \mathcal{H} |n\rangle = E_n |n\rangle, \]

where

\[ E_n = \hbar [\omega_0 n + \omega_1 (n^2 - n)]. \]

Note that

\[ \frac{E_{n+1} - E_n}{\hbar} = \omega_0 + 2\omega_1 n, \]

thus \( E_{n+1} > E_n \).

b) Using the relations

\begin{align}
x &= \sqrt{\frac{\hbar}{2m\omega_0}} (a^\dagger + a), \\
p &= i \sqrt{\frac{m\hbar}{2\omega_0}} (a^\dagger - a), \\
x^2 &= \frac{\hbar}{2m\omega_0} (a^\dagger a^\dagger + aa + 2N + 1), \\
p^2 &= \frac{m\hbar\omega_0}{2} (-a^\dagger a^\dagger - aa + 2N + 1), \\
a |n\rangle &= \sqrt{n} |n - 1\rangle, \\
a^\dagger |n\rangle &= \sqrt{n + 1} |n + 1\rangle,
\end{align}

one finds
5.4. Solutions

i. $\langle 0 | x | 0 \rangle = 0$

ii. $\langle 0 | p | 0 \rangle = 0$

iii. $\langle 0 | (\Delta x)^2 | 0 \rangle = \frac{\hbar}{2m_{\text{mc}}}$

iv. $\langle 0 | (\Delta p)^2 | 0 \rangle = \frac{m_{\text{mc}} \omega^2}{2}$

30. The proof of the clue is:

$$N^2 = b^\dagger b b^\dagger b = b^\dagger (1 - b^\dagger b) b = N.$$  \hfill (5.287)

Moreover, $N$ is Hermitian, thus $N$ is a projector.

a) Let $| n \rangle$ be the eigenvectors of $N$ and $n$ the corresponding real eigenvalues ($N$ is Hermitian)

$$N | n \rangle = n | n \rangle .$$  \hfill (5.288)

Using the clue one finds that $n^2 = n$, thus the possible values of $n$ are 0 (ground state) and 1 (excited state). Thus, the eigenvalues of $\mathcal{H}$ are 0 and $\epsilon$.

b) To verify the statement in the clue we calculate

$$Nb^\dagger | 0 \rangle = b^\dagger b b^\dagger | 0 \rangle = b^\dagger (1 - N) | 0 \rangle = b^\dagger | 0 \rangle ,$$  \hfill (5.289)

thus the state $b^\dagger | 0 \rangle$ is indeed an eigenvector of $N$ with eigenvalue 1 (excited state). In what follows we use the notation

$$| 1 \rangle = b^\dagger | 0 \rangle .$$  \hfill (5.290)

Note that $| 1 \rangle$ is normalized since

$$\langle 1 | 1 \rangle = \langle 0 | b b^\dagger | 0 \rangle = \langle 0 | (1 - N) | 0 \rangle = \langle 0 | 0 \rangle = 1 .$$  \hfill (5.291)

Moreover, since $| 0 \rangle$ and $| 1 \rangle$ are eigenvectors of an Hermitian operator with different eigenvalues they must be orthogonal to each other

$$\langle 0 | 1 \rangle = 0 .$$  \hfill (5.292)

Using Eqs. (5.290), (5.291) and (5.292) one finds

$$\langle + | + \rangle = 2 | A_+ |^2 ,$$  \hfill (5.293)

$$\langle - | - \rangle = 2 | A_- |^2 .$$  \hfill (5.294)

choosing the normalization constants to be non-negative real numbers lead to

$$A_+ = A_- = \frac{1}{\sqrt{2}} .$$  \hfill (5.295)
c) Using $N^2 = N$ one finds
\[
\exp \left( -\frac{i\mathcal{H}t}{\hbar} \right) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left( -\frac{i\mathcal{H}t}{\hbar} \right)^n = 1 + N \sum_{n=1}^{\infty} \frac{1}{n!} \left( -\frac{i\epsilon t}{\hbar} \right)^n = 1 + N \left( -1 + \sum_{n=0}^{\infty} \frac{1}{n!} \left( -\frac{i\epsilon t}{\hbar} \right)^n \right) = 1 + N \left( -1 + \exp \left( -\frac{i\epsilon t}{\hbar} \right) \right).
\]

Thus
\[
p_0(t) = \left| \langle \psi \left\lfloor \right. \langle 0 | - (1) \right\rangle \left[ 1 + N \left( -1 + \exp \left( -\frac{i\epsilon t}{\hbar} \right) \right) \right] \right| (|0\rangle + |1\rangle)^2 = \frac{1}{4} \left| 1 - \exp \left( -\frac{i\epsilon t}{\hbar} \right) \right|^2 = \sin^2 \left( \frac{\epsilon t}{2\hbar} \right).
\]

(5.296)

31. The closure relation (5.31) can be written as
\[
1 = |n\rangle \langle m| \delta_{n,m}.
\]

(5.297)

With the help of Eq. (5.32) together with the relation
\[
\frac{1}{n!} \left( \frac{d}{d\varsigma} \right)^n \varsigma^m \bigg|_{\varsigma=0} = \delta_{n,m},
\]

(5.298)

which is obtained using the Taylor power expansion series of the function $\varsigma^m$, one finds that
1 = \infty \sum_{n,m=0} |n\rangle \langle m| \delta_{n,m}

= \infty \sum_{n,m=0} \frac{1}{\sqrt{n!}\sqrt{m!}} |n\rangle \langle m| \left( \frac{d}{d\zeta} \right)^n \zeta^m \big|_{\zeta = 0}

= \infty \sum_{n,m=0} \frac{(a^\dagger)^n}{n!} |0\rangle \langle 0| \frac{a^m}{m!} \left( \frac{d}{d\zeta} \right)^n \zeta^m \big|_{\zeta = 0}

= \left( \infty \sum_{n=0} \frac{(a^\dagger)^n}{n!} \left( \frac{d}{d\zeta} \right)^n \right) |0\rangle \langle 0| \left( \infty \sum_{m=0} \frac{a^m}{m!} \right) \big|_{\zeta = 0}

= \exp \left( a^\dagger \frac{d}{d\zeta} \right) |0\rangle \langle 0| \exp (a\zeta) \big|_{\zeta = 0} \cdot (5.300)

Denote the normal ordering representation of the operator |0\rangle \langle 0| by Z, i.e.

|0\rangle \langle 0| =: Z \cdot (5.301)

For general operators X and Y it is easy to show that the following holds

\langle X : Y : \rangle = \langle XY : \rangle \cdot (5.302)

Thus

1 = \exp \left( a^\dagger \frac{d}{d\zeta} \right) \cdot Z : \exp (a\zeta) \big|_{\zeta = 0}

=: \exp \left( a^\dagger \frac{d}{d\zeta} \right) Z \exp (a\zeta) \big|_{\zeta = 0} :

=: \exp (a^\dagger a) Z:

=: \exp (a^\dagger a) ( : Z : ) \cdot , (5.303)

and therefore

\langle 0\rangle \langle 0| =: \exp (-a^\dagger a) : \cdot (5.304)

Using again Eq. (5.32) one finds that

\langle n\rangle \langle n| = \frac{1}{n!} \langle a\rangle^n \exp (-a^\dagger a) (a^\dagger)^n : \cdot (5.305)

32. The Hamiltonian H, which is given by

\[ H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} + xf(t) \cdot , (5.306) \]
can be expressed in terms of the annihilation $a$ and creation $a^\dagger$ operators [see Eqs. (5.11) and (5.12)] as
\[
H = \hbar \omega \left( a^\dagger a + \frac{1}{2} \right) + f(t) \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) .
\] (5.307)

The Heisenberg equation of motion for the operator $a$ is given by [see Eq. (4.37)]
\[
\frac{da}{dt} = -i\omega a - i\sqrt{\frac{1}{2m\omega}} f(t) .
\] (5.308)

The solution of this first order differential equation is given by
\[
a(t) = e^{-i\omega(t-t_0)} a(t_0) - i\sqrt{\frac{1}{2m\omega}} \int_{t_0}^t dt' \ e^{-i\omega(t-t')} f(t') ,
\] (5.309)

where the initial time $t_0$ will be taken below to be $-\infty$. The operator $a^\dagger(t)$ is found from the Hermitian conjugate of the last result. Let $P_n(t)$ be the Heisenberg representation of the projector $|n\rangle \langle n|$. The probability $p_n(t)$ to find the oscillator in the number state $|n\rangle$ at time $t$ is given by
\[
p_n(t) = \langle 0| P_n(t) |0\rangle .
\] (5.310)

To evaluate $p_n(t)$ it is convenient to employ the normal ordering representation of the operator $P_n (5.91)$. In normal ordering the first term of Eq. (5.309), which is proportional to $a(t_0)$ does not contribute to $p_n(t)$ since $a(t_0) |0\rangle = 0$ and also $\langle 0| a^\dagger(t_0) = 0$. To evaluate $p_n = p_n (t \to \infty)$ the integral in the second term of Eq. (5.309) is evaluate from $t_0 = -\infty$ to $t = +\infty$. Thus one finds that
\[
p_n = \frac{e^{-\mu} \mu^n}{n!} ,
\] (5.311)

where
\[
\mu = \frac{1}{2m\omega} \left| \int_{-\infty}^\infty dt' \ e^{i\omega t'} f(t') \right|^2 .
\] (5.312)
6. Angular Momentum

Consider a point particle moving in three dimensional space. The \textit{orbital} angular momentum $L$ is given by

$$L = \mathbf{r} \times \mathbf{p} = \det \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{pmatrix},$$

where $\mathbf{r} = (x, y, z)$ is the position vector and where $\mathbf{p} = (p_x, p_y, p_z)$ is the momentum vector. In classical physics the following holds:

\textit{Claim.}

$$\{L_i, L_j\} = \varepsilon_{ijk} L_k,$$

where

$$\varepsilon_{ijk} = \begin{cases} 
0 & i, j, k \text{ are not all different} \\
1 & i, j, k \text{ is an even permutation of } x, y, z \\
-1 & i, j, k \text{ is an odd permutation of } x, y, z 
\end{cases}$$

\textit{Proof.} Clearly, Eq. (6.1) holds for the case $i = j$. Using Eq. (1.48), which reads

$$\{x_i, p_j\} = \delta_{ij},$$

one has

$$\{L_x, L_y\} = \{yp_z - zp_y, zp_x - xp_z\}$$
$$= \{yp_z, zp_x\} + \{zp_y, xp_z\}$$
$$= y\{p_z, z\} p_x + x\{z, p_z\} p_y$$
$$= -yp_x + xp_y$$
$$= L_z.$$ \hfill (6.4)

In a similar way one finds that $\{L_y, L_z\} = L_x$ and $\{L_z, L_x\} = L_y$. These results together with Eq. (1.49) complete the proof.

Using the rule (4.41) $\{,\} \to (1/i\hbar) [,]$ one concludes that in quantum mechanics the following holds:

$$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k.$$

(6.5)
6.1 Angular Momentum and Rotation

We have seen before that the unitary operator $u(t, t_0)$ is the generator of time evolution [see Eq. (4.4)]. Similarly, we have seen that the unitary operator

$$J(\Delta) = \exp\left(-\frac{i\Delta \cdot \mathbf{p}}{\hbar}\right)$$

[see Eq. (3.72)] is the generator of linear translations:

$$J(\Delta) |r'\rangle = |r' + \Delta\rangle.$$  

Below we will see that one can define a unitary operator that generates rotations.

**Exercise 6.1.1.** Show that

$$D^\dagger_z(\phi) \begin{pmatrix} x \\ y \\ z \end{pmatrix} D_z(\phi) = R_z \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

where

$$D_z(\phi) = \exp\left(-\frac{i\phi L_z}{\hbar}\right),$$

and where

$$R_z = \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$  

**Solution 6.1.1.** Equation (6.8) is made of 3 identities:

$$D_z(\phi) x D_z(\phi) = x \cos \phi - y \sin \phi,$$

$$D_z(\phi) y D_z(\phi) = x \sin \phi + y \cos \phi,$$

$$D_z(\phi) z D_z(\phi) = z.$$

As an example, we prove below the first one. Using the identity (2.174), which is given by

$$e^{Lz}Ae^{-Lz} = A + [L, A] + \frac{1}{2!} [L, [L, A]] + \frac{1}{3!} [L, [L, [L, A]]] + \cdots,$$

one has

$$D_z(\phi) x D_z(\phi) = x + \frac{i\phi}{\hbar} [L_z, x] + \frac{1}{2!} \left(\frac{i\phi}{\hbar}\right)^2 [L_z, [L_z, x]] + \frac{1}{3!} \left(\frac{i\phi}{\hbar}\right)^3 [L_z, [L_z, [L_z, x]]] + \cdots.$$
6.1. Angular Momentum and Rotation

Furthermore with the help of

$$L_z = xp_y - yp_x ,$$  \hspace{1cm} (6.16)

$$[x_i, p_j] = i\hbar \delta_{ij} ,$$  \hspace{1cm} (6.17)

one finds that

$$[L_z, x] = -y [p_x, x] = i\hbar y ,$$

$$[L_z, [L_z, x]] = i\hbar x [p_y, y] = - (i\hbar)^2 x ,$$

$$[L_z, [L_z, [L_z, x]]] = - (i\hbar)^2 [L_z, x] = - (i\hbar)^3 y ,$$

$$[L_z, [L_z, [L_z, [L_z, x]]]] = (i\hbar)^4 x ,$$

$$\vdots$$  \hspace{1cm} (6.18)

thus

$$\begin{aligned}
D^\dagger_\hat{z}(\phi) x D_\hat{z}(\phi) &= x \left( 1 - \frac{\phi^2}{2!} + \frac{\phi^4}{4!} + \cdots \right) - y \left( \phi - \frac{\phi^3}{3!} + \cdots \right) \\
&= x \cos \phi - y \sin \phi .
\end{aligned} \hspace{1cm} (6.19)
$$

The other 2 identities in Eq. (6.8) can be proven in a similar way.

The matrix $R_\hat{z}$ [see Eq. (6.10)] represents a geometrical rotation around the $z$ axis with angle $\phi$. Therefore, in view of the above result, we refer to the operator $D_\hat{z}(\phi)$ as the generator of rotation around the $z$ axis with angle $\phi$. It is straightforward to generalize the above results and to show that rotation around an arbitrary unit vector $\hat{n}$ axis with angle $\phi$ is given by

$$D_\hat{n}(\phi) = \exp \left( -i\frac{\phi \mathbf{L} \cdot \hat{n}}{\hbar} \right) . \hspace{1cm} (6.20)$$

In view of Eq. (3.72), it can be said that linear momentum $\mathbf{p}$ generates translations. Similarly, in view of the above equation (6.20), angular momentum $\mathbf{L}$ generates rotation. However, there is an important distinction between these two types of geometrical transformations. On one hand, according to Eq. (3.7) the observables $p_x, p_y$ and $p_z$ commute with each other, and consequently translation operators with different translation vectors commute

$$[J(\Delta_1), J(\Delta_2)] = 0 . \hspace{1cm} (6.21)$$

On the other hand, as can be seen from Eq. (6.5), different components of $\mathbf{L}$ do not commute and therefore rotation operators $D_\hat{n}(\phi)$ with different rotations axes $\hat{n}$ need not commute. Both the above results, which were obtained from commutation relations between quantum operators, demonstrate two well known geometrical facts: (i) different linear translations commute, whereas (ii) generally, different rotations do not commute.
6.2 General Angular Momentum

Elementary particles carry angular momentum in two different forms. The first one is the above discussed orbital angular momentum, which is commonly labeled as $L$. This contribution $L = r \times p$ has a classical analogue, which was employed above to derive the commutation relations (6.5) from the corresponding Poisson’s brackets relations. The other form of angular momentum is spin, which is commonly labeled as $S$. Contrary to the orbital angular momentum, the spin does not have any classical analogue. In a general discussion on angular momentum in quantum mechanics the label $J$ is commonly employed.

$L$ - orbital angular momentum
$S$ - spin angular momentum
$J$ - general angular momentum

In the discussion below we derive some properties of angular momentum in quantum mechanics, where our only assumption is that the components of the angular momentum vector of operators $J = (J_x, J_y, J_z)$ obey the following commutation relations

$$[J_i, J_j] = i\hbar\varepsilon_{ijk}J_k.$$  \hspace{1cm} (6.22)

Namely, we assume that Eq. (6.5), which was obtained from the corresponding Poisson’s brackets relations for the case of orbital angular momentum holds for general angular momentum.

6.3 Simultaneous Diagonalization of $J^2$ and $J_z$

As we have seen in chapter 2, commuting operators can be simultaneously diagonalized. In this section we seek such simultaneous diagonalization of the operators $J^2$ and $J_z$, where

$$J^2 = J_x^2 + J_y^2 + J_z^2.$$  \hspace{1cm} (6.23)

As is shown by the claim below, these operators commute.

Claim. The following holds

$$[J^2, J_x] = [J^2, J_y] = [J^2, J_z] = 0.$$  \hspace{1cm} (6.24)

Proof. Using Eq. (6.22) one finds that

$$[J^2, J_z] = [J_x^2, J_z] + [J_y^2, J_z]$$

$$= i\hbar(-J_xJ_y - J_yJ_x + J_yJ_x + J_xJ_y) = 0.$$  \hspace{1cm} (6.24)

In a similar way one can show that $[J^2, J_x] = [J^2, J_y] = 0.$
6.3. Simultaneous Diagonalization of $J^2$ and $J_z$

The common eigenvectors of the operators $J^2$ and $J_z$ are labeled as $|a, b\rangle$, and the corresponding eigenvalues are labeled as $a\hbar^2$ and $b\hbar$ respectively.

\[
J^2 |a, b\rangle = a\hbar^2 |a, b\rangle, \quad (6.25)
\]
\[
J_z |a, b\rangle = b\hbar |a, b\rangle. \quad (6.26)
\]

Recall that we have shown in chapter 5 for the case of harmonic oscillator that the ket-vectors $|n\rangle$ and $a^\dagger |n\rangle$ are eigenvectors of the number operator $N$ provided that $|n\rangle$ is an eigenvector of $N$. Somewhat similar claim can be made regarding the current problem under consideration of simultaneous diagonalization of $J^2$ and $J_z$:

**Theorem 6.3.1.** Let $|a, b\rangle$ be a normalized simultaneous eigenvector of the operators $J^2$ and $J_z$ with eigenvalues $a\hbar^2$ and $b\hbar$ respectively, i.e.

\[
J^2 |a, b\rangle = a\hbar^2 |a, b\rangle, \quad (6.27)
\]
\[
J_z |a, b\rangle = b\hbar |a, b\rangle, \quad (6.28)
\]
\[
\langle a, b | a, b \rangle = 1. \quad (6.29)
\]

Then (i) the vector

\[
|a, b + 1\rangle \equiv \hbar^{-1} [a - b (b + 1)]^{-1/2} J^+_|a, b\rangle \quad (6.30)
\]

where

\[
J^+_ = J_x + iJ_y, \quad (6.31)
\]

is a normalized simultaneous eigenvector of the operators $J^2$ and $J_z$ with eigenvalues $a\hbar^2$ and $b (b + 1)$ respectively, namely

\[
J^2 |a, b + 1\rangle = a\hbar^2 |a, b + 1\rangle, \quad (6.32)
\]
\[
J_z |a, b + 1\rangle = (b + 1) b |a, b + 1\rangle. \quad (6.33)
\]

(ii) The vector

\[
|a, b - 1\rangle \equiv \hbar^{-1} [a - b (b - 1)]^{-1/2} J^-|a, b\rangle \quad (6.34)
\]

where

\[
J^- = J_x - iJ_y, \quad (6.35)
\]

is a normalized simultaneous eigenvector of the operators $J^2$ and $J_z$ with eigenvalues $a\hbar^2$ and $b (b - 1)$ respectively, namely

\[
J^2 |a, b - 1\rangle = a\hbar^2 |a, b - 1\rangle, \quad (6.36)
\]
\[
J_z |a, b - 1\rangle = (b - 1) b |a, b - 1\rangle. \quad (6.37)
\]
Proof. The following holds

\[ \mathbf{J}^2 (\mathbf{J}_\pm |a, b\rangle) = \left( \mathbf{J}_x^2 + \mathbf{J}_y^2 \right) |a, b\rangle = ah^2 (\mathbf{J}_\pm |a, b\rangle) . \]  

(6.38)

Similarly

\[ J_z (\mathbf{J}_\pm |a, b\rangle) = ([J_z, \mathbf{J}_\pm] + \mathbf{J}_\pm J_z) |a, b\rangle , \]

where

\[ [J_z, \mathbf{J}_\pm] = [J_z, J_x \pm iJ_y] = h (iJ_y \pm J_x) = \pm h J_\pm , \]

thus

\[ J_z (\mathbf{J}_\pm |a, b\rangle) = (b \pm 1) h (\mathbf{J}_\pm |a, b\rangle) . \]  

(6.39)

Using the following relations

\[ J_+ J_- = J_+ J_- \\
= (J_x + iJ_y) (J_x - iJ_y) \\
= J_x^2 + J_y^2 + i [J_x, J_y] \\
= \mathbf{J}^2 - J_z^2 - h J_z , \]

(6.40)

one finds that

\[ \langle a, b | J_+ J_+ |a, b\rangle = \langle a, b | \mathbf{J}^2 |a, b\rangle - \langle a, b | J_z (J_z + h) |a, b\rangle \\
= h^2 [a - b (b + 1)] , \]

(6.41)

and

\[ \langle a, b | J_+ J_- |a, b\rangle = \langle a, b | \mathbf{J}^2 |a, b\rangle - \langle a, b | J_z (J_z - h) |a, b\rangle \\
= h^2 [a - b (b - 1)] . \]

(6.42)

Thus the states \(|a, b + 1\rangle\) and \(|a, b - 1\rangle\) are both normalized.
What are the possible values of $b$? Recall that we have shown in chapter 5 for the case of harmonic oscillator that the eigenvalues of the number operator $N$ must be nonnegative since the operator $N$ is positive-definite. Below we employ a similar approach to show that:

**Claim.** $b^2 \leq a$

**Proof.** Both $J_x^2$ and $J_y^2$ are positive-definite, therefore

$$\langle j, b | J_x^2 + J_y^2 | j, b \rangle \geq 0. \quad (6.46)$$

On the other hand, $J_x^2 + J_y^2 = J^2 - J_z^2$, therefore $a - b^2 \geq 0$.

As we did in chapter 5 for the case of the possible eigenvalues $n$ of the number operator $N$, also in the present case the requirement $b^2 \leq a$ restricts the possible values that $b$ can take:

**Claim.** For a given value of $a$ the possible values of $b$ are \{-$b_{\text{max}}$, -$b_{\text{max}} + 1$, $\cdots$, $b_{\text{max}} - 1$, $b_{\text{max}}$\} where $a = b_{\text{max}} (b_{\text{max}} + 1)$. Moreover, the possible values of $b_{\text{max}}$ are $0$, $1/2$, $1$, $3/2$, $2$, $\cdots$.

**Proof.** There must be a maximum value $b_{\text{max}}$ for which

$$J_+ |a, b_{\text{max}}\rangle = 0. \quad (6.47)$$

Thus, also

$$J_+^\dagger J_+ |a, b_{\text{max}}\rangle = 0 \quad (6.48)$$

holds. With the help of Eq. (6.42) this can be written as

$$\left(J^2 - J_z^2 - b J_z\right) |a, b_{\text{max}}\rangle = [a - b_{\text{max}} (b_{\text{max}} + 1)] \hbar^2 |a, b_{\text{max}}\rangle = 0. \quad (6.49)$$

Since $|a, b_{\text{max}}\rangle \neq 0$ one has

$$a - b_{\text{max}} (b_{\text{max}} + 1) = 0, \quad (6.50)$$

or

$$a = b_{\text{max}} (b_{\text{max}} + 1). \quad (6.51)$$

In a similar way with the help of Eq. (6.43) one can show that there exists a minimum value $b_{\text{min}}$ for which

$$a = b_{\text{min}} (b_{\text{min}} - 1). \quad (6.52)$$

From the last two equations one finds that

$$b_{\text{max}} (b_{\text{max}} + 1) = b_{\text{min}} (b_{\text{min}} - 1), \quad (6.53)$$

or
Thus, since $b_{\text{max}} - b_{\text{min}} + 1 > 0$ one finds that
\begin{equation}
\label{eq:6.55}
b_{\text{min}} = -b_{\text{max}}.
\end{equation}

The formal solutions of Eqs. (6.51) and (6.52) are given by
\begin{equation}
\label{eq:6.56}
b_{\text{max}} = -\frac{1}{2} \pm \frac{1}{2} \sqrt{1 + 4a},
\end{equation}
and
\begin{equation}
\label{eq:6.57}
b_{\text{min}} = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 + 4a}.
\end{equation}

Furthermore, $a$ is an eigenvalue of a positive-definite operator $J^2$, therefore $a \geq 0$. Consequently, the only possible solutions for which $b_{\text{max}} \geq b_{\text{min}}$ are
\begin{equation}
\label{eq:6.58}
b_{\text{max}} = -\frac{1}{2} + \frac{1}{2} \sqrt{1 + 4a} \geq 0,
\end{equation}
and
\begin{equation}
\label{eq:6.59}
b_{\text{min}} = \frac{1}{2} - \frac{1}{2} \sqrt{1 + 4a} = -b_{\text{max}} \leq 0.
\end{equation}

That is, for a given value of $a$, both $b_{\text{max}}$ and $b_{\text{min}}$ are uniquely determined. The value $b_{\text{min}}$ is obtained by successively applying the operator $J_-$ to the state $|a, b_{\text{max}}\rangle$ an integer number of times, and therefore $b_{\text{max}} - b_{\text{min}} = 2b_{\text{max}}$ must be an integer. Consequently, the possible values of $b_{\text{max}}$ are $0, 1/2, 1, 3/2, \cdots$.

We now change the notation $|a, b\rangle$ for the simultaneous eigenvectors to the more common notation $|j, m\rangle$, where
\begin{equation}
\label{eq:6.60}
j = b_{\text{max}},
\end{equation}
\begin{equation}
\label{eq:6.61}
m = b.
\end{equation}

Our results can be summarized by the following relations
\begin{equation}
\label{eq:6.62}
J^2 |j, m\rangle = j (j + 1) \hbar^2 |j, m\rangle,
\end{equation}
\begin{equation}
\label{eq:6.63}
J_z |j, m\rangle = m \hbar |j, m\rangle,
\end{equation}
\begin{equation}
\label{eq:6.64}
J_+ |j, m\rangle = \sqrt{j (j + 1) - m (m + 1)} \hbar |j, m + 1\rangle,
\end{equation}
\begin{equation}
\label{eq:6.65}
J_- |j, m\rangle = \sqrt{j (j + 1) - m (m - 1)} \hbar |j, m - 1\rangle,
\end{equation}
where the possible values $j$ can take are
\begin{equation}
\label{eq:6.66}
j = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots,
\end{equation}
and for each given $j$, the quantum number $m$ can take any of the $2j + 1$ possible values
\begin{equation}
\label{eq:6.67}
m = -j, -j + 1, \cdots, j - 1, j.
\end{equation}
6.4 Example - Spin 1/2

The vector space of a spin 1/2 system is the subspace spanned by the ket-vectors $|\frac{1}{2}, \frac{-1}{2}\rangle$ and $|\frac{1}{2}, \frac{1}{2}\rangle$. In this subspace the spin angular momentum is labeled using the letter $S$, as we have discussed above. The matrix representation of some operators of interest in this basis can be easily found with the help of Eqs. (6.62), (6.63), (6.64) and (6.65):

\[
S^2 = \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},
\]

\[
S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \equiv \frac{\hbar}{2} \sigma_z,
\]

\[
S_+ = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},
\]

\[
S_- = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ i & 0 \end{pmatrix}.
\]

The above results for $S_+$ and $S_-$ together with the identities

\[
S_x = \frac{S_+ + S_-}{2},
\]

\[
S_y = \frac{S_+ - S_-}{2i},
\]

can be used to find the matrix representation of $S_x$ and $S_y$

\[
S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv \frac{\hbar}{2} \sigma_x,
\]

\[
S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv \frac{\hbar}{2} \sigma_y.
\]

The matrices $\sigma_x$, $\sigma_y$, and $\sigma_z$ are called Pauli’s matrices, and are related to the corresponding spin angular momentum operators by the relation

\[
S_k = \frac{\hbar}{2} \sigma_k.
\]

6.5 Orbital Angular Momentum

As we have discussed above, orbital angular momentum $L = r \times p$ refers to spatial motion. For this case the states $|l, m\rangle$ (here, the letter $l$ is used instead of $j$ since we are dealing with orbital angular momentum) can be described using wave functions. In this section we calculate these wave functions. For this purpose it is convenient to employ the transformation from Cartesian to spherical coordinates.
\[
\begin{align*}
  x &= r \sin \theta \cos \phi, \\
  y &= r \sin \theta \sin \phi, \\
  x &= r \cos \theta,
\end{align*}
\]

where
\[
\begin{align*}
  r &\geq 0, \\
  0 &\leq \theta \leq \pi, \\
  0 &\leq \phi \leq 2\pi.
\end{align*}
\]

**Exercise 6.5.1.** Show that:

1. 
\[
\langle \mathbf{r}' | L_z | \alpha \rangle = -i\hbar \frac{\partial}{\partial \phi} \langle \mathbf{r}' | \alpha \rangle.
\]

2. 
\[
\langle \mathbf{r}' | L_\pm | \alpha \rangle = -i\hbar \exp(\pm i\phi) \left( \pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \mathbf{r}' | \alpha \rangle.
\]

3. 
\[
\langle \mathbf{r}' | L^2 | \alpha \rangle = -\hbar^2 \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right] \langle \mathbf{r}' | \alpha \rangle.
\]

**Solution 6.5.1.** Using the relations
\[
\mathbf{L} = \mathbf{r} \times \mathbf{p} = \text{det} \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{pmatrix},
\]

\[
\langle \mathbf{r}' | \mathbf{r} | \alpha \rangle = \delta_{\mathbf{r} \mathbf{r}'} | \alpha \rangle,
\]

\[
\langle \mathbf{r}' | \mathbf{p} | \alpha \rangle = \frac{\hbar}{i} \nabla \langle \mathbf{r}' | \alpha \rangle,
\]

[see Eqs. (3.21) and (3.29)] one finds that
\[
\langle \mathbf{r}' | L_x | \alpha \rangle = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \psi_\alpha (\mathbf{r}'),
\]

\[
\langle \mathbf{r}' | L_y | \alpha \rangle = \frac{\hbar}{i} \left( \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \psi_\alpha (\mathbf{r}'),
\]

\[
\langle \mathbf{r}' | L_z | \alpha \rangle = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \psi_\alpha (\mathbf{r}'),
\]

where
\[
\psi_\alpha (\mathbf{r}') = \langle \mathbf{r}' | \alpha \rangle.
\]
The inverse transformation is given by
\[ r = \sqrt{x^2 + y^2 + z^2}, \quad (6.93) \]
\[ \cos \theta = \frac{z}{\sqrt{x^2 + y^2 + z^2}}, \quad (6.94) \]
\[ \cot \phi = \frac{x}{y}. \quad (6.95) \]

1. The following holds
\[ \frac{\partial}{\partial \phi} = \frac{\partial x}{\partial \phi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \phi} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \phi} \frac{\partial}{\partial z} \]
\[ = -r \sin \theta \sin \phi \frac{\partial}{\partial x} + r \sin \theta \cos \phi \frac{\partial}{\partial y} \]
\[ = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}, \quad (6.96) \]

thus using Eq. (6.91) one has
\[ (r'|L_z|\alpha) = -i\hbar \frac{\partial}{\partial \phi} \psi_\alpha (r'). \quad (6.97) \]

2. Using Eqs. (6.89) and (6.90) together with the relation \( L_+ = L_x + iL_y \) one has
\[ \frac{i}{\hbar} \langle r'|L_+|\alpha \rangle = \frac{i}{\hbar} \langle r'|L_x + iL_y|\alpha \rangle \]
\[ = \left( y \frac{\partial}{\partial z} - \frac{z}{\partial y} \frac{\partial}{\partial x} + iz \frac{\partial}{\partial x} - ix \frac{\partial}{\partial z} \right) \psi_\alpha (r') \]
\[ = \left[ z \left( i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) - i (x + iy) \frac{\partial}{\partial z} \right] \psi_\alpha (r') \]
\[ = \left[ z \left( i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) - ir \sin \theta e^{i\phi} \frac{\partial}{\partial z} \right] \psi_\alpha (r'). \quad (6.98) \]

Thus, by using the identity
\[ \frac{\partial}{\partial \theta} = \frac{\partial x}{\partial \theta} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \theta} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \theta} \frac{\partial}{\partial z} \]
\[ = r \cos \theta \left( \cos \phi \frac{\partial}{\partial x} + \sin \phi \frac{\partial}{\partial y} \right) - r \sin \theta \frac{\partial}{\partial z}, \quad (6.99) \]

or
\[ r \sin \theta \frac{\partial}{\partial z} = r \cos \theta \left( \cos \phi \frac{\partial}{\partial x} + \sin \phi \frac{\partial}{\partial y} \right) - \frac{\partial}{\partial \theta}, \quad (6.100) \]
one finds that
\[ \frac{i}{\hbar} \langle r' | L_+ | \alpha \rangle = \left[ z \left( i \frac{\partial}{\partial x} - \frac{\partial}{\partial y} \right) - i e^{i\phi} \left( \cot \theta \left( x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} \right) - \frac{\partial}{\partial \theta} \right) \right] \psi_\alpha (r') \]
\[ = i \left( z - e^{i\phi} x \cot \theta \right) \frac{\partial}{\partial x} - \left( z + ie^{i\phi} y \cot \theta \right) \frac{\partial}{\partial y} + i e^{i\phi} \frac{\partial}{\partial \theta} \psi_\alpha (r') \]
\[ = e^{i\phi} \left[ i \cot \theta \left( \frac{e^{-i\phi} \tan \theta - x}{x - iy} \right) \frac{\partial}{\partial x} - \cot \theta \left( \frac{e^{-i\phi} \tan \theta + iy}{x - iy} \right) \frac{\partial}{\partial y} + i \frac{\partial}{\partial \theta} \right] \psi_\alpha (r') \]
\[ = e^{i\phi} \left( i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \psi_\alpha (r') . \]

(6.101)

In a similar way one evaluates \( \langle r' | L_\mp | \alpha \rangle \). Both results can be expressed as
\[ \langle r' | L_\pm | \alpha \rangle = -i \hbar \exp (\pm i\phi) \left( \pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \psi_\alpha (r') . \]

(6.102)

3. Using the result of the previous section one has
\[ \langle r' | L_x | \alpha \rangle = \frac{1}{2} \langle r' | (L_+ + L_-) | \alpha \rangle \]
\[ = \frac{i\hbar}{2} \left[ e^{i\phi} \left( \cot \theta \frac{\partial}{\partial \phi} - i \frac{\partial}{\partial \theta} \right) + e^{-i\phi} \left( \cot \theta \frac{\partial}{\partial \phi} + i \frac{\partial}{\partial \theta} \right) \right] \psi_\alpha (r') \]
\[ = i\hbar \left( \cos \phi \cot \theta \frac{\partial}{\partial \phi} + \sin \phi \frac{\partial}{\partial \theta} \right) \psi_\alpha (r') . \]

(6.103)

Similarly
\[ \langle r' | L_y | \alpha \rangle = i\hbar \left( \sin \phi \cot \theta \frac{\partial}{\partial \phi} - \cos \phi \frac{\partial}{\partial \theta} \right) \psi_\alpha (r') , \]

(6.104)

thus
\[ \langle r' | L_z^2 | \alpha \rangle = \langle r' | L_x^2 + L_y^2 + L_z^2 | \alpha \rangle \]
\[ = -\hbar^2 \left[ \left\{ \cos \phi \cot \theta \frac{\partial}{\partial \phi} + \sin \phi \frac{\partial}{\partial \theta} \right\}^2 + \left\{ \sin \phi \cot \theta \frac{\partial}{\partial \phi} - \cos \phi \frac{\partial}{\partial \theta} \right\}^2 + \left( \frac{\partial}{\partial \phi} \right)^2 \right] \psi_\alpha (r') \]
\[ = -\hbar^2 \left[ \left( 1 + \cot^2 \theta \right) \frac{\partial^2}{\partial \phi^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{\partial^2}{\partial \theta^2} \right] \psi_\alpha (r') \]
\[ = -\hbar^2 \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right] \psi_\alpha (r') . \]

(6.105)
Spherical Harmonics. The above exercise allows translating the relations (6.62) and (6.63), which are given by
\[
\begin{align*}
L^2 |l, m\rangle &= l (l + 1) \hbar^2 |l, m\rangle, \\
L_z |l, m\rangle &= m \hbar |l, m\rangle,
\end{align*}
\]
into differential equations for the corresponding wavefunctions
\[
- \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right] \psi_{\alpha} (\mathbf{r}') = l (l + 1) \psi_{\alpha} (\mathbf{r}') ,
\]
(6.108)
\[
- \frac{\partial}{\partial \phi} \psi_{\alpha} (\mathbf{r}') = m \psi_{\alpha} (\mathbf{r}') ,
\]
(6.109)

where \( m = -l, -l + 1, \ldots, l - 1, l \).

We seek solutions having the form
\[
\psi_{\alpha} (\mathbf{r}') = f (r) Y_{l m} (\theta, \phi) .
\]
(6.111)

We require that both \( f (r) \) and \( Y_{l m} (\theta, \phi) \) are normalized
\[
1 = \int_{0}^{\infty} dr r^2 |f (r)|^2 ,
\]
(6.112)
\[
1 = \int_{0}^{\pi} d\theta \sin \theta \int_{0}^{2\pi} d\phi |Y_{l m} (\theta, \phi)|^2 .
\]
(6.113)

These normalization requirements guarantee that the total wavefunction is normalized
\[
1 = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz |\psi_{\alpha} (\mathbf{r}')|^2 .
\]
(6.114)

Substituting into Eqs. (6.108) and (6.109) yields
\[
- \left[ \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) \right] Y_{l m} = l (l + 1) Y_{l m} ,
\]
(6.115)
\[
- \frac{\partial}{\partial \phi} Y_{l m} = m Y_{l m} .
\]
(6.116)

The functions \( Y_{l m} (\theta, \phi) \) are called spherical harmonics.

In the previous section, which discusses the case of general angular momentum, we have seen that the quantum number \( m \) can take any half integer value \( 0, 1/2, 1, 3/2, \ldots \) [see Eq. (6.66)]. Recall that the only assumption employed in order to obtain this result was the commutation relations (6.22).
However, as is shown by the claim below, only integer values are allowed for the case of orbital angular momentum. In view of this result, one may argue that the existence of spin, which corresponds to half integer values, is in fact predicted by the commutation relations (6.22) only.

Claim. The variable $m$ must be an integer.

Proof. Consider a solution having the form

$$Y_l^m (\theta, \phi) = F_l^m (\theta) e^{im\phi}.$$  \hfill (6.117)

Clearly, Eq. (6.116) is satisfied. The requirement

$$Y_l^m (\theta, \phi) = Y_l^m (\theta, \phi + 2\pi),$$  \hfill (6.118)

namely, the requirement that $Y_l^m (\theta, \phi)$ is continuous, leads to

$$e^{2\pi im} = 1,$$  \hfill (6.119)

thus $m$ must be an integer.

The spherical harmonics $Y_l^m (\theta, \phi)$ can be obtained by solving Eqs. (6.115) and (6.116). However, we will employ an alternative approach, in which in the first step we find the spherical harmonics $Y_l^l (\theta, \phi)$ by solving the equation

$$L_+ |l, l\rangle = 0,$$  \hfill (6.120)

which is of first order [contrary to Eq. (6.115), which is of the second order]. Using the identity (6.84), which is given by

$$\langle \alpha' | L_+ | \alpha \rangle = -i h e^{i\phi} \left( i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \alpha' | \alpha \rangle,$$  \hfill (6.121)

one has

$$\left( \frac{\partial}{\partial \theta} - l \cot \theta \right) F_l^l (\theta) = 0.$$  \hfill (6.122)

The solution is given by

$$F_l^l (\theta) = C_l (\sin \theta)^l,$$  \hfill (6.123)

where $C_l$ is a normalization constant. Thus, $Y_l^l$ is given by

$$Y_l^l (\theta, \phi) = C_l (\sin \theta)^l e^{i\phi}.$$  \hfill (6.124)

In the second step we employ the identity (6.65), which is given by

$$J_- |j, m\rangle = \sqrt{j (j + 1) - m (m - 1)h} |j, m - 1\rangle,$$  \hfill (6.125)
and Eq. (6.84), which is given by

$$\langle \kappa' | L_\pm | \alpha \rangle = -i\hbar \exp (\pm i\phi) \left( \pm i \frac{\partial}{\partial \theta} - \cot \theta \frac{\partial}{\partial \phi} \right) \langle \kappa' | \alpha \rangle ,$$

(6.126)

to derive the following recursive relation

$$e^{-i\phi} \left( - \frac{\partial}{\partial \theta} - m \cot \theta \right) Y^m_l (\theta, \phi) = \sqrt{l(l+1) - m(m-1)} Y^{m-1}_l (\theta, \phi) ,$$

(6.127)

which allows finding $Y^m_l (\theta, \phi)$ for all possible values of $m$ provided that $Y^l_l (\theta, \phi)$ is given. The normalized spherical harmonics are found using this method to be given by

$$Y^m_l (\theta, \phi) = \frac{(-1)^l}{2^l l!} \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}} e^{im\phi} (\sin \theta)^{-m} \frac{d^{l-m}}{d(\cos \theta)^{l-m}} (\sin \theta)^2 .$$

(6.128)

As an example, closed form expressions for the cases $l = 0$ and $l = 1$ are given below

$$Y^0_0 (\theta, \phi) = \frac{1}{\sqrt{4\pi}} ,$$

(6.129)

$$Y^\pm_1 (\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi} ,$$

(6.130)

$$Y^0_1 (\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta .$$

(6.131)

### 6.6 Problems

1. Let $R_i$ (where $i \in \{x, y, z\}$ ) be the 3×3 rotation matrices (as defined in the lecture). Show that for infinitesimal angle $\phi$ the following holds

$$[R_x (\phi) , R_y (\phi)] = 1 - R_z (\phi^2) ,$$

(6.132)

where

$$[R_x (\phi) , R_y (\phi)] = R_z (\phi) R_y (\phi) - R_y (\phi) R_z (\phi) .$$

(6.133)

2. Show that

$$\exp \left( \frac{iJ_z \phi}{\hbar} \right) J_x \exp \left( - \frac{iJ_z \phi}{\hbar} \right) = J_x \cos \phi - J_y \sin \phi .$$

(6.134)
3. The components of the Pauli matrix vector $\sigma$ are given by:

$$
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

(6.135)

a) Show that

$$(\sigma \cdot a)(\sigma \cdot b) = a \cdot b + i\sigma \cdot (a \times b),$$

where $a$ and $b$ are vector operators which commute with $\sigma$, but not necessarily commute with each other.

b) Show that

$$\exp\left(\frac{-i\sigma \cdot \hat{n} \phi}{2}\right) = \mathbf{1} \cos \frac{\phi}{2} - i\sigma \cdot \hat{n} \sin \frac{\phi}{2},$$

(6.137)

where $\hat{n}$ is a unit vector and where $\mathbf{1}$ is the $2 \times 2$ identity matrix.

4. Find the eigenvectors and eigenvalues of the matrix $\sigma \cdot \hat{n}$ ($\hat{n}$ is a unit vector).

5. Consider an electron in a state in which the component of its spin along the $z$ axis is $+\hbar/2$. What is the probability that the component of the spin along an axis $z'$, which makes an angle $\theta$ with the $z$ axis, will be measured to be $+\hbar/2$ or $-\hbar/2$? What is the average value of the component of the spin along this axis?

6. The $2 \times 2$ matrix $U$ is given by

$$U = \frac{1 + i\alpha (\sigma \cdot \hat{n})}{1 - i\alpha (\sigma \cdot \hat{n})},$$

(6.138)

where

$$\sigma = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}$$

(6.139)

is the Pauli vector matrix,

$$\hat{n} = n_x \hat{x} + n_y \hat{y} + n_z \hat{z}$$

(6.140)

is a unit vector, i.e. $\hat{n} \cdot \hat{n} = 1$, and $n_x, n_y, n_z$ and $\alpha$ are all real parameters. Note that generally for a matrix or an operator $\frac{1}{A} \equiv A^{-1}$.

a) show that $U$ is unitary.

b) Show that

$$\frac{dU}{dr} = \frac{2i (\sigma \cdot \hat{n})}{1 + \alpha^2} U.$$

(6.141)

c) Calculate $U$ by solving the differential equation in the previous section.
6.6. Problems

7. A particle is located in a box, which is divided into a left and right sections. The corresponding vector states are denoted as $|L\rangle$ and $|R\rangle$ respectively. The Hamiltonian of the system is given by

$$\mathcal{H} = E_L |L\rangle \langle L| + E_R |R\rangle \langle R| + \Delta (|L\rangle \langle R| + |R\rangle \langle L|).$$  \hfill (6.142)

The particle at time $t = 0$ is in the left section

$$|\psi (t = 0)\rangle = |L\rangle.$$  \hfill (6.143)

Calculate the probability $p_R (t)$ to find the particle in the state $|R\rangle$ at time $t$.

8. A magnetic field given by

$$\mathbf{B} (t) = B_0 \hat{z} + B_1 (\hat{x} \cos (\omega_1 t) + \hat{y} \sin (\omega_1 t))$$  \hfill (6.144)

is applied to a spin 1/2 particle. At time $t = 0$ the state is given by

$$|\alpha\rangle (t = 0) = |\uparrow; \hat{z}\rangle.$$  \hfill (6.145)

Calculate the probability $P_{\uparrow\downarrow} (t)$ to find the system in the state $|\downarrow; \hat{z}\rangle$ at time $t > 0$.

9. Find the time evolution of the state vector of a spin 1/2 particle in a magnetic field along the $z$ direction with time dependent magnitude $\mathbf{B} (t) = B (t) \hat{z}$. A magnetic field given by $\mathbf{B} = B \cos (\omega t) \hat{z}$, where $B$ is a constant, is applied to a spin 1/2. At time $t = 0$ the spin is in state $|\psi (t)\rangle$, which satisfies

$$S_x |\psi (t = 0)\rangle = \hbar \frac{1}{2} |\psi (t = 0)\rangle,$$  \hfill (6.146)

Calculate the expectation value $\langle S_z \rangle$ at time $t \geq 0$.

10. Consider a spin 1/2 particle. The time dependent Hamiltonian is given by

$$\mathcal{H} = -\frac{4\omega S_z}{1 + (\omega t)^2},$$  \hfill (6.147)

where $\omega$ is a real non-negative constant and $S_z$ is the z component of the angular momentum operator. Calculate the time evolution operator $u$ of the system.

11. A magnetic field given by $\mathbf{B} = B \cos (\omega t) \hat{z}$, where $B$ is a constant, is applied to a spin 1/2. At time $t = 0$ the spin is in state $|\psi (t)\rangle$, which satisfies

$$S_x |\psi (t = 0)\rangle = \hbar \frac{1}{2} |\psi (t = 0)\rangle,$$  \hfill (6.146)

Calculate the expectation value $\langle S_z \rangle$ at time $t \geq 0$.

12. Consider a spin 1/2 particle in an eigenstate of the operator $\mathbf{S} \cdot \hat{n}$ with eigenvalue $+\hbar/2$, where $\mathbf{S}$ is the vector operator of angular momentum and where $\hat{n}$ is a unit vector. The angle between the unit vector $\hat{n}$ and the $z$ axis is $\theta$. Calculate the expectation values

a) $\langle S_z \rangle$
13. An ensemble of spin 1/2 particles are in a normalized state
\[ |\psi\rangle = \alpha |+\rangle + \beta |-\rangle, \]
where the states |+\rangle and |--\rangle are the eigenstates of \( S_z \) (the z component of the angular momentum operator). At what direction the magnetic field should be aligned in a Stern-Gerlach experiment in order for the beam not to split.

14. Consider a spin 1/2 particle having gyromagnetic ratio \( \gamma \) in a magnetic field given by \( B(t) \hat{u} \). The unit vector is given by
\[
\hat{u} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta),
\]
where \( \theta, \varphi \) are angles in spherical coordinates. The field intensity is given by
\[
B(t) = \begin{cases} 
0 & t < 0 \\
B_0 & 0 < t < \tau \\
0 & t > \tau 
\end{cases}.
\]
At times \( t < 0 \) the spin was in state |+\rangle, namely in eigenstate of \( S_z \) with positive eigenvalue. Calculate the probability \( P_{-}(t) \) to find the spin in state |−\rangle at time \( t \), where \( t > \tau \).

15. Consider a spin 1/2 particle. The Hamiltonian is given by
\[
\mathcal{H} = \omega S_x,
\]
where \( \omega \) is a Larmor frequency and where \( S_x \) is the x component of the angular momentum operator. The z component of the angular momentum is measured at the times \( t_n = nT/N \) where \( n = 0, 1, 2, \cdots, N \), \( N \) is integer and \( T \) is the time of the last measurement.

a) Find the matrix representation of the time evolution operator \( u(t) \) in the basis of \( \{|\pm\rangle \} \) states.

b) What is the probability \( p_{\text{same}} \) to get the same result in all \( N + 1 \) measurements. Note that the initial state of the particle is unknown.

c) For a fixed \( T \) calculate the limit \( \lim_{N \to \infty} p_{\text{same}} \).

16. Consider a spin 1/2 particle. No external magnetic field is applied. Three measurements are done one after the other. In the first one the z component of the angular momentum is measured, in the second one the component along the direction \( \hat{u} \) is measured and in the third measurement, again the z component is measured. The unit vector \( \hat{u} \) is described using the angles \( \theta \) and \( \varphi \)
\[
\hat{u} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta).
\]
Calculate the probability \( p_{\text{same}} \) to have the same result in the 1st and 3rd measurements.
17. Let \( \langle \mu \rangle(t) \) be the expectation value of the magnetic moment associated with spin 1/2 particle \( \mu = \gamma S \), where \( S \) is the angular momentum and \( \gamma \) is the gyromagnetic ratio. Show that in the presence of a time varying magnetic field \( B(t) \) the following holds
\[
\frac{d}{dt} \langle \mu \rangle (t) = \gamma \langle \mu \rangle (t) \times B(t) .
\] (6.152)

18. The Hamiltonian of an electron of mass \( m \), charge \( q \), spin 1/2, placed in electromagnetic field described by the vector potential \( A(r,t) \) and the scalar potential \( \varphi(r,t) \), can be written as [see Eq. (1.62)]
\[
H = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 + q\varphi - \frac{q\hbar}{2mc} \mathbf{\sigma} \cdot \mathbf{B} ,
\] (6.153)
where \( \mathbf{B} = \nabla \times \mathbf{A} \). Show that this Hamiltonian can also be written as
\[
H = \frac{1}{2m} \left[ \mathbf{\sigma} \cdot \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right) \right]^2 + q\varphi .
\] (6.154)

19. Show that
\[
\langle j, m \rangle \left[ (\Delta J_x)^2 + (\Delta J_y)^2 \right] |j, m\rangle = \hbar^2 \left( j^2 + j - m^2 \right) .
\] (6.155)

20. Find the condition under which the Hamiltonian of a charged particle in a magnetic field
\[
H = \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 .
\] (6.156)
can be written as
\[
H = \frac{1}{2m} \mathbf{p}^2 - \frac{q}{mc} \mathbf{\sigma} \cdot \mathbf{p} + \frac{q^2}{2mc^2} \mathbf{A}^2 .
\] (6.157)

21. Consider a point particle having mass \( m \) and charge \( q \) moving under the influence of electric field \( \mathbf{E} \) and magnetic field \( \mathbf{B} \), which are related to the scalar potential \( \varphi \) and to the vector potential \( \mathbf{A} \) by
\[
\mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} ,
\] (6.158)
and
\[
\mathbf{B} = \nabla \times \mathbf{A} .
\] (6.159)
Find the coordinates representation of the time-independent Schrödinger equation \( \mathcal{H} |\alpha\rangle = E |\alpha\rangle \).
22. A particle of mass $m$ and charge $e$ interacts with a vector potential
\begin{align*}
A_x &= A_z = 0, \\
A_y &= Bx.
\end{align*}
(6.160)
(6.161)
Calculate the ground state energy. Clue: Consider a wave function of the form
\[ \psi(x, y, z) = \chi(x) \exp(ik_xy) \exp(ik_z z). \]
(6.162)

23. Find the energy spectrum of a charged particle having mass $m$ and charge $q$ moving in uniform and time-independent magnetic field $B = B\hat{z}$ and electric field $E = E\hat{x}$.

24. Consider a particle having mass $m$ and charge $e$ moving in the $xy$ plane under the influence of the potential $U(y) = \frac{1}{2}m\omega^2 y^2$. A uniform and time-independent magnetic field given by $B = B\hat{z}$ is applied perpendicularly to the $xy$ plane. Calculate the eigenenergies of the particle.

25. Consider a particle with charge $q$ and mass $\mu$ confined to move on a circle of radius $a$ in the $xy$ plane, but is otherwise free. A uniform and time-independent magnetic field $B$ is applied in the $z$ direction.
   a) Find the eigenenergies.
   b) Calculate the current $J_m$ for each of the eigenstates of the system.

26. The Hamiltonian of a non isotropic rigid rotator is given by
\[ H = \frac{L_x^2}{2I_{xy}} + \frac{L_y^2}{2I_{xy}} + \frac{L_z^2}{2I_z}, \]
(6.163)
where $L$ is the vector angular momentum operator. At time $t = 0$ the state of the system is described by the wavefunction
\[ \psi(\theta, \phi) = A \sin \theta \cos \phi, \]
(6.164)
where $\theta, \phi$ are angles in spherical coordinates and $A$ is a normalization constant. Calculate the expectation value $\langle L_z \rangle$ at time $t > 0$.

27. The eigenstates of the angular momentum operators $L^2$ and $L_z$ with $l = 1$ and $m = -1, 0, 1$ are denoted as $|1, -1\rangle$, $|1, 0\rangle$ and $|1, 1\rangle$.
   a) Write the $3 \times 3$ matrix of the operator $L_x$ in this $l = 1$ subspace.
   b) Calculate the expectation value $\langle L_x \rangle$ for the state $\frac{1}{\sqrt{2}} \left[ |1, 1\rangle + \sqrt{2} |1, 0\rangle + |1, -1\rangle \right]$.
   c) The same as the previous section for the state $\frac{1}{\sqrt{2}} \left[ |1, 1\rangle - |1, -1\rangle \right]$.
   d) Write the $3 \times 3$ matrix representation in this basis of the rotation operator at angle $\phi$ around the $z$ axis.
   e) The same as in the previous section for an infinitesimal rotation with angle $d\phi$ around the $x$ axis.

28. Consider a particle of mass $m$ in a 3D harmonic potential
\[ V(x, y, z) = \frac{1}{2}m\omega^2 \left( x^2 + y^2 + z^2 \right). \]
(6.165)
6.6. Problems

The state vector $|\psi\rangle$ of the particle satisfy

\begin{align*}
    a_x |\psi\rangle &= \alpha_x |\psi\rangle, \\
    a_y |\psi\rangle &= \alpha_y |\psi\rangle, \\
    a_z |\psi\rangle &= \alpha_z |\psi\rangle,
\end{align*}

(6.166)

(6.167)

(6.168)

where $\alpha_x$, $\alpha_y$ and $\alpha_z$ are complex and $a_x$, $a_y$ and $a_z$ are annihilation operators.

\begin{align*}
    a_x &= \sqrt{\frac{m\omega}{2\hbar}} \left( x + \frac{ip_x}{m\omega} \right), \\
    a_y &= \sqrt{\frac{m\omega}{2\hbar}} \left( y + \frac{ip_y}{m\omega} \right), \\
    a_z &= \sqrt{\frac{m\omega}{2\hbar}} \left( z + \frac{ip_z}{m\omega} \right),
\end{align*}

(6.169)

(6.170)

(6.171)

Let $\mathbf{L}$ be the vector operator of the orbital angular momentum.

a) Calculate $\langle L_z \rangle$.

b) Calculate $\Delta L_z$.

29. A rigid rotator is prepared in a state

\begin{equation}
    |\alpha\rangle = A (|1, 1\rangle - |1, -1\rangle),
\end{equation}

(6.172)

where $A$ is a normalization constant, and where the symbol $|l, m\rangle$ denotes an angular momentum state with quantum numbers $l$ and $m$. Calculate

a) $\langle L_z \rangle$.

b) $\langle (\Delta L_x)^2 \rangle$.

30. The Hamiltonian of a top is given by

\begin{equation}
    \mathcal{H} = \frac{L_x^2}{2I_1} + \frac{L_y^2}{2I_2} + \frac{L_z^2}{2I_2},
\end{equation}

(6.173)

where $\mathbf{L}$ is the angular momentum vector operator. Let $|\psi_0\rangle$ be the ground state of the system.

a) Calculate the quantity $A_z(\phi)$, which is defined as

\begin{equation}
    A_z(\phi) = \langle \psi_0 | \exp \left( \frac{iL_z\phi}{\hbar} \right) \mathcal{H} \exp \left( -\frac{iL_z\phi}{\hbar} \right) |\psi_0\rangle.
\end{equation}

(6.174)

b) Calculate the quantity $A_x(\phi)$, which is defined as

\begin{equation}
    A_x(\phi) = \langle \psi_0 | \exp \left( \frac{iL_x\phi}{\hbar} \right) \mathcal{H} \exp \left( -\frac{iL_x\phi}{\hbar} \right) |\psi_0\rangle.
\end{equation}
6.7 Solutions

1. By cyclic permutation of

\[
R_{\hat{z}} = \begin{pmatrix}
\cos \phi & -\sin \phi & 0 \\
\sin \phi & \cos \phi & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

one has

\[
R_{\hat{x}} = \begin{pmatrix}
1 & 0 & 0 \\
0 & \cos \phi - \sin \phi & 0 \\
0 & \sin \phi & \cos \phi
\end{pmatrix},
\]

\[
R_{\hat{y}} = \begin{pmatrix}
\cos \phi & 0 & -\sin \phi \\
0 & 1 & 0 \\
\sin \phi & 0 & \cos \phi
\end{pmatrix}.
\]

On one hand

\[
1 - [R_{\hat{z}} (\phi), R_{\hat{y}} (\phi)] = \begin{pmatrix}
1 & 1 & -1 + \cos^2 \phi & \sin \phi - \sin \phi \cos \phi \\
1 & 1 & -\sin \phi - \sin \phi \cos \phi & 1 \sin \phi \cos \phi - \sin \phi \\
\sin \phi - \sin \phi \cos \phi & 1 & \sin \phi \cos \phi \cos \phi - \sin \phi & 1
\end{pmatrix}
\]

\[
= \begin{pmatrix}
1 & 1 - \phi^2 & 0 \\
\phi^2 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix} + O (\phi^3).
\]

(6.178)

On the other hand

\[
R_{\hat{z}} (\phi^2) = \begin{pmatrix}
\cos \phi^2 & -\sin \phi^2 & 0 \\
\sin \phi^2 & \cos \phi^2 & 0 \\
0 & 0 & 1
\end{pmatrix} = \begin{pmatrix}
1 & -\phi^2 & 0 \\
\phi^2 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix} + O (\phi^3),
\]

(6.179)

thus

\[
1 - [R_{\hat{z}} (\phi), R_{\hat{y}} (\phi)] = R_{\hat{z}} (\phi^2) + O (\phi^3).
\]

(6.180)

2. Using the identity (2.174), which is given by

\[
e^L A e^{-L} = A + [L, A] + \frac{1}{2!} [L, [L, A]] + \frac{1}{3!} [L, [L, [L, A]]] + \cdots,
\]

(6.181)

and the commutation relations (6.22), which are given by

\[
[J_i, J_j] = i \hbar \varepsilon_{ijk} J_k,
\]

(6.182)

one has
6.7. Solutions

\[
\exp \left( \frac{i J_z \phi}{\hbar} \right) J_x \exp \left( -\frac{i J_x \phi}{\hbar} \right)
\]

\[= J_x + \frac{i \phi}{\hbar} [J_z, J_x] + \frac{1}{2!} \left( \frac{i \phi}{\hbar} \right)^2 [J_z, [J_z, J_x]] + \frac{1}{3!} \left( \frac{i \phi}{\hbar} \right)^3 [J_z, [J_z, [J_z, J_x]]] + \cdots
\]

\[= J_x \left( 1 - \frac{1}{2!} \phi^2 + \cdots \right) - J_y \left( \phi - \frac{1}{3!} \phi^3 + \cdots \right)\]

\[J_x \cos \phi - J_y \sin \phi. \quad (6.183)
\]

3. The components of the Pauli matrix vector \( \sigma \) are given by:

\[\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (6.184)\]

a) The following holds

\[\sigma \cdot a = \begin{pmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{pmatrix}, \quad (6.185)\]

\[\sigma \cdot b = \begin{pmatrix} b_z & b_x - ib_y \\ b_x + ib_y & -b_z \end{pmatrix}, \quad (6.186)\]

thus

\[(\sigma \cdot a) (\sigma \cdot b) = \begin{pmatrix} a_z b_z + (a_x - ia_y) (b_x + ib_y) a_z (b_x - ib_y) - (a_x - ia_y) b_z \\ (a_x + ia_y) b_z - a_z (b_x + ib_y) a_z b_z + (a_x + ia_y) (b_x - ib_y) \end{pmatrix}\]

\[= a \cdot b \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}
\]

\[+i (a_yb_z - a_z b_y) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

\[+i (a_z b_x - a_x b_z) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}
\]

\[+i (a_x b_y - a_y b_x) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

\[= a \cdot b + i \sigma \cdot (a \times b). \quad (6.187)\]

b) Using (a) one has

\[(\sigma \cdot \hat{n})^2 = 1, \quad (6.188)\]

thus with the help of the Taylor expansion of the functions \( \cos(x) \) and \( \sin(x) \) one finds
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\[
\exp \left( -\frac{i \sigma \cdot \hat{n} \phi}{2} \right) = \cos \left( \frac{\sigma \cdot \hat{n} \phi}{2} \right) - i \sin \left( \frac{\sigma \cdot \hat{n} \phi}{2} \right) = 1 \cos \frac{\phi}{2} - i \sigma \cdot \hat{n} \sin \frac{\phi}{2}.
\]  

(6.189)

4. In spherical coordinates the unit vectors \( \hat{n} \) is expressed as

\[
\hat{n} = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta),
\]

(6.190)

thus

\[
\sigma \cdot \hat{n} = \begin{pmatrix}
\cos \theta & \sin \theta e^{-i\varphi} \\
\sin \theta e^{i\varphi} & -\cos \theta
\end{pmatrix}.
\]

(6.191)

The eigen values \( \lambda_+ \) and \( \lambda_- \) are found solving

\[
\lambda_+ + \lambda_- = \text{Tr} (\sigma \cdot \hat{n}) = 0,
\]

(6.192)

and

\[
\lambda_+ \lambda_- = \text{Det} (\sigma \cdot \hat{n}) = -1,
\]

(6.193)

thus

\[
\lambda_{\pm} = \pm 1.
\]

(6.194)

The normalized eigenvectors can be chosen to be given by

\[
|+\rangle = \begin{pmatrix}
\cos \frac{\theta}{2} \exp \left( -\frac{i\varphi}{2} \right) \\
\sin \frac{\theta}{2} \exp \left( \frac{i\varphi}{2} \right)
\end{pmatrix},
\]

(6.195)

\[
|\rangle = \begin{pmatrix}
-\sin \frac{\theta}{2} \exp \left( -\frac{i\varphi}{2} \right) \\
\cos \frac{\theta}{2} \exp \left( \frac{i\varphi}{2} \right)
\end{pmatrix}.
\]

(6.196)

5. Using Eq. (6.195) one finds the probability \( p_+ \) to measure +h/2 is given by

\[
p_+ = \left| \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix}
\cos \frac{\theta}{2} \exp \left( -\frac{i\varphi}{2} \right) \\
\sin \frac{\theta}{2} \exp \left( \frac{i\varphi}{2} \right)
\end{pmatrix} \right|^2 = \cos^2 \frac{\theta}{2},
\]

(6.197)

and the probability \( p_- \) to measure -h/2 is

\[
p_- = 1 - p_+ = \sin^2 \frac{\theta}{2}.
\]

(6.198)

The average value of the component of the spin along \( z' \) axis is thus

\[
\frac{\hbar}{2} \left( \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \right) = \frac{\hbar}{2} \cos \theta.
\]

(6.199)
6. In general, note that all smooth functions of the matrix \((\sigma \cdot \hat{n})\) commute, a fact that greatly simplifies the calculations.

a) The following holds
\[
\frac{1}{1 - i\alpha (\sigma \cdot \hat{n})} = 1 + i\alpha (\sigma \cdot \hat{n}) + [i\alpha (\sigma \cdot \hat{n})]^2 + \cdots ,
\] (6.200)
thus
\[
\left(\frac{1}{1 - i\alpha (\sigma \cdot \hat{n})}\right)^\dagger = 1 - i\alpha (\sigma \cdot \hat{n}) + [(1) \alpha (\sigma \cdot \hat{n})] + \cdots = \frac{1}{1 + i\alpha (\sigma \cdot \hat{n})},
\] (6.201)
therefore
\[
UU^\dagger = 1 + i\alpha (\sigma \cdot \hat{n}) \left(1 - i\alpha (\sigma \cdot \hat{n})\right) + \cdots = 1,
\] (6.202)
and similarly \(U^\dagger U = 1\).

b) Exploiting again the fact that all smooth functions of the matrix \((\sigma \cdot \hat{n})\) commute and using Eq. (6.188) one has
\[
\frac{dU}{d\alpha} = i\left[1 - i\alpha (\sigma \cdot \hat{n})\right] (\sigma \cdot \hat{n}) + [1 + i\alpha (\sigma \cdot \hat{n})] (\sigma \cdot \hat{n})
\[
= i\frac{2 (\sigma \cdot \hat{n})}{[1 - i\alpha (\sigma \cdot \hat{n})]^2}
\[
= i\frac{2 (\sigma \cdot \hat{n})}{[1 - i\alpha (\sigma \cdot \hat{n})]}\frac{1 + i\alpha (\sigma \cdot \hat{n})}{1 - i\alpha (\sigma \cdot \hat{n})}
\[
= \frac{2i (\sigma \cdot \hat{n})}{1 + \alpha^2} U .
\] (6.203)

c) By integration one has
\[
U = U_0 \exp \left(2i (\sigma \cdot \hat{n}) \int_0^\alpha \frac{d\alpha'}{1 + \alpha'^2}\right)
\[
U_0 \exp \left(2i (\sigma \cdot \hat{n}) \tan^{-1} \alpha \right) ,
\] (6.204)
where \(U_0\) is a the matrix \(U\) at \(\alpha = 0\). With the help of Eq. (6.137) one thus finds that
\[
U = U_0 \left[1 \cos \left(2 \tan^{-1} \alpha \right) + i\sigma \cdot \hat{n} \sin \left(2 \tan^{-1} \alpha \right)\right] ,
\] (6.205)
Using the identities
\[
\cos \left(2 \tan^{-1} \alpha \right) = \frac{1 - \alpha^2}{1 + \alpha^2} ,
\] (6.206)
\[
\sin \left(2 \tan^{-1} \alpha \right) = \frac{2\alpha}{1 + \alpha^2} ,
\] (6.207)
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and assuming \( U_0 = 1 \) one finds that

\[
U = \frac{1 - \alpha^2}{1 + \alpha^2} + i \mathbf{\sigma} \cdot \mathbf{\hat{n}} \frac{2\alpha}{1 + \alpha^2}.
\]

(6.208)

7. In terms of Pauli matrices

\[
H \approx E_a \sigma_0 + \Delta \sigma_x + E_d \sigma_z,
\]

(6.209)

where

\[
E_a = \frac{E_L + E_R}{2}, \quad E_d = \frac{E_L - E_R}{2},
\]

(6.210)

and

\[
\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
\]

(6.211)

Using Eq. (6.137), which is given by

\[
\exp\left(-\frac{i \mathbf{\sigma} \cdot \mathbf{\hat{n}} \phi}{2}\right) = \cos \frac{\phi}{2} - i \mathbf{\sigma} \cdot \mathbf{\hat{n}} \sin \frac{\phi}{2},
\]

(6.212)

the time evolution operator \( u(t) \) can be calculated

\[
u(t) = \exp\left(-\frac{iH t}{\hbar}\right)
\]

\[
= \exp\left(-\frac{iE_a \sigma_0 t}{\hbar}\right) \exp\left(-\frac{i(\Delta \sigma_x + E_d \sigma_z) t}{\hbar}\right)
\]

\[
= \exp\left(-\frac{iE_a t}{\hbar}\right) \exp\left(-i \mathbf{\sigma} \cdot \mathbf{\hat{n}} \frac{\sqrt{\Delta^2 + E_d^2} t}{\hbar}\right),
\]

(6.213)

where

\[
\mathbf{\sigma} \cdot \mathbf{\hat{n}} = \mathbf{\sigma} \cdot \frac{(\Delta, 0, E_d)}{\sqrt{\Delta^2 + E_d^2}}.
\]

(6.214)

thus

\[
u(t) = \exp\left(-\frac{iE_a t}{\hbar}\right) \left( \cos \frac{\sqrt{\Delta^2 + E_d^2} t}{\hbar} - i \frac{\Delta \sigma_x + E_d \sigma_z}{\sqrt{\Delta^2 + E_d^2}} \sin \frac{\sqrt{\Delta^2 + E_d^2} t}{\hbar} \right).
\]

(6.215)

The probability \( p_R(t) \) is thus given by
6.7. Solutions

\[ p_R(t) = |\langle R | u(t) | \psi(t = 0) \rangle|^2 \]
\[ = |\langle R | u(t) | L \rangle|^2 \]
\[ = \frac{\Delta^2}{\Delta^2 + (E_R - E_L)^2} \sin^2 \left( \frac{t \sqrt{\Delta^2 + (E_R - E_L)^2}}{\hbar} \right). \]  

(6.216)

8. The Hamiltonian is given by

\[ \mathcal{H} = \omega_0 S_z + \omega_1 (\cos(\omega t) S_x + \sin(\omega t) S_y), \]  

(6.217)

where

\[ \omega_0 = \frac{|e| B_0}{mc}, \]  

(6.218)

\[ \omega_1 = \frac{|e| B_1}{mc}. \]  

(6.219)

The matrix representation in the basis \{\ket{+}, \ket{-}\} (where \ket{+} = \ket{+; \hat{z}} and \ket{-} = \ket{-; \hat{z}}) is found using Eqs. (6.69), (6.74) and (6.75)

\[ \mathcal{H} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 \exp(-i\omega t) \\ \omega_1 \exp(i\omega t) & -\omega_0 \end{pmatrix}. \]  

(6.220)

The Schrödinger equation is given by

\[ i\hbar \frac{d}{dt} |\alpha\rangle = \mathcal{H} |\alpha\rangle. \]  

(6.221)

It is convenient to express the general solution as

\[ |\alpha\rangle(t) = b_+(t) \exp\left(-\frac{i\omega t}{2}\right) |+\rangle + b_-(t) \exp\left(\frac{i\omega t}{2}\right) |-\rangle. \]  

(6.222)

Substituting into the Schrödinger equation yields

\[ i\frac{d}{dt} \begin{pmatrix} e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} \begin{pmatrix} b_+ \\ b_- \end{pmatrix} \]
\[ = \frac{1}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} \begin{pmatrix} b_+ \\ b_- \end{pmatrix}. \]  

(6.223)

or

\[ i\frac{\omega}{2} \begin{pmatrix} -e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} \begin{pmatrix} b_+ \\ b_- \end{pmatrix} + \begin{pmatrix} e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} \begin{pmatrix} \dot{b}_+ \\ \dot{b}_- \end{pmatrix} \]
\[ = -\frac{i}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{-i\omega t} \\ \omega_1 e^{i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} e^{-\frac{i\omega t}{2}} & 0 \\ 0 & e^{\frac{i\omega t}{2}} \end{pmatrix} \begin{pmatrix} b_+ \\ b_- \end{pmatrix}. \]  

(6.224)
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By multiplying from the left by
\[
\begin{pmatrix}
  e^{i\omega t} & 0 \\
  0 & e^{-i\omega t}
\end{pmatrix}
\]
one has
\[
\frac{i\omega}{2} \begin{pmatrix}
  -1 & 0 \\
  0 & 1
\end{pmatrix} \begin{pmatrix}
  b_+ \\
  b_-
\end{pmatrix} + \begin{pmatrix}
  \dot{b}_+ \\
  \dot{b}_-
\end{pmatrix} = -\frac{i}{2} \begin{pmatrix}
  \omega_0 & \omega_1 \\
  \omega_1 & -\omega_0
\end{pmatrix} \begin{pmatrix}
  b_+ \\
  b_-
\end{pmatrix},
\]
(6.225)

or
\[
i \begin{pmatrix}
  \dot{b}_+ \\
  \dot{b}_-
\end{pmatrix} = \frac{\Omega}{2} \begin{pmatrix}
  b_+ \\
  b_-
\end{pmatrix},
\]
(6.226)

where
\[
\Omega = \begin{pmatrix}
  \Delta \omega & \omega_1 \\
  \omega_1 & -\Delta \omega
\end{pmatrix} = \Delta \omega \sigma_z + \omega_1 \sigma_x,
\]
(6.227)

and
\[
\Delta \omega = \omega_0 - \omega.
\]
(6.228)

At time \(t = 0\)
\[
\begin{pmatrix}
  b_+ (0) \\
  b_- (0)
\end{pmatrix} = \begin{pmatrix}
  1 \\
  0
\end{pmatrix}.
\]
(6.229)

The time evolution is found using Eq. (6.137)
\[
\begin{pmatrix}
  b_+ (t) \\
  b_- (t)
\end{pmatrix} = \exp \left( -\frac{i\Omega t}{2} \right) \begin{pmatrix}
  b_+ (0) \\
  b_- (0)
\end{pmatrix}
\]
\[
= \begin{pmatrix}
  \cos \theta - i \frac{\Delta \omega \sin \theta}{\sqrt{\omega_1^2 + (\Delta \omega)^2}} & -i \frac{\omega_1 \sin \theta}{\sqrt{\omega_1^2 + (\Delta \omega)^2}} \\
  -i \frac{\omega_1 \sin \theta}{\sqrt{\omega_1^2 + (\Delta \omega)^2}} & \cos \theta + i \frac{\Delta \omega \sin \theta}{\sqrt{\omega_1^2 + (\Delta \omega)^2}}
\end{pmatrix} \begin{pmatrix}
  1 \\
  0
\end{pmatrix},
\]
(6.230)

where
\[
\theta = \sqrt{\frac{\omega_1^2 + (\Delta \omega)^2 t}{2}}.
\]
(6.231)

The probability is thus given by
\[
P_{+-} (t) = \frac{\omega_1^2}{\omega_1^2 + (\Delta \omega)^2} \sin^2 \sqrt{\frac{\omega_1^2 + (\Delta \omega)^2 t}{2}}.
\]
(6.232)
9. The Schrödinger equation is given by

\[ i\hbar \frac{d}{dt} |\alpha\rangle = \mathcal{H} |\alpha\rangle, \quad (6.233) \]

where

\[ \mathcal{H} = \omega S_z, \quad (6.234) \]

and

\[ \omega (t) = \frac{|e| B(t)}{m_e c}. \quad (6.235) \]

In the basis of the eigenvectors of \( S_z \) one has

\[ |\alpha\rangle = c_+ |+\rangle + c_- |-- \rangle, \quad (6.236) \]

and

\[ i\hbar (\dot{c}_+ |+\rangle + \dot{c}_- |-- \rangle) = \omega S_z (c_+ |+\rangle + c_- |-- \rangle), \quad (6.237) \]

where

\[ S_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle, \quad (6.238) \]

thus one gets 2 decoupled equations

\[ \dot{c}_+ = -\frac{i \omega}{2} c_+, \quad (6.239) \]

\[ \dot{c}_- = \frac{i \omega}{2} c_- . \quad (6.240) \]

The solution is given by

\[ c_\pm (t) = c_\pm (0) \exp \left( \pm \frac{i}{2} \int_0^t \omega (t') dt' \right) \]

\[ = c_\pm (0) \exp \left( \pm \frac{i |e|}{2m_c c} \int_0^t B (t') dt' \right). \quad (6.241) \]

10. At time \( t = 0 \)

\[ |\psi (t = 0)\rangle = \frac{1}{\sqrt{2}} (|+\rangle + |-- \rangle). \quad (6.242) \]

Using the result of the previous problem and the notation

\[ \omega_c = \frac{eB}{mc}. \quad (6.243) \]
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one finds

\[ |\psi(t)\rangle = \frac{1}{\sqrt{2}} \left\{ \exp \left( -\frac{i\omega_c}{2} \int_0^t \cos(\omega t') \, dt' \right) |+\rangle + \exp \left( \frac{i\omega_c}{2} \int_0^t \cos(\omega t') \, dt' \right) |-\rangle \right\} \]

\[ = \frac{1}{\sqrt{2}} \left[ \exp \left( -\frac{i\omega_c \sin \omega t}{2\omega} \right) |+\rangle + \exp \left( \frac{i\omega_c \sin \omega t}{2\omega} \right) |-\rangle \right] , \]

(6.244)

thus

\[ \langle S_z \rangle (t) = \langle \psi(t) | S_z | \psi(t) \rangle = 0 . \] (6.245)

11. The Schrödinger equation for \( u \) is given by

\[ i\hbar \frac{du}{dt} = \mathcal{H} u , \] (6.246)

thus

\[ \frac{du}{dt} = -\frac{4i\omega S_z}{\hbar} \frac{1}{1 + (\omega t)^2} u . \] (6.247)

By integration one finds

\[ u(t) = u(0) \exp \left( -\frac{4i\omega S_z}{\hbar} \int_0^t \frac{dt'}{1 + (\omega t')^2} \right) \]

\[ = u(0) \exp \left( \frac{4iS_z}{\hbar} \tan^{-1}(\omega t) \right) . \] (6.248)

Setting an initial condition \( u(t=0) = 1 \) yields

\[ u(t) = \exp \left( \frac{4iS_z}{\hbar} \tan^{-1}(\omega t) \right) . \] (6.249)

The matrix elements of \( u(t) \) in the basis of the eigenstates \( |\pm\rangle \) of \( S_z \) are given by

\[ \langle + | u(t) | + \rangle = \exp \left( 2i \tan^{-1}(\omega t) \right) = \frac{1 + i\omega t}{1 - i\omega t} , \] (6.250)

\[ \langle - | u(t) | - \rangle = \exp \left( -2i \tan^{-1}(\omega t) \right) = \frac{1 - i\omega t}{1 + i\omega t} , \] (6.251)

\[ \langle + | u(t) | - \rangle = \langle - | u(t) | + \rangle = 0 . \] (6.252)

12. The eigenvector of \( \mathbf{S} \cdot \hat{n} \), where \( \hat{n} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \) with eigenvalue \( +\hbar/2 \) is given by [see Eq. (6.195)]
6.7. Solutions

\[ |+; S \cdot \mathbf{n} \rangle = \cos \frac{\theta}{2} e^{-i \frac{\varphi}{2}} |+\rangle + \sin \frac{\theta}{2} e^{i \frac{\varphi}{2}} |-\rangle \ . \quad (6.253) \]

The operator \( S_z \) is written as

\[ S_z = \frac{\hbar}{2} (|+\rangle \langle +| - |-\rangle \langle -|) \ . \quad (6.254) \]

(a) Thus

\[ \langle +; S \cdot \mathbf{n} | S_z | +; S \cdot \mathbf{n} \rangle = \frac{\hbar}{2} \left( \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \right) = \frac{\hbar}{2} \cos \theta \ . \quad (6.255) \]

(b) Since \( S_z^2 \) is the identity operator times \( \frac{\hbar^2}{4} \) one has

\[ \langle (\Delta S_z)^2 \rangle = \langle S_z^2 \rangle - \langle S_z \rangle^2 = \frac{\hbar^2}{4} (1 - \cos^2 \theta) = \frac{\hbar^2}{4} \sin^2 \theta \ . \quad (6.256) \]

13. We seek a unit vector \( \mathbf{n} \) such that

\[ |\psi\rangle = |+; S \cdot \mathbf{n} \rangle \ , \quad (6.257) \]

where \( |+; S \cdot \mathbf{n} \rangle \) is given by Eq. (6.195)

\[ |+; S \cdot \mathbf{n} \rangle = \cos \frac{\theta}{2} \exp \left( -i \frac{\varphi}{2} \right) |+\rangle + \sin \frac{\theta}{2} \exp \left( i \frac{\varphi}{2} \right) |-\rangle \ , \quad (6.258) \]

thus the following hold

\[ \cot \frac{\theta}{2} = \left| \frac{\alpha}{\beta} \right| \ , \quad (6.259) \]

and

\[ \varphi_+ = \arg (\beta) - \arg (\alpha) \ . \quad (6.260) \]

Similarly, by requiring that

\[ |\psi\rangle = |-; S \cdot \mathbf{n} \rangle \ , \quad (6.261) \]

where

\[ |-; S \cdot \mathbf{n} \rangle = - \sin \frac{\theta}{2} \exp \left( -i \frac{\varphi}{2} \right) |+\rangle + \cos \frac{\theta}{2} \exp \left( i \frac{\varphi}{2} \right) |-\rangle \ , \quad (6.262) \]

one finds

\[ \tan \frac{\theta}{2} = \left| \frac{\alpha}{\beta} \right| \ , \quad (6.263) \]

\[ \varphi_- = \arg (\beta) - \arg (\alpha) + \pi \ . \quad (6.264) \]
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14. The Hamiltonian at the time interval $0 < t < \tau$ is given by

$$ H = -\gamma B_0 (S \cdot \hat{u}) , \quad (6.265) $$

where $\gamma$ is the gyromagnetic ratio and $S$ is the angular momentum operator. The eigenvectors of $S \cdot \hat{u}$ with eigenvalue $\pm \hbar / 2$ are given by [see Eqs. (6.195) and (6.196)]

$$ |+; S \cdot \hat{u} \rangle = \cos \frac{\theta}{2} e^{-i\frac{\tau}{2}} |+\rangle + \sin \frac{\theta}{2} e^{i\frac{\tau}{2}} |-\rangle , \quad (6.266) $$

$$ |--; S \cdot \hat{u} \rangle = -\sin \frac{\theta}{2} e^{-i\frac{\tau}{2}} |+\rangle + \cos \frac{\theta}{2} e^{i\frac{\tau}{2}} |-\rangle , \quad (6.267) $$

Thus in the time interval $0 < t < \tau$ the state vector is given by

$$ |\alpha \rangle = |+; S \cdot \hat{u} \rangle \langle +; S \cdot \hat{u} |+\rangle \exp \left( \frac{i\gamma B_0 t}{2} \right) + |--; S \cdot \hat{u} \rangle \langle -; S \cdot \hat{u} |+\rangle \exp \left( -\frac{i\gamma B_0 t}{2} \right) $$

$$ = |+; S \cdot \hat{u} \rangle \cos \frac{\theta}{2} e^{i\frac{\tau}{2}} \exp \left( \frac{i\gamma B_0 t}{2} \right) - |--; S \cdot \hat{u} \rangle \sin \frac{\theta}{2} e^{i\frac{\tau}{2}} \exp \left( -\frac{i\gamma B_0 t}{2} \right) $$

$$ = e^{i\phi} \left[ \cos^2 \frac{\theta}{2} \exp \left( \frac{i\gamma B_0 t}{2} \right) + \sin^2 \frac{\theta}{2} \exp \left( -\frac{i\gamma B_0 t}{2} \right) \right] |+\rangle $$

$$ + \sin \frac{\theta}{2} \cos \frac{\theta}{2} \left[ \exp \left( \frac{i\gamma B_0 t}{2} \right) - \exp \left( -\frac{i\gamma B_0 t}{2} \right) \right] |-\rangle $$

$$ = e^{i\phi} \left[ \frac{1 + \cos \theta}{2} \exp \left( \frac{i\gamma B_0 t}{2} \right) + \frac{1 - \cos \theta}{2} \exp \left( -\frac{i\gamma B_0 t}{2} \right) \right] |+\rangle $$

$$ + i \sin \theta \sin \left( \frac{\gamma B_0 \tau}{2} \right) |-\rangle $$

$$ = e^{i\phi} \left[ \cos \left( \frac{\gamma B_0 \tau}{2} \right) + i \cos \theta \sin \left( \frac{\gamma B_0 \tau}{2} \right) \right] |+\rangle + i \sin \theta \sin \left( \frac{\gamma B_0 \tau}{2} \right) |-\rangle . \quad (6.268) $$

Thus for $t > \tau$

$$ P_\rightarrow (t) = \sin^2 \theta \sin^2 \left( \frac{\gamma B_0 \tau}{2} \right) . \quad (6.269) $$

An alternative solution - The Hamiltonian in the basis of $|\pm\rangle$ states is given by

$$ H = -\gamma B_0 \hbar (\sigma \cdot \hat{u}) , \quad (6.270) $$

where $\sigma$ is the Pauli matrix vector

$$ \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \quad (6.271) $$
The time evolution operator is given by

\[ u(t) = \exp \left( -\frac{i\mathcal{H}t}{\hbar} \right) = \exp \left[ i\gamma B_0 t \frac{\mathbf{\sigma} \cdot \hat{u}}{2} \right]. \]  

(6.272)

Using the identity (6.137) one finds

\[
\begin{pmatrix}
I 
\end{pmatrix}
\cos \left( \frac{\gamma B_0 t}{2} \right)
+ i \hat{u} \cdot \mathbf{\sigma} 
\sin \left( \frac{\gamma B_0 t}{2} \right)

= \left( \begin{pmatrix}
\cos \left( \frac{\gamma B_0 t}{2} \right) + i \cos \theta \sin \left( \frac{\gamma B_0 t}{2} \right) & i \sin \theta e^{-i\phi} \sin \left( \frac{\gamma B_0 t}{2} \right) \\
i \sin \theta e^{i\phi} \sin \left( \frac{\gamma B_0 t}{2} \right) & \cos \left( \frac{\gamma B_0 t}{2} \right) - i \cos \theta \sin \left( \frac{\gamma B_0 t}{2} \right) 
\end{pmatrix} \right) , \]

(6.273)

thus for \( t > \tau \)

\[
P_.(t) = \left| \begin{pmatrix}
0 
1
\end{pmatrix} u(t) \begin{pmatrix}
1 
0
\end{pmatrix} \right|^2 = \sin^2 \theta \sin^2 \left( \frac{\gamma B_0 \tau}{2} \right). \]  

(6.274)

15. The matrix representation of the Hamiltonian in the basis of \( |\pm; S_z \rangle \) states is given by

\[ \mathcal{H} = \frac{\hbar \omega}{2} (\hat{x} \cdot \mathbf{\sigma}) , \]  

(6.275)

where \( \mathbf{\sigma} \) is the Pauli matrix vector

\[
\sigma_x = \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}
0 & -i \\
i & 0
\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix} . \]

(6.276)

a) The time evolution operator is given by

\[
u(t) = \exp \left( -\frac{i\mathcal{H}t}{\hbar} \right) = \exp \left( -\frac{i\omega t}{2} (\hat{x} \cdot \mathbf{\sigma}) \right) . \]  

(6.277)

Using the identity

\[
\exp (i \mathbf{u} \cdot \mathbf{\sigma}) = \mathbf{1} \cos \alpha + i \mathbf{\hat{u}} \cdot \mathbf{\sigma} \sin \alpha , \]

(6.278)

where \( \mathbf{u} = \alpha \hat{u} \) is a three-dimensional real vector and \( \mathbf{\hat{u}} \) is a three-dimensional real unit vector, one finds

\[
u(t) = \mathbf{1} \cos \left( \frac{\omega t}{2} \right) - i \sigma_1 \sin \left( \frac{\omega t}{2} \right) 
\begin{pmatrix}
\cos \left( \frac{\omega t}{2} \right) & -i \sin \left( \frac{\omega t}{2} \right) \\
-i \sin \left( \frac{\omega t}{2} \right) & \cos \left( \frac{\omega t}{2} \right) 
\end{pmatrix} . \]

(6.279)
b) Let \( P_{++}(t) \) be the probability to measure \( S_z = +h/2 \) at time \( t > 0 \) given that at time \( t = 0 \) the spin was found to have \( S_z = +h/2 \). Similarly, \( P_{--}(t) \) is the probability to measure \( S_z = -h/2 \) at time \( t > 0 \) given that at time \( t = 0 \) the spin was found to have \( S_z = -h/2 \).

These probabilities are given by

\[
P_{++}(t) = \left| \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} u(t) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = \cos^2 \frac{\omega t}{2}, \tag{6.280}
\]

\[
P_{--}(t) = \left| \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} u(t) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right|^2 = \cos^2 \frac{\omega t}{2}. \tag{6.281}
\]

Thus, assuming that the first measurement has yielded \( S_z = +h/2 \) one finds \( p_{\text{same}} = \left[ P_{++} \left( \frac{\omega T}{2N} \right) \right]^N \), whereas assuming that the first measurement has yielded \( S_z = -h/2 \) one finds \( p_{\text{same}} = \left[ P_{--} \left( \frac{\omega T}{2N} \right) \right]^N \).

Thus in general independently on the result of the first measurement one has

\[
p_{\text{same}} = \cos^{2N} \frac{\omega T}{2N}. \tag{6.282}
\]

\[c)\] Using

\[
p_{\text{same}} = \exp \left( 2N \log \left( \cos \frac{\omega T}{2N} \right) \right) = \exp \left( 2N \log \left( 1 - \frac{1}{2} \left( \frac{\omega T}{2N} \right)^2 + O \left( \frac{1}{N} \right)^4 \right) \right) = \exp \left( -\frac{(\omega T)^2}{4N} + O \left( \frac{1}{N} \right)^3 \right). \tag{6.283}
\]

one finds

\[
\lim_{N \to \infty} p_{\text{same}} = 1. \tag{6.284}
\]

This somewhat surprising result is called the quantum Zeno effect or the 'watched pot never boils' effect.

16. The eigenvectors of \( \mathbf{S} \cdot \hat{\mathbf{u}} \) with eigenvalues \( \pm h/2 \) are given by

\[
|\pm; \hat{\mathbf{u}} \rangle = \cos \frac{\theta}{2} e^{-i\frac{\pi}{2}} |+\rangle + \sin \frac{\theta}{2} e^{i\frac{\pi}{2}} |-\rangle, \tag{6.285a}
\]

\[
|\mp; \hat{\mathbf{u}} \rangle = -\sin \frac{\theta}{2} e^{-i\frac{\pi}{2}} |+\rangle + \cos \frac{\theta}{2} e^{i\frac{\pi}{2}} |-\rangle, \tag{6.285b}
\]

where the states \(|\pm\rangle\) are eigenvectors of \( \mathbf{S} \cdot \hat{\mathbf{z}} \). Let \( P(\sigma_3, \sigma_2 | \sigma_1) \) be the probability to measure \( \mathbf{S} \cdot \hat{\mathbf{u}} = \sigma_2 (h/2) \) in the second measurement and to measure \( \mathbf{S} \cdot \hat{\mathbf{z}} = \sigma_3 (h/2) \) in the third measurement given that the result of the first measurement was \( \mathbf{S} \cdot \hat{\mathbf{z}} = \sigma_1 (h/2) \), and where \( \sigma_n \in \{\pm, -\} \).

The following holds
6.7. Solutions

\[ P(\pm, \pm\pm) = \left| \langle \pm\pm; \hat{\mathbf{u}} \rangle \right|^2 = \cos^4 \frac{\theta}{2}, \quad (6.286a) \]
\[ P(\pm, -\pm\pm) = \left| \langle \pm\pm; \hat{\mathbf{u}} \rangle \right|^2 = \sin^4 \frac{\theta}{2}, \quad (6.286b) \]
\[ P(-, -\pm\pm) = \left| \langle -\pm\pm; \hat{\mathbf{u}} \rangle \right|^2 = \cos^4 \frac{\theta}{2}, \quad (6.286c) \]
\[ P(-, +\pm\pm) = \left| \langle -\pm\pm; \hat{\mathbf{u}} \rangle \right|^2 = \sin^4 \frac{\theta}{2}, \quad (6.286d) \]

thus independently on what was the result of the first measurement one has

\[ p_{\text{same}} = \cos^4 \frac{\theta}{2} + \sin^4 \frac{\theta}{2} = 1 - \frac{1}{2} \sin^2 \theta. \quad (6.287) \]

17. The Hamiltonian is given by

\[ \mathcal{H} = -\mathbf{\mu} \cdot \mathbf{B}. \quad (6.288) \]

Using Eq. (4.38) for \( \mu_z \) one has

\[ \frac{d}{dt} \langle \mu_z \rangle = \frac{1}{\hbar} \langle [\mu_z, \mathcal{H}] \rangle \]
\[ = -\frac{\gamma^2}{\hbar} (B_x [S_z, S_x] + B_y [S_z, S_y]) \]
\[ = \gamma^2 (B_y S_x - B_x S_y) \]
\[ = \gamma (\mathbf{\mu} \times \mathbf{B}) \cdot \hat{\mathbf{z}}. \quad (6.289) \]

Similar expressions are obtained for \( \mu_x \) and \( \mu_y \) that together can be written in a vector form as

\[ \frac{d}{dt} \langle \mathbf{\mu} \rangle (t) = \gamma \langle \mathbf{\mu} \rangle (t) \times \mathbf{B} (t). \quad (6.290) \]

18. Using Eq. (6.136), which is given by

\[ (\sigma \cdot \mathbf{a}) (\sigma \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i \sigma \cdot (\mathbf{a} \times \mathbf{b}), \quad (6.291) \]

one has

\[ \left[ \sigma \cdot \left( \mathbf{p} - \frac{\mathbf{q}}{c} \mathbf{A} \right) \right]^2 = \left( \mathbf{p} - \frac{\mathbf{q}}{c} \mathbf{A} \right)^2 + i \sigma \cdot ((\mathbf{p} - \mathbf{q}) \times (\mathbf{p} - \mathbf{q} \mathbf{A})) \]
\[ = \left( \mathbf{p} - \frac{\mathbf{q}}{c} \mathbf{A} \right)^2 - \frac{\mathbf{q}}{c} \sigma \cdot (\mathbf{A} \times \mathbf{p} + \mathbf{p} \times \mathbf{A}). \quad (6.292) \]

The \( z \) component of the term \((\mathbf{A} \times \mathbf{p} + \mathbf{p} \times \mathbf{A})\) can be expressed as

\[ (\mathbf{A} \times \mathbf{p} + \mathbf{p} \times \mathbf{A}) \cdot \hat{\mathbf{z}} = A_x p_y - A_y p_x + p_x A_y - p_y A_x \]
\[ = [A_x, p_y] - [A_y, p_x], \quad (6.293) \]
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thus, with the help of Eq. (3.75) one finds that

$$(\mathbf{A} \times \mathbf{p} + \mathbf{p} \times \mathbf{A}) \cdot \hat{z} = i\hbar \left( \frac{dA_y}{dy} - \frac{dA_x}{dx} \right) = -i\hbar (\nabla \times \mathbf{A}) \cdot \hat{z}.$$  \hspace{1cm} (6.294)

Similar results can be obtained for the $x$ and $y$ components, thus

$$\left[ \sigma \cdot \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right) \right]^2 = \left( \mathbf{p} - \frac{q}{c} \mathbf{A} \right)^2 - \frac{q\hbar}{c} \sigma \cdot \mathbf{B}.$$  \hspace{1cm} (6.295)

19. Since

$$\langle j, m | J_x | j, m \rangle = \langle j, m | J_y | j, m \rangle = 0,$$  \hspace{1cm} (6.296)

and

$$J_x^2 + J_y^2 = \mathbf{J}^2 - J_z^2,$$  \hspace{1cm} (6.297)

one finds that

$$\langle j, m | \left[ (\Delta J_x)^2 + (\Delta J_y)^2 \right] | j, m \rangle = \langle j, m | \mathbf{J}^2 | j, m \rangle - \langle j, m | J_z^2 | j, m \rangle = \hbar^2 (j^2 + j - m^2).$$  \hspace{1cm} (6.298)

20. The condition is

$$\mathbf{p} \cdot \mathbf{A} = \mathbf{A} \cdot \mathbf{p},$$  \hspace{1cm} (6.299)

or

$$[p_x, A_x] + [p_y, A_y] + [p_z, A_z] = 0,$$  \hspace{1cm} (6.300)

or using Eq. (3.75)

$$\frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} = 0,$$  \hspace{1cm} (6.301)

or

$$\nabla \cdot \mathbf{A} = 0.$$  \hspace{1cm} (6.302)

21. The Hamiltonian is given by Eq. (1.62)

$$\mathcal{H} = \frac{(\mathbf{p} - \frac{2}{c} \mathbf{A})^2}{2m} + q\varphi,$$  \hspace{1cm} (6.303)

thus, the the coordinates representation of $\mathcal{H} |\alpha\rangle = E |\alpha\rangle$ is given by

$$\langle \mathbf{r}' | \mathcal{H} |\alpha\rangle = E \langle \mathbf{r}' |\alpha\rangle.$$  \hspace{1cm} (6.304)
Using the notation
\[ (r' | \alpha) = \psi(r') \] (6.305)
for the wavefunction together with Eqs. (3.23) and (3.29) one has
\[
\left[ \frac{1}{2m} \left( -i\hbar \nabla - \frac{q}{c} A \right)^2 + q\varphi \right] \psi(r') = E\psi(r').
\] (6.306)

22. The Hamiltonian is given by
\[
H = \left( \frac{\hat{p}^2}{2m} \right) + \frac{p_x^2 + p_y^2}{2m} + \left( \frac{p_y - \frac{eB}{c}}{2m} \right)^2
\]
\[
= \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2 \left( x - \frac{cp_y}{eB} \right)^2 + \frac{p_y^2}{2m}
\] (6.307)
where
\[ \omega_c = \frac{eB}{mc} . \] (6.308)

Using the clue
\[ \psi(x, y, z) = \chi(x) \exp(ik_y y) \exp(ik_z z) \] (6.309)
one finds that the time independent Schrödinger equation for the wavefunction \( \chi(x) \) is thus given by
\[
\left[ \frac{p_x^2}{2m} + \frac{1}{2}m\omega_c^2 \left( x - \frac{cp_y}{eB} \right)^2 \right] \chi(x) = \left( E - \frac{\hbar^2 k_y^2}{2m} \right) \chi(x) ,
\] (6.310)
where \( \hat{p}_x = -i\hbar\partial/\partial x \), thus the eigen energies are given by
\[ E_{n,k} = \hbar\omega_c \left( n + \frac{1}{2} \right) + \frac{\hbar^2 k_y^2}{2m} , \] (6.311)
where \( n \) is integer and \( k \) is real, and the ground state energy is
\[ E_{n=0,k=0} = \frac{\hbar\omega_c}{2} . \] (6.312)

23. Using the gauge \( A = Bx\hat{y} \) the Hamiltonian is given by [see Eq. (1.62)]
\[
H = \left( \frac{\hat{p}^2}{2m} \right) - qEx
\]
\[
= \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \left( \frac{p_y - \frac{eB}{c}}{2m} \right)^2 - qEx .
\] (6.313)
The last two terms can be written as
\[
\left(\frac{p_y - qBx}{e}\right)^2 - qEx = \frac{p_y^2}{2m} + \frac{1}{2}m\omega_c^2 \left[(x - x_0)^2 - x_0^2\right], \tag{6.314}
\]
where
\[
\omega_c = \frac{qB}{mc}, \tag{6.315}
\]
and
\[
x_0 = \frac{me^2}{q^2B^2} \left(qE + \frac{qpy}{mc}\right). \tag{6.316}
\]
Substituting the trial wavefunction
\[
\psi(x, y, z) = \varphi(x) \exp(\text{i}ky) \exp(\text{i}kz), \tag{6.317}
\]
into the three dimensional Schrödinger equation yields a one dimensional Schrödinger equation
\[
\left[ \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega_c^2 (x - \tilde{x}_0)^2 - \frac{1}{2}m\omega_c^2 \tilde{x}_0^2 + \frac{h^2k_y^2 + h^2k_z^2}{2m} \right] \varphi(x) = E\varphi(x), \tag{6.318}
\]
where \(\hat{p}_x = -\text{i}\hbar \frac{\partial}{\partial x}\) and where
\[
\tilde{x}_0 = \frac{mc^2}{q^2B^2} \left(qE + \frac{qhk_y}{mcB}\right). \tag{6.319}
\]
This equation describes a harmonic oscillator with a minimum potential at \(x = \tilde{x}_0\), with added constant terms that give rise to a shift in the energy level, which are thus given by
\[
E_{n, k_y, k_z} = \hbar\omega_c \left(n + \frac{1}{2}\right) - \frac{1}{2}m\omega_c^2 \tilde{x}_0^2 + \frac{\hbar^2k_y^2 + \hbar^2k_z^2}{2m} \\
= \hbar\omega_c \left(n + \frac{1}{2}\right) - \frac{mc^2E^2}{2B^2} - \frac{\text{ch}k_yE}{B} + \frac{\hbar^2k_z^2}{2m}, \tag{6.320}
\]
where \(n = 0, 1, 2, \cdots\) and where the momentum variables \(k_y\) and \(k_z\) can take any real value.

24. The Schrödinger equation reads
\[
\left[ \frac{\left(\hat{p} - \frac{qA}{e}\right)^2}{2m} + U(y) \right] \psi(x, y) = E\psi(x, y), \tag{6.321}
\]
6.7. Solutions

Employing the gauge \( A = -By\hat{x} \) one has

\[
\frac{\hat{p}^2}{2m} + \frac{(\hat{p}_x + \frac{e}{\hbar}By)^2}{2m} + \frac{\hat{p}_y^2}{2m} + U(y) \psi(x, y) = E\psi(x, y) ,
\]

(6.322)

where \( \hat{p}_x = -i\hbar \partial/\partial x \) and \( \hat{p}_y = -i\hbar \partial/\partial y \). By substituting the trial wavefunction

\[
\psi(x, y) = \exp(ikx) \chi(y) ,
\]

(6.323)

one obtains a one dimensional Schrödinger equation for \( \chi(y) \)

\[
\frac{\hat{p}_y^2}{2m} + \left( \frac{\hat{p}_x + \frac{e}{\hbar}By + \hbar k}{2m} \right)^2 + \frac{1}{2}m\omega^2_0 y^2 \chi(y) = E\chi(y) ,
\]

(6.324)

or

\[
\frac{\hat{p}_y^2}{2m} + \frac{\hbar^2 k^2}{2m} + \frac{1}{2}m\omega^2_0 y^2 - \frac{eB\hbar k}{mc} y \chi(y) = E\chi(y) ,
\]

(6.325)

where \( \omega^2_0 \equiv \omega^2 + \omega^2_0 \) and \( \omega = |e| B/mc \). This can also be written as

\[
\frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega^2_0 \left( y - \frac{eB\hbar k}{m^2\omega^2_0} \right)^2 + \frac{\hbar^2 k^2}{2m} \frac{\omega^2_0}{\omega^2_{c0}} \chi(y) = E\chi(y) .
\]

(6.326)

This is basically a one-dimensional Schrödinger equation with a parabolic potential of an harmonic oscillator and the eigenenergies are thus given by:

\[
E(n, k) = \hbar \omega_{c0} \left( n + \frac{1}{2} \right) + \hbar^2 k^2 \frac{\omega^2}{2m} \frac{\omega^2_{c0}}{\omega^2_{c0}} ,
\]

where \( n = 0, 1, 2, \cdots \) and \( k \) is real.

25. It is convenient to choose a gauge having cylindrical symmetry, namely

\[
A = -\frac{\hbar}{2} r \times B .
\]

(6.327)

For this gauge \( \nabla \cdot A = 0 \), thus according to Eq. (6.157) the Hamiltonian is given by

\[
\mathcal{H} = \frac{1}{2\mu} p^2 - \frac{q}{\mu c} p \cdot A + \frac{q^2}{2\mu c^2} A^2 .
\]

(6.328)
Chapter 6. Angular Momentum

The Schrödinger equation in cylindrical coordinates \((\rho, z, \phi)\) is given by (note that \(A = \left(\frac{\rho B}{2}\right) \hat{\phi}\))

\[ -\frac{\hbar^2}{2\mu} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + \frac{i\hbar B}{2\mu c} \frac{\partial \psi}{\partial \phi} + \frac{q^2}{2\mu c^2} \left( \frac{\rho B}{2} \right)^2 \psi = E\psi . \] (6.329)

The particle is constrained to move along the ring, which is located at \(z = 0\) and \(\rho = a\), thus the effective one dimensional Schrödinger equation of the system is given by

\[ -\frac{\hbar^2}{2\mu a^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{i\hbar q B}{2\mu c} \frac{\partial \psi}{\partial \phi} + \frac{q^2 a^2 B^2}{8\mu c^2} \psi = E\psi . \] (6.330)

a) Consider a solution of the form

\[ \psi (\phi) = \frac{1}{\sqrt{2\pi a}} \exp (im\phi) , \] (6.331)

where the pre factor \((2\pi a)^{-1/2}\) ensures normalization. The continuity requirement that \(\psi (2\pi) = \psi (0)\) implies that \(m\) must be an integer. Substituting this solution into the Schrödinger equation (6.330) yields

\[ E_m = \frac{\hbar^2 m^2}{2\mu a^2} - \frac{\hbar q B m}{2\mu c} + \frac{q^2 a^2 B^2}{8\mu c^2} \]
\[ = \frac{\hbar^2}{2\mu a^2} \left( m^2 - \frac{q B a^2}{ch} m + \frac{1}{4} \left( \frac{q B a^2}{ch} \right)^2 \right) \]
\[ = \frac{\hbar^2}{2\mu a^2} \left( m - \frac{q B a^2}{2ch} \right)^2 \]
\[ = \frac{\hbar^2}{2\mu a^2} \left( m - \frac{\phi}{\Phi_0} \right)^2 , \] (6.332)

where

\[ \Phi = B\pi a^2 , \] (6.333)

is the magnetic flux threading the ring and

\[ \Phi_0 = \frac{ch}{q} . \] (6.334)

b) In general the current density is given by Eq. (4.159). For a wavefunction having the form

\[ \psi (r) = \alpha (r) e^{i\beta(r)} , \] (6.335)
where both $\alpha$ and $\beta$ are real, one has
\[
J = \frac{\hbar}{\mu} \operatorname{Im} [\alpha (\nabla (\alpha) + \alpha \nabla (i\beta))] - q \frac{\mu c}{\mu c^2} (\rho A)
\]
\[
= \frac{\hbar \alpha^2}{\mu} \nabla (\beta) - q \frac{\mu c}{\mu c^2} A
\]
\[
= \frac{|\psi|^2}{\mu} \left( \hbar \nabla (\beta) - \frac{q}{c} A \right).
\]

(6.336)

In the present case one has
\[
A = \frac{\rho B \hat{\phi}}{2},
\]
\[
\nabla (\beta) = \frac{m}{a} \hat{\phi},
\]
and the normalized wavefunctions are
\[
\psi_m (\phi) = \frac{1}{\sqrt{2\pi a}} \exp (im\phi),
\]
\[
(6.339)
\]

thus
\[
J_m = \frac{1}{2\pi a \mu} \left( \frac{ma}{a} \frac{q a B}{c \cdot 2} \hat{\phi} = \frac{h}{2\pi a^2 \mu} \left( m - \frac{\hat{\phi}}{\Phi_0} \right) \hat{\phi}.
\]
\[
(6.340)
\]

Note that the following holds
\[
|J_m| = \frac{c}{q} \frac{\partial E_m}{\partial \hat{\Phi}}.
\]
\[
(6.341)
\]

26. The Hamiltonian can be written as
\[
\mathcal{H} = \frac{L_z^2}{2I_{xy}} + \frac{L_z^2}{2I_z}
\]
\[
= \frac{L_z^2}{2I_{xy}} + \left( \frac{1}{2I_z} - \frac{1}{2I_{xy}} \right) L_z^2,
\]
\[
(6.342)
\]

Thus the states $|l, m\rangle$ (the standard eigenstates of $L_z$ and $L_z$) are eigenstates of $\mathcal{H}$ and the following holds
\[
\mathcal{H} |l, m\rangle = E_{l,m} |l, m\rangle,
\]
\[
(6.343)
\]

where
\[
E_{l,m} = \hbar^2 \left[ \frac{l(l+1)}{2I_{xy}} + \left( \frac{1}{2I_z} - \frac{1}{2I_{xy}} \right) m^2 \right].
\]
\[
(6.344)
\]

Using the expression
Chapter 6. Angular Momentum

\[ Y^\pm_1 (\theta, \phi) = \mp \sqrt{3 \over 8\pi} \sin \theta e^{\pm i \phi}, \quad (6.345) \]

one finds that
\[ \sin \theta \cos \phi = \sqrt{2 \pi \over 3} (Y^{-1}_1 - Y^1_1), \quad (6.346) \]

thus the normalized state at \( t = 0 \) can be written as
\[ |\psi(0)\rangle = \frac{1}{\sqrt{2}} (|1, -1\rangle - |1, 1\rangle), \quad (6.347) \]

Since \( E_1, -1 = E_1, 1 \) the state \( |\psi(0)\rangle \) is stationary. Moreover
\[
\langle \psi(t) | L_z | \psi(t) \rangle = \langle \psi(0) | L_z | \psi(0) \rangle \\
= \frac{1}{2} \left( \langle (1, -1) - (1, 1) \rangle L_z \langle (1, -1) - (1, 1) \rangle \right) \\
= \frac{1}{2} \left( \langle (1, -1) - (1, 1) \rangle \langle -1, -1 - |1, 1\rangle \rangle \right) \\
= 0. \quad (6.348)
\]

27. With the help of the relations
\[
L_x = \frac{L_+ + L_-}{2}, \quad (6.349) \\
L_+ |l, m\rangle = \hbar \sqrt{l(l+1) - m(m+1)} |l, m+1\rangle, \quad (6.350) \\
L_- |l, m\rangle = \hbar \sqrt{l(l+1) - m(m-1)} |l, m-1\rangle. \quad (6.351)
\]

one finds
a)
\[
L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (6.352)
\]

b)
\[
\langle L_x \rangle = \frac{\hbar}{\sqrt{2}} \left( \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \right) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2} \\ \sqrt{2} \end{pmatrix} = \hbar. \quad (6.353)
\]

c)
\[
\langle L_x \rangle = \frac{\hbar}{\sqrt{2}} \left( -\frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \right) \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -\frac{1}{\sqrt{2}} \\ 0 \end{pmatrix} = 0. \quad (6.354)
\]
d) 
\[ D_z(\phi) = \exp \left( -\frac{i\phi L_z}{\hbar} \right) = \begin{pmatrix} 
\exp(-i\phi) & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & \exp(i\phi) 
\end{pmatrix} \] . \quad (6.355)

e) In general
\[ D_\hat{n}(d\phi) = \exp \left( \frac{i(d\phi) \hat{L} \cdot \hat{\mathbf{n}}}{\hbar} \right) = 1 - \frac{i(d\phi) \hat{L} \cdot \hat{\mathbf{n}}}{\hbar} + O \left( (d\phi)^2 \right) , \] 
thus
\[ D_\hat{x}(d\phi) = \begin{pmatrix} 
1 - \frac{i(d\phi)}{\sqrt{2}} & 0 & 0 \\
0 & 1 & \frac{i(d\phi)}{\sqrt{2}} \\
0 & \frac{i(d\phi)}{\sqrt{2}} & 1 
\end{pmatrix} + O \left( (d\phi)^2 \right) . \quad (6.357)

28. Using
\[ L_z = xp_y - yp_x \ , \] \quad (6.358)
\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a_x + a_x^\dagger) \ , \] \quad (6.359)
\[ y = \sqrt{\frac{\hbar}{2m\omega}} (a_y + a_y^\dagger) \ , \] \quad (6.360)
\[ p_x = i \sqrt{\frac{m\hbar}{2}} (a_x + a_x^\dagger) \ , \] \quad (6.361)
\[ p_y = i \sqrt{\frac{m\hbar}{2}} (a_y + a_y^\dagger) \ , \] \quad (6.362)
one finds
\[ L_z = \frac{i\hbar}{2} \left[ (a_x + a_x^\dagger)(-a_y + a_y^\dagger) - (a_y + a_y^\dagger)(-a_x + a_x^\dagger) \right] \]
\[ = i\hbar \left( a_x a_y^\dagger - a_x^\dagger a_y \right) . \] \quad (6.363)
a) Thus
\[ \langle L_z \rangle = i\hbar \left( a_x a_y^\dagger - a_x^\dagger a_y \right) . \] \quad (6.364)
b) Using the commutation relations
\[ [a_x, a_y^\dagger] = 1 \ , \] \quad (6.365)
\[ [a_y, a_y^\dagger] = 1 \ , \] \quad (6.366)
one finds
\[ \langle L_z^2 \rangle = -\hbar^2 (\alpha_x, \alpha_y, \alpha_z) (\alpha_x \alpha_y^* - \alpha_y \alpha_x^*) (\alpha_x \alpha_y^* - \alpha_y \alpha_x^*) \langle \alpha_x, \alpha_y, \alpha_z \rangle \]
\[ = \hbar^2 \left[ |\alpha_x|^2 \left( 1 + |\alpha_y|^2 \right) + |\alpha_y|^2 \left( 1 + |\alpha_x|^2 \right) - (\alpha_x \alpha_y^*)^2 - (\alpha_y \alpha_x^*)^2 \right], \]
(6.367)

thus
\[ (\Delta L_z)^2 = \hbar^2 \left[ |\alpha_x|^2 \left( 1 + |\alpha_y|^2 \right) + |\alpha_y|^2 \left( 1 + |\alpha_x|^2 \right) + (\alpha_x \alpha_y^*)^2 - (\alpha_y \alpha_x^*)^2 \right] \]
\[ = \hbar^2 \left[ (|\alpha_x|^2 + |\alpha_y|^2) \right], \]
(6.368)

\[ \Delta L_z = \hbar \sqrt{|\alpha_x|^2 + |\alpha_y|^2}. \] (6.369)

29. The normalization constant can be chosen to be \( A = 1/\sqrt{2} \). In general:
\[ L_x = \frac{L_+ + L_-}{2}, \] (6.370)
\[ L_+ |l, m\rangle = \sqrt{l(l+1) - m(m+1)} |l, m+1\rangle, \] (6.371)
\[ L_- |l, m\rangle = \sqrt{l(l+1) - m(m-1)} |l, m-1\rangle. \] (6.372)

a) The following holds
\[ L_x |\alpha\rangle = \frac{(L_- |l, 1\rangle - L_+ |l, -1\rangle)}{2\sqrt{2}} \]
\[ = \frac{\hbar (|1, 0\rangle - |1, 0\rangle)}{2} = 0, \] (6.373)

thus
\[ \langle L_x \rangle = 0. \] (6.374)

b) Using \( L_x |\alpha\rangle = 0 \) one finds
\[ \left\langle (\Delta L_x)^2 \right\rangle = \langle L_x^2 \rangle - \langle L_x \rangle^2 = 0 - 0 = 0. \] (6.375)

30. The Hamiltonian can be expressed as
\[ \mathcal{H} = \frac{L_x^2}{2I_1} + \frac{L_y^2}{2I_2} - \frac{L_z^2}{2I_1} = \frac{L_x^2}{2I_1} + \frac{L_z^2}{2I_e}, \] (6.376)

where
\[ I_e = \frac{I_1 I_2}{I_1 - I_2}. \] (6.377)

Thus, the angular momentum states \(|l, m\rangle\), which satisfy
6.7. Solutions

\( L^2 |l, m\rangle = l(l + 1) \hbar^2 |l, m\rangle \),  \( (6.378) \)
\( L_z |l, m\rangle = m \hbar |l, m\rangle \),  \( (6.379) \)

are eigenvector of \( \mathcal{H} \)

\( \mathcal{H} |l, m\rangle = E_{l,m} |l, m\rangle \),  \( (6.380) \)

where

\[
E_{l,m} = \frac{l(l+1)\hbar^2}{2I_1} + \frac{m^2\hbar^2}{2I_c} = \frac{\hbar^2}{2I_1} \left( l(l+1) - m^2 + m^2 \frac{I_1}{I_2} \right). \quad (6.381)
\]

a) Since \([\mathcal{H}, L_z] = 0\) one has

\[
\exp \left( \frac{iL_z \phi}{\hbar} \right) \mathcal{H} \exp \left( -\frac{iL_z \phi}{\hbar} \right) = \mathcal{H},
\]

thus for the ground state \( l = m = 0 \)

\[ A_z (\phi) = \langle \psi_0 | \mathcal{H} | \psi_0 \rangle = E_{0,0} = 0. \quad (6.383) \]

b) The operator \( L_x \) can be expressed as

\[
L_x = \frac{L_+ + L_-}{2}. \quad (6.384)
\]

In general

\[
L_+ |l, m\rangle = \hbar \sqrt{I(l+1) - m(m+1)} |l, m+1\rangle, \quad (6.385)
\]
\[
L_- |l, m\rangle = \hbar \sqrt{I(l+1) - m(m-1)} |l, m-1\rangle, \quad (6.386)
\]

thus

\[
L_+ |0, 0\rangle = L_- |0, 0\rangle = 0, \quad (6.387)
\]

and consequently

\[
\exp \left( -\frac{iL_x \phi}{\hbar} \right) |\psi_0\rangle = |\psi_0\rangle, \quad (6.388)
\]

thus

\[ A_x (\phi) = \langle \psi_0 | \mathcal{H} | \psi_0 \rangle = E_{0,0} = 0. \quad (6.389) \]
7. Central Potential

Consider a particle having mass $m$ in a central potential, namely a potential $V(r)$ that depends only on the distance

$$r = \sqrt{x^2 + y^2 + z^2}$$

(7.1)

from the origin. The Hamiltonian is given by

$$\mathcal{H} = \frac{p^2}{2m} + V(r).$$

(7.2)

**Exercise 7.0.1.** Show that

$$[\mathcal{H}, L_z] = 0,$$

(7.3)

$$[\mathcal{H}, L^2] = 0.$$  

(7.4)

**Solution 7.0.1.** Using

$$[x_i, p_j] = i\hbar \delta_{ij},$$

$$L_z = xp_y - yp_x,$$

(7.5)

(7.6)

one has

$$[p^2, L_z] = \left[ p_x^2, L_z \right] + \left[ p_y^2, L_z \right] + \left[ p_z^2, L_z \right]$$

$$= \left[ p_x^2, xp_y \right] - \left[ p_y^2, yp_x \right]$$

$$= i\hbar (-2pxp_y + 2pypx)$$

$$= 0,$$

(7.7)

and

$$[r^2, L_z] = \left[ x^2, L_z \right] + \left[ y^2, L_z \right] + \left[ z^2, L_z \right]$$

$$= -y \left[ x^2, px \right] + \left[ y^2, py \right] x$$

$$= 0.$$  

(7.8)

Thus $L_z$ commutes with any smooth function of $r^2$, and consequently $[\mathcal{H}, L_z] = 0$. In a similar way one can show that $[\mathcal{H}, L_x] = [\mathcal{H}, L_y] = 0$, and therefore $[\mathcal{H}, L^2] = 0$. 
Chapter 7. Central Potential

In classical physics the corresponding Poisson's brackets relations hold

\[ \{ \mathcal{H}, L_x \} = \{ \mathcal{H}, L_y \} = \{ \mathcal{H}, L_z \} = 0 , \tag{7.9} \]

and

\[ \{ \mathcal{H}, L^2 \} = 0 . \tag{7.10} \]

These relations imply that classically the angular momentum is a constant of the motion [see Eq. (1.40)]. On the other in quantum mechanics, as we have seen in section 2.12 of chapter 2, the commutation relations

\[ [\mathcal{H}, L_z] = 0 , \tag{7.11} \]
\[ [\mathcal{H}, L^2] = 0 , \tag{7.12} \]

imply that it is possible to find a basis for the vector space made of common eigenvectors of the operators \( \mathcal{H}, L^2 \) and \( L_z \).

7.1 Simultaneous Diagonalization of the Operators \( \mathcal{H}, L^2 \) and \( L_z \)

We start by proving some useful relations:

Exercise 7.1.1. Show that

\[ L^2 = r^2 p^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i \hbar \mathbf{r} \cdot \mathbf{p} . \tag{7.13} \]

Solution 7.1.1. The following holds

\[ L_z^2 = (xp_y - yp_x)^2 \]
\[ = x^2 p_y^2 + y^2 p_x^2 - xp_y y p_x - yp_x x p_y \]
\[ = x^2 y^2 p_x^2 + y^2 x^2 p_y^2 - x^2 p_x p_y - y^2 p_x p_y \]
\[ = x^2 p_y^2 + y^2 p_x^2 - x p_x y p_y - y p_y x p_x + i \hbar (x p_x + y p_y) . \tag{7.14} \]

Using the relation

\[ xp_x p_x = x ([p_x, x] + xp_x) p_x = -i \hbar p_x + x^2 p_x^2 , \tag{7.15} \]

or

\[ i \hbar p_x = x^2 p_x^2 - xp_x p_x , \tag{7.16} \]

one has
Exercise 7.1.2. Show that

\[ L_z^2 = x^2 p_y^2 + y^2 p_z^2 - xp_y y p_y - y p_y x p_x + \frac{i \hbar}{2} (x p_x + y p_y) + \frac{1}{2} (x^2 p_z^2 - x p_x x p_z + y^2 p_y^2 - y p_y y p_y) . \]  

(7.17)

By cyclic permutation one obtains similar expression for \( L_x^2 \) and for \( L_y^2 \). Combining these expressions lead to

\[ \mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2 \]

\[ = y^2 p_z^2 + z^2 p_y^2 - y p_y z p_z - z p_z y p_y + \frac{i \hbar}{2} (y p_y + z p_z) + \frac{1}{2} (y^2 p_z^2 - y p_y z p_z + z^2 p_y^2 - z p_z y p_y) \]

\[ + z^2 p_z^2 + x^2 p_y^2 - z p_z x p_z - x p_z z p_z + \frac{i \hbar}{2} (z p_z + x p_x) + \frac{1}{2} (z^2 p_z^2 - z p_z x p_z + x^2 p_y^2 - x p_y z p_y) \]

\[ + x^2 p_y^2 + y^2 p_z^2 - x p_x y p_x - y p_y y p_y + \frac{i \hbar}{2} (x p_x + y p_y) + \frac{1}{2} (x^2 p_z^2 - x p_x y p_x + y^2 p_y^2 - y p_y y p_y) \]

\[ = (x^2 + y^2 + z^2) (p_x^2 + p_y^2 + p_z^2) - (x p_x + y p_y + z p_z)^2 + i \hbar (x p_x + y p_y + z p_z) \]

\[ = r^2 \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i \hbar \mathbf{r} \cdot \mathbf{p} . \]  

(7.18)

Exercise 7.1.2. Show that

\[ \langle \mathbf{r}' \mid \mathbf{p}^2 \mid \alpha \rangle = -\hbar^2 \left( \frac{1}{r^2} \frac{\partial^2}{\partial r^2} \langle \mathbf{r}' \mid \alpha \rangle - \frac{1}{r^2} \langle \mathbf{r}' \mid \mathbf{L}^2 \mid \alpha \rangle \right) . \]  

(7.19)

Solution 7.1.2. Using the identities

\[ \mathbf{L}^2 = r^2 \mathbf{p}^2 - (\mathbf{r} \cdot \mathbf{p})^2 + i \hbar \mathbf{r} \cdot \mathbf{p} , \]

\[ \langle \mathbf{r}' \mid \mathbf{r} \mid \alpha \rangle = r' \langle \mathbf{r}' \mid \alpha \rangle , \]  

(7.20)

(7.21)

and

\[ \langle \mathbf{r}' \mid \mathbf{p} \mid \alpha \rangle = \frac{\hbar}{i} \nabla \langle \mathbf{r}' \mid \alpha \rangle , \]  

(7.22)

one finds that

\[ \langle \mathbf{r}' \mid \mathbf{L}^2 \mid \alpha \rangle = \langle \mathbf{r}' \mid r^2 \mathbf{p}^2 \mid \alpha \rangle - \langle \mathbf{r}' \mid (\mathbf{r} \cdot \mathbf{p})^2 \mid \alpha \rangle + i \hbar \langle \mathbf{r}' \mid \mathbf{r} \cdot \mathbf{p} \mid \alpha \rangle . \]  

(7.23)

The following hold

\[ \langle \mathbf{r}' \mid \mathbf{r} \cdot \mathbf{p} \mid \alpha \rangle = -i \hbar \mathbf{r}' \cdot \nabla \langle \mathbf{r}' \mid \alpha \rangle = -i \hbar \mathbf{r}' \frac{\partial}{\partial \mathbf{r}'} \langle \mathbf{r}' \mid \alpha \rangle , \]  

(7.24)

\[ \langle \mathbf{r}' \mid (\mathbf{r} \cdot \mathbf{p})^2 \mid \alpha \rangle = -\hbar^2 \left( \mathbf{r}' \frac{\partial}{\partial \mathbf{r}'} \right)^2 \langle \mathbf{r}' \mid \alpha \rangle \]

\[ = -\hbar^2 \left( \mathbf{r}'^2 \frac{\partial^2}{\partial \mathbf{r}'^2} + \mathbf{r}' \frac{\partial}{\partial \mathbf{r}'} \right) \langle \mathbf{r}' \mid \alpha \rangle , \]  

(7.25)
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\[ \langle r' | r^2 \mathbf{p}^2 | \alpha \rangle = r'^2 \langle r' | \mathbf{p}^2 | \alpha \rangle , \]  

(7.26)

thus

\[ \langle r' | \mathbf{p}^2 | \alpha \rangle = -\hbar^2 \left[ \left( \frac{\partial^2}{\partial r'^2} + \frac{2}{r'} \frac{\partial}{\partial r'} \right) \langle r' | \alpha \rangle - \frac{1}{\hbar^2 r'^2} \langle r' | \mathbf{L}^2 | \alpha \rangle \right] , \]  

(7.27)

or

\[ \langle r' | \mathbf{p}^2 | \alpha \rangle = -\hbar^2 \left( \frac{1}{r'} \frac{\partial^2}{\partial r'^2} r' \langle r' | \alpha \rangle - \frac{1}{\hbar^2 r'^2} \langle r' | \mathbf{L}^2 | \alpha \rangle \right) . \]  

(7.28)

The time-independent Schrödinger equation in the coordinates representation

\[ \langle r' | \mathcal{H} | \alpha \rangle = E \langle r' | \alpha \rangle , \]  

(7.29)

where the Hamiltonian \( \mathcal{H} \) is given by Eq. (7.2), can thus be written using the above results as

\[ \langle r' | \mathcal{H} | \alpha \rangle = -\frac{\hbar^2}{2m} \left[ \frac{1}{r'} \frac{\partial^2}{\partial r'^2} r' \langle r' | \alpha \rangle - \frac{1}{\hbar^2 r'^2} \langle r' | \mathbf{L}^2 | \alpha \rangle \right] + V(r') \langle r' | \alpha \rangle . \]  

(7.30)

7.2 The Radial Equation

Consider a solution having the form

\[ \langle r' | \alpha \rangle = \varphi(r') = R(r') Y_{lm}^m (\theta', \phi') . \]  

(7.31)

With the help of Eq. (6.106) one finds that

\[ \langle r' | \mathbf{L}^2 | \alpha \rangle = \hbar^2 l(l + 1) \varphi(r') . \]  

(7.32)

Substituting into Eq. (7.30) yields an equation for \( R(r) \)

\[ -\frac{\hbar^2}{2m} \left[ \frac{1}{r} \frac{d^2}{dr^2} r R(r) - \frac{1}{r^2} l(l + 1) R(r) \right] + V(r) R(r) = E R(r) . \]  

(7.33)

The above equation, which is called the radial equation, depends on the quantum number \( l \), however, it is independent on the quantum number \( m \). The different solutions for a given \( l \) are labeled using the index \( k \)

\[ -\frac{\hbar^2}{2m} \left[ \frac{1}{r} \frac{d^2}{dr^2} r R_{kl} - \frac{1}{r^2} l(l + 1) R_{kl} \right] + V R_{kl} = E R_{kl} . \]  

(7.34)

It is convenient to introduce the function \( u_{kl}(r) \), which is related to \( R_{kl}(r) \) by the following relation

\[ R_{kl}(r) = \frac{1}{r} u_{kl}(r) . \]  

(7.35)
Substituting into Eq. (7.34) yields an equation for \( u_{kl}(r) \)

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right) u_{kl}(r) = E_{kl} u_{kl}(r),
\]

(7.36)

where the effective potential \( V_{\text{eff}}(r) \) is given by

\[
V_{\text{eff}}(r) = \frac{l(l+1)\hbar^2}{2mr^2} + V(r).
\]

(7.37)

The total wave function is thus given by

\[
\varphi_{klm}(r) = \frac{1}{r} u_{kl}(r) Y^m_l(\theta, \phi).
\]

(7.38)

Since the spherical harmonic \( Y^m_l(\theta, \phi) \) is assumed to be normalized [see Eq. (6.113)], to ensure that \( \varphi_{klm}(r) \) is normalized we require that

\[
1 = \int_0^\infty dr r^2 |R_{kl}(r)|^2 = \int_0^\infty dr |u_{kl}(r)|^2.
\]

(7.39)

In addition solutions with different \( k \) are expected to be orthogonal, thus

\[
\int_0^\infty dr u_{kl}^*(r) u_{k'l}(r) = \delta_{kk'}.
\]

(7.40)

The wave functions \( \varphi_{klm}(r) \) represent common eigenstates of the operators \( \mathcal{H}, L_z \) and \( L^2 \), which are denoted as \( |klm\rangle \) and which satisfy the following relations

\[
\varphi_{klm}(r') = \langle r' |klm\rangle,
\]

(7.41)

and

\[
\mathcal{H} |klm\rangle = E_{kl} |klm\rangle,
\]

(7.42)

\[
L^2 |klm\rangle = l(l+1)\hbar^2 |klm\rangle,
\]

(7.43)

\[
L_z |klm\rangle = mh |klm\rangle.
\]

(7.44)

The following claim reveals an important property of the radial wavefunction near the origin \( r = 0 \):

Claim. If the potential energy \( V(r) \) does not diverge more rapidly than \( 1/r \) near the origin then

\[
\lim_{r \to 0} u(r) = 0.
\]

(7.45)
Proof. Consider the case where near the origin \( u(r) \) has a dominant power term having the form \( r^s \) (namely, all other terms are of order higher than \( s \), and thus become negligibly small for sufficiently small \( r \)). Substituting into Eq. (7.36) and keeping only the dominant terms (of lowest order in \( r \)) lead to

\[
-\frac{\hbar^2}{2m} s(s-1) r^{s-2} + \frac{l(l+1)\hbar^2}{2m} r^{s-2} = 0,
\]

thus \( s = -l \) or \( s = l + 1 \). However, the solution \( s = -l \) for \( l \geq 1 \) must be rejected since for this case the normalization condition (7.39) cannot be satisfied as the integral diverges near \( r = 0 \). Moreover, also for \( l = 0 \) the solution \( s = -l \) must be rejected. For this case \( \varphi(r) \propto 1/r \) near the origin, however, such a solution contradicts Eq. (7.30), which can be written as

\[
-\frac{\hbar^2}{2m} \nabla^2 \varphi(r) + V(r) \varphi(r) = E \varphi(r).
\]

since

\[
\nabla^2 \frac{1}{r} = -4\pi \delta(r).
\]

We thus conclude that only the solution \( s = l + 1 \) is acceptable, and consequently \( \lim_{r \to 0} u(r) = 0 \).

### 7.3 Hydrogen Atom

The Hydrogen atom is made of two particles, an electron and a proton. It is convenient to employ the center of mass coordinates system. As is shown below, in this reference frame the two body problem is reduced into a central potential problem of effectively a single particle.

**Exercise 7.3.1.** Consider two point particles having mass \( m_1 \) and \( m_2 \) respectively. The potential energy \( V(r) \) depends only on the relative coordinate \( r = r_1 - r_2 \). Show that the Hamiltonian of the system in the center of mass frame is given by

\[
\mathcal{H} = \frac{p^2}{2\mu} + V(r),
\]

where the reduced mass \( \mu \) is given by

\[
\mu = \frac{m_1 m_2}{m_1 + m_2}.
\]
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Solution 7.3.1. The Lagrangian is given by

\[ \mathcal{L} = \frac{m_1 \dot{r}_1^2}{2} + \frac{m_2 \dot{r}_2^2}{2} - V(r_1 - r_2) . \]  

(7.51)

In terms of center of mass \( r_0 \) and relative \( r \) coordinates, which are given by

\[ r_0 = \frac{m_1 r_1 + m_2 r_2}{m_1 + m_2} , \]  

(7.52)
\[ r = r_1 - r_2 , \]  

(7.53)

the Lagrangian is given by

\[
\mathcal{L} = \frac{m_1 \left( \dot{r}_0 + \frac{m_2}{m_1 + m_2} \dot{k} \right)^2}{2} + \frac{m_2 \left( \dot{r}_0 - \frac{m_1}{m_1 + m_2} \dot{k} \right)^2}{2} - V(r) \\
= \frac{M \dot{r}_0^2}{2} + \frac{\mu \dot{k}^2}{2} - V(r) ,
\]  

(7.54)

where the total mass \( M \) is given by

\[ M = m_1 + m_2 , \]  

(7.55)

and the reduced mass by

\[ \mu = \frac{m_1 m_2}{m_1 + m_2} . \]  

(7.56)

Note that the Euler Lagrange equation for the coordinate \( r_0 \) yields that \( \ddot{r}_0 = 0 \) (since the potential is independent on \( r_0 \)). In the center of mass frame \( r_0 = 0 \). The momentum canonically conjugate to \( r \) is given by

\[ p = \frac{\partial \mathcal{L}}{\partial \dot{r}} . \]  

(7.57)

Thus the Hamiltonian is given by

\[ \mathcal{H} = p \cdot \dot{r} - \mathcal{L} = \frac{p^2}{2\mu} + V(r) . \]  

(7.58)

For the case of Hydrogen atom the potential between the electron having charge \(-e\) and the proton having charge \(e\) is given by

\[ V(r) = \frac{-e^2}{r} . \]  

(7.59)

Since the proton’s mass \( m_p \) is significantly larger than the electron’s mass \( m_e \) \((m_p \simeq 1800 m_e)\) the reduced mass is very close to \( m_e \)

\[ \mu = \frac{m_e m_p}{m_e + m_p} \simeq m_e . \]  

(7.60)
The radial equation (7.36) for the present case is given by
\[
\left( -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_{\text{eff}}(r) \right) u_{kl}(r) = E_{kl}u_{kl}(r) ,
\]
where
\[
V_{\text{eff}}(r) = -\frac{e^2}{r} + \frac{l(l+1)\hbar^2}{2\mu r^2}.
\]
In terms of the dimensionless radial coordinate
\[
\rho = \frac{r}{a_0},
\]
where
\[
a_0 = \frac{\hbar^2}{\mu e^2} = 0.53 \times 10^{-10} \text{ m} ,
\]
is the Bohr’s radius, and in terms of the dimensionless parameter
\[
\lambda_{kl} = \sqrt{\frac{E_{kl}}{E_l}} ,
\]
where
\[
E_l = \frac{\mu e^4}{2\hbar^2} = 13.6 \text{ eV} ,
\]
is the ionization energy, the radial equation becomes
\[
\left( -\frac{d^2}{d\rho^2} + V_l(\rho) + \lambda_{kl}^2 \right) u_{kl} = 0
\]
where
\[
V_l(\rho) = -\frac{2}{\rho} + \frac{l(l+1)}{\rho^2} .
\]

The function $V_l(\rho)$ for $l = 0$ (solid line) and $l = 1$ (dashed line).
We seek solutions of Eq. (7.67) that represent bound states, for which \( E_{kl} \) is negative, and thus \( \lambda_{kl} \) is a nonvanishing real positive. In the limit \( \rho \to \infty \) the potential \( V_l(\rho) \to 0 \), and thus it becomes negligibly small in comparison with \( \lambda_{kl} \) [see Eq. (7.67)]. Therefore, in this limit the solution is expected to be asymptotically proportional to \( e^{\pm \lambda_{kl} \rho} \). To ensure that the solution is normalizable the exponentially diverging solution \( e^{+ \lambda_{kl} \rho} \) is excluded. Moreover, as we have seen above, for small \( \rho \) the solution is expected to be proportional to \( \rho^{l+1} \). Due to these considerations we express \( u_{kl}(r) \) as

\[
\begin{align*}
  u_{kl}(r) &= y(\rho) \rho^{l+1} e^{-\lambda_{kl} \rho} .
\end{align*}
\]

Substituting into Eq. (7.67) yields an equation for the function \( y(\rho) \)

\[
\left[ \frac{d^2}{d\rho^2} + 2 \left( \frac{l+1}{\rho} - \lambda_{kl} \right) \frac{d}{d\rho} + \frac{2(1 - \lambda_{kl}(l+1))}{\rho} \right] y = 0 .
\]

Consider a power series expansion of the function \( y(\rho) \)

\[
y(\rho) = \sum_{q=0}^{\infty} c_q \rho^q .
\]

Substituting into Eq. (7.70) yields

\[
\begin{align*}
  \sum_{q=0}^{\infty} q(q-1)c_q \rho^{q-2} + 2(l+1) \sum_{q=0}^{\infty} c_q \rho^{q-2} \\
  -2\lambda_{kl} \sum_{q=0}^{\infty} q c_q \rho^{q-1} + 2(1 - \lambda_{kl}(l+1)) \sum_{q=0}^{\infty} c_q \rho^{q-1} &= 0 ,
\end{align*}
\]

thus

\[
\frac{c_q}{c_{q-1}} = \frac{2[\lambda_{kl}(q+l) - 1]}{q(q+2l+1)} .
\]

We argue below that for physically acceptable solutions \( y(\rho) \) must be a polynomial function [i.e. the series (7.71) needs to be finite]. To see this note that for large \( q \) Eq. (7.73) implies that

\[
\lim_{q \to \infty} \frac{c_q}{c_{q-1}} = \frac{2\lambda_{kl}}{q} .
\]

Similar recursion relation holds for the coefficients of the power series expansion of the function \( e^{2\lambda_{kl} \rho} \)

\[
e^{2\lambda_{kl} \rho} = \sum_{q=0}^{\infty} \tilde{c}_q \rho^q ,
\]

where
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\[ \tilde{c}_q = \frac{(2\lambda_{kl})^q}{q!}, \]  

(7.76)

thus

\[ \frac{\tilde{c}_q}{\tilde{c}_{q-1}} = \frac{2\lambda_{kl}}{q}. \]  

(7.77)

This observation suggests that for large \( \rho \) the function \( u_{kl} \) asymptotically becomes proportional to \( e^{\lambda_{kl}\rho} \). However, such an exponentially diverging solution must be excluded since it cannot be normalized. Therefore, to avoid such a discrepancy, we require that \( y(\rho) \) must be a polynomial function.

As can be seen from Eq. (7.73), this requirement is satisfied provided that \( \lambda_{kl} (q + l) - 1 = 0 \) for some \( q \). A polynomial function of order \( k - 1 \) is obtained when \( \lambda_{kl} \) is taken to be given by

\[ \lambda_{kl} = \frac{1}{k + l}, \]  

(7.78)

where \( k = 1, 2, 3, \ldots \). With the help of Eq. (7.73) the polynomial function can be evaluated. Some examples are given below

\[ y_{k=1,l=0}(\rho) = c_0, \]  

(7.79)

\[ y_{k=1,l=1}(\rho) = c_0, \]  

(7.80)

\[ y_{k=2,l=0}(\rho) = c_0 \left( 1 - \frac{\rho}{2} \right), \]  

(7.81)

\[ y_{k=2,l=1}(\rho) = c_0 \left( 1 - \frac{\rho}{6} \right). \]  

(7.82)

The coefficient \( c_0 \) can be determined from the normalization condition.

As can be seen from Eqs. (7.65) and (7.78), all states having the same sum \( k + l \), which is denoted as

\[ n = k + l, \]  

(7.83)

have the same energy. The index \( n \) is called the principle quantum number. Due to this degeneracy, which is sometimes called accidental degeneracy, it is common to label the states with the indices \( n, l \) and \( m \), instead of \( k, l \) and \( m \). In such labeling the eigenenergies are given by

\[ E_n = -\frac{E_1}{n^2}, \]  

(7.84)

where

\[ n = 1, 2, \ldots. \]  

(7.85)

For a given \( n \) the quantum number \( l \) can take any of the possible values

\[ l = 0, 1, 2, \ldots, n - 1, \]  

(7.86)
and the quantum number \( m \) can take any of the possible values

\[
m = -l, -l + 1, \ldots, l - 1, l.
\]  

(7.87)

The level of degeneracy of the level \( E_n \) is given by

\[
g_n = 2 \sum_{l=0}^{n-1} (2l + 1) = 2 \left( \frac{(n-1)n}{2} + n \right) = 2n^2.
\]

(7.88)

Note that the factor of 2 is due to spin. The normalized radial wave functions of the states with \( n = 1 \) and \( n = 2 \) are found to be given by

\[
R_{10}(r) = 2 \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0},
\]

(7.89)

\[
R_{20}(r) = \left( 2 - \frac{r}{a_0} \right) \left( \frac{1}{2a_0} \right)^{3/2} e^{-r/a_0},
\]

(7.90)

\[
R_{21}(r) = \left( \frac{1}{2a_0} \right)^{3/2} \frac{r}{\sqrt{3} a_0} e^{-r/3a_0}.
\]

(7.91)

The wavefunction \( \varphi_{n,l,m}(r) \) of an eigenstate with quantum numbers \( n, l \) and \( m \) is given by

\[
\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_{l}^{m}(\theta,\phi).
\]

(7.92)

While the index \( n \) labels the shell number, the index \( l \) labels the sub-shell. In spectroscopy it is common to label different sub-shells with letters:

\[
\begin{align*}
  l = 0 & \text{ s} \\
  l = 1 & \text{ p} \\
  l = 2 & \text{ d} \\
  l = 3 & \text{ f} \\
  l = 4 & \text{ g}
\end{align*}
\]

7.4 Problems

1. Consider the wave function with quantum numbers \( n, l, \) and \( m \) of a hydrogen atom \( \varphi_{n,l,m}(r) \).
   a) Show that the probability current in spherical coordinates \( r, \theta, \varphi \) is given by

\[
J_{n,l,m}(r) = \frac{\hbar}{\mu} m \left| \frac{\varphi_{n,l,m}(r)}{r \sin \theta} \right|^2 \hat{\phi},
\]

(7.93)

where \( \mu \) is the reduced mass and \( \hat{\phi} \) is a unit vector orthogonal to \( \hat{z} \) and \( \hat{r} \).
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b) Use the result of the previous section to show that the total angular momentum is given by \( L = m \hat{\mathbf{z}} \).

2. Show that the average electrostatic potential in the neighborhood of an Hydrogen atom in its ground state is given by

\[
\varphi = e \left( \frac{1}{a_0} + \frac{1}{r} \right) \exp \left( -\frac{2r}{a_0} \right),
\]

where \( a_0 \) is the Bohr radius.

3. An hydrogen atom is in its ground state. The distance \( r \) between the electron and the proton is measured. Calculate the expectation value \( \langle r \rangle \) and the most probable value \( r_0 \) (at which the probability density obtains a maximum).

4. Tritium, which is labeled as \(^3\text{H}\), is a radioactive isotope of hydrogen. The nucleus of tritium contains 1 proton and two neutrons. An atom of tritium is in its ground state, when the nucleus suddenly decays into a Helium nucleus, with the emission of a fast electron, which leaves the atom without perturbing the extra-nuclear electron. Find the probability that the resulting \( \text{He}^+ \) ion will be left in:

a) 1s state.

b) 2s state.

c) a state with \( l \neq 0 \).

5. At time \( t = 0 \) an Hydrogen atom is in the state

\[
|\alpha(t=0)\rangle = A (|2, 1, -1\rangle + |2, 1, 1\rangle),
\]

where \( A \) is a normalization constant and where \( |n, l, m\rangle \) denotes the eigenstate with quantum numbers \( n, l \) and \( m \). Calculate the expectation value \( \langle x \rangle \) at time \( t \).

6. Consider a particle having mass \( m \) in a 3D potential given by

\[
V(r) = -A\delta(r-a),
\]

where \( r = \sqrt{x^2 + y^2 + z^2} \) is the radial coordinate, the length \( a \) is a constant and \( \delta() \) is the delta function. For what range of values of the constant \( A \) the particle has a bound state.

7. A spinless point particle is in state \( |\gamma\rangle \). The state vector \( |\gamma\rangle \) is an eigenvector of the operators \( L_x, L_y \) and \( L_z \) (the \( x, y \) and \( z \) components of the angular momentum vector operator). What can be said about the wavefunction \( \psi(r') \) of the state \( |\gamma\rangle \)?

7.5 Solutions

1. In general the current density is given by Eq. (4.159). For a wavefunction having the form
7.5. Solutions

\[ \psi(r) = \alpha(r) e^{i\beta(r)}, \]  

(7.96)

where both \( \alpha \) and \( \beta \) are real, one has

\[ J = \frac{\hbar}{\mu} \text{Im} [\alpha (\nabla (\alpha) + \alpha \nabla (i\beta))] \]
\[ = \frac{\hbar \alpha^2}{\mu} \nabla (\beta) \]
\[ = \frac{\hbar |\psi|^2}{\mu} \nabla (\beta). \]  

(7.97)

\( a) \) The wavefunction \( \varphi_{n,l,m}(r) \) is given by

\[ \psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{ml}^{m}(\theta, \phi) = R_{nl}(r) F_{ml}^{m}(\theta) e^{im\phi}, \]  

(7.98)

where both \( R_{nl} \) and \( F_{ml}^{m} \) are real, thus

\[ J_{n,l,m}(r) = \frac{\hbar}{\mu} \frac{|\varphi_{n,l,m}(r)|^2}{r} \nabla (m\phi). \]  

(7.99)

In spherical coordinates one has

\[ \nabla = \hat{\mathbf{r}} \frac{\partial}{\partial r} + \hat{\mathbf{\theta}} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\mathbf{\phi}} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}, \]  

(7.100)

thus

\[ J_{n,l,m}(r) = \frac{\hbar}{\mu} \frac{|\varphi_{n,l,m}(r)|^2}{r \sin \theta} \hat{\mathbf{\phi}}. \]  

(7.101)

\( b) \) The contribution of the volume element \( d^3r \) to the angular momentum with respect to the origin is given by \( dL = \mu r \times J_{n,l,m}(r) d^3r \).

In spherical coordinates the total angular momentum is given by

\[ L = \int \mu r \times J_{n,l,m}(r) d^3r = m \hbar \int \frac{|\varphi_{n,l,m}(r)|^2}{r \sin \theta} r \times \hat{\varphi} d^3r. \]  

(7.102)

By symmetry, only the component along \( \hat{\mathbf{z}} \) of \( r \times \varphi \) contributes, thus

\[ L = m \hbar \hat{\mathbf{z}}. \]  

(7.103)

2. The charge density of the electron in the ground state is given by

\[ \rho = -e |\varphi_{1,0,0}(r)|^2 = -\frac{e}{\pi a_0^3} \exp \left( -\frac{2r}{a_0} \right). \]  

(7.104)
Chapter 7. Central Potential

The Poisson's equation is given by

\[ \nabla^2 \phi = -4\pi \rho. \]  \hspace{1cm} (7.105)

To verify that the electrostatic potential given by Eq. (7.94) solves this equation we calculate

\[
\nabla^2 \phi = \frac{1}{r} \frac{d^2}{dr^2} (r \phi)
= e \frac{d^2}{dr^2} \left( \frac{r}{a_0} + 1 \right) \exp \left( -\frac{2r}{a_0} \right)
= \frac{4e \exp \left( -\frac{2r}{a_0} \right)}{a_0^2}
= -4\pi \rho.
\]  \hspace{1cm} (7.106)

Note also that

\[ \lim_{r \to \infty} \phi (r) = 0, \]  \hspace{1cm} (7.107)

as is required for a neutral atom.

3. The radial wave function of the ground state is given by

\[ R_{10}(r) = 2 \left( \frac{1}{a_0} \right)^{3/2} \exp \left( -\frac{r}{a_0} \right) \]  \hspace{1cm} (7.108)

thus the probability density of the variable \( r \) is given by

\[ f(r) = |rR_{10}(r)|^2 = \frac{4}{r} \left( \frac{r}{a_0} \right)^3 \exp \left( -\frac{2r}{a_0} \right). \]  \hspace{1cm} (7.109)

Thus

\[ \langle r \rangle = \int_0^\infty r f(r) \, dr = 4a_0 \int_0^\infty x^3 \exp (-2x) \, dx = \frac{3}{2} a_0. \]  \hspace{1cm} (7.110)

The most probable value \( r_0 \) is found from the condition

\[ 0 = \frac{df}{dr} = \frac{8r_0}{a_0^2} \exp \left( -\frac{2r_0}{a_0} \right) (a_0 - r_0), \]  \hspace{1cm} (7.111)

thus

\[ r_0 = a_0. \]  \hspace{1cm} (7.112)

4. The radial wave function of a hydrogen-like atom with a nucleus having charge \( Ze \) is found by substituting \( e^2 \) by \( Ze^2 \) in Eqs. (7.89), (7.90) and (7.91), namely
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\[
R_{10}^{(Z)}(r) = 2 \left( \frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0},
\]

\[
R_{20}^{(Z)}(r) = (2 - Zr/a_0) \left( \frac{Z}{2a_0} \right)^{3/2} e^{-Zr/a_0},
\]

\[
R_{21}^{(Z)}(r) = \left( \frac{Z}{2a_0} \right)^{3/2} \frac{Zr}{\sqrt{3a_0}} e^{-Zr/a_0}.
\]

The change in reduced mass is neglected. Therefore

a) For the 1s state

\[
Pr(1s) = \left( \int_0^\infty dr^2 R_{10}^{(Z=1)} R_{10}^{(Z=2)} \right)^2 = \frac{27}{a_0^3} \left( \frac{2a_0^3}{3} \right)^2 = 0.702.
\]

b) For the 2s state

\[
Pr(2s) = \left( \int_0^\infty dr^2 R_{20}^{(Z=1)} R_{20}^{(Z=2)} \right)^2 = \frac{16}{a_0^6} \left( \frac{a_0^3}{8} (2 - 3) \right)^2 = 0.25.
\]

c) For this case the probability vanishes due to the orthogonality between spherical harmonics with different \( l \).

5. The normalization constant is chosen to be \( A = 1/\sqrt{2} \). Since both states \( |2,1,-1\rangle \) and \( |2,1,1\rangle \) have the same energy the state \( |\alpha\rangle \) is stationary. The following holds

\[
\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{ml}^m(\theta, \phi),
\]

\[
R_{21}(r) = \left( \frac{1}{2a_0} \right)^{3/2} \frac{r}{\sqrt{3a_0}} e^{-Zr/a_0},
\]

\[
Y_{-1}^1(\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-i\phi},
\]

\[
Y_{1}^1(\theta, \phi) = -\frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{i\phi},
\]

\[
x = r \sin \theta \cos \phi.
\]

In general

\[
\langle n'l'm'|x|nlm \rangle = \int_0^\infty dr^2 R_{n'l'}(r) R_{nl}(r) \int_{-1}^1 d(\cos \theta) \int_0^{2\pi} d\phi \sin \theta \cos \phi \left( Y_{l'm'}^m \right)^* Y_{lm}^m.
\]

thus
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\[ \langle 2, 1, 1 | x | 2, 1, 1 \rangle \propto \int_0^{2\pi} d\phi \cos \phi = 0 , \quad (7.115) \]

\[ \langle 2, 1, -1 | x | 2, 1, -1 \rangle \propto \int_0^{2\pi} d\phi \cos \phi = 0 , \quad (7.116) \]

\[ \langle 2, 1, 1 | x | 2, 1, -1 \rangle \propto \int_0^{2\pi} d\phi \cos \phi e^{-2i\phi} = 0 , \quad (7.117) \]

\[ \langle 2, 1, -1 | x | 2, 1, 1 \rangle \propto \int_0^{2\pi} d\phi \cos \phi e^{2i\phi} = 0 , \quad (7.118) \]

and therefore

\[ \langle x \rangle (t) = 0 . \quad (7.119) \]

6. The radial equation is given by

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right] u_{k,l}(r) = E_{k,l} u_{k,l}(r) . \quad (7.120) \]

The boundary conditions imposed upon \( u(r) \) by the potential are

\[ u(0) = 0 , \quad (7.121) \]

\[ u(a^+) = u(a^-) \quad (7.122) \]

\[ \frac{du(a^+)}{dr} - \frac{du(a^-)}{dr} = -\frac{2}{a_0} u(a) . \quad (7.123) \]

where \( a_0 = \frac{\hbar^2}{mA} . \quad (7.124) \)

Since the centrifugal term \( l(l+1)\hbar^2/2mr^2 \) is non-negative the ground state is obtained with \( l = 0 \). We seek a solution for that case having the form

\[ u(r) = \begin{cases} \sinh(\kappa r) & r < a \\ \sinh(\kappa a) \exp(-\kappa (r-a)) & r > a \end{cases} , \quad (7.125) \]

where

\[ \kappa = \sqrt{-2mE} \frac{\hbar}{\hbar} . \quad (7.126) \]

The condition (7.123) yields
7.5. Solutions

\[
-k \sinh (ka) - k \cosh (ka) = -\frac{2}{a_0} \sinh (ka),
\]

(7.127)

or

\[
\frac{ka_0}{2} = \frac{1}{1 + \coth (ka)}.
\]

A real solution exists only if

\[
a_0 > \frac{2}{2m}\,
\]

(7.128)

or

\[
a_0 < a,
\]

(7.129)

7. The state vector \(|\gamma\rangle\) is an eigenvector of the operators \(L_x, L_y\), therefore it is easy to see that it consequently must be an eigenvector of the operator \([L_x, L_y]\) with a zero eigenvalue. Thus, since \([L_x, L_y] = i\hbar L_z\), one has \(L_z |\gamma\rangle = 0\). Similarly, one finds that \(L_z |\gamma\rangle = L_y |\gamma\rangle = 0\). Therefore, \(|\gamma\rangle\) is also an eigenvector of the operator \(L^2 = L_x^2 + L_y^2 + L_z^2\) with a zero eigenvalue. Therefore the wavefunction has the form

\[
\psi (r') = R (r') Y_{l=0} (\theta', \phi') = \frac{R (r')}{\sqrt{4\pi}},
\]

(7.130)

where the radial function \(R (r')\) is an arbitrary normalized function.
8. Density Operator

Consider an ensemble of \( N \) identical copies of a quantum system. The ensemble can be divided into subsets, where all systems belonging to the same subset have the same state vector. Let \( Nw_i \) be the number of systems having state vector \( |\alpha^{(i)}\rangle \), where

\[
0 \leq w_i \leq 1 , 
\tag{8.1}
\]

and where

\[
\sum_i w_i = 1. 
\tag{8.2}
\]

The state vectors are all assumed to be normalized

\[
\langle \alpha^{(i)} | \alpha^{(i)} \rangle = 1. 
\tag{8.3}
\]

Consider a measurement of an observable \( A \), having a set of eigenvalues \( \{a_n\} \) and corresponding set of eigenvectors \( \{|a_n\}\) \n
\[
A |a_n\rangle = a_n |a_n\rangle. 
\tag{8.4}
\]

The set of eigenvectors \( \{|a_n\}\) is assumed to be orthonormal and complete

\[
\langle a_m | a_n \rangle = \delta_{nm}, 
\tag{8.5}
\]

\[
\sum_n |a_n\rangle \langle a_n| = 1. 
\tag{8.6}
\]

Consider a measurement of the observable \( A \) done on a system that is randomly chosen from the ensemble. The probability to choose a system having state vector \( |\alpha^{(i)}\rangle \) is \( w_i \). Given that the state vector is \( |\alpha^{(i)}\rangle \), the expectation value of \( A \) is \( \langle \alpha^{(i)} | A | \alpha^{(i)} \rangle \) [see Eq. (2.84)]. Thus, the expectation (average) value of such a measurement done on a system that is randomly chosen from the ensemble is given by

\[
\langle A \rangle = \sum_i w_i \langle \alpha^{(i)} | A | \alpha^{(i)} \rangle = \sum_i \sum_n w_i \langle a_n | \alpha^{(i)} \rangle^2 a_n. 
\tag{8.7}
\]
Chapter 8. Density Operator

Claim. The expectation value can be expressed as

\[ \langle A \rangle = \text{Tr}(\rho A) \]  
(8.8)

where

\[ \rho = \sum_i w_i |\alpha^{(i)}\rangle \langle \alpha^{(i)}| \]  
(8.9)

is the density operator.

Proof. Let \{ \{b_m\} \} be an orthonormal and complete basis for the vector space

\[ \sum_m \langle b_m | b_m \rangle = 1 \]  
(8.10)

The following holds

\begin{align*}
\langle A \rangle &= \sum_i w_i \langle \alpha^{(i)} | A | \alpha^{(i)} \rangle \\
&= \sum_i \sum_m w_i \langle \alpha^{(i)} | A | b_m \rangle \langle b_m | \alpha^{(i)} \rangle \\
&= \sum_m \langle b_m | \sum_i w_i |\alpha^{(i)}\rangle \langle \alpha^{(i)} | A | b_m \rangle \\
&= \text{Tr}(\rho A) ,
\end{align*}

(8.11)

where

\[ \rho = \sum_i w_i |\alpha^{(i)}\rangle \langle \alpha^{(i)}| . \]

Below we discuss some basic properties of the density operator:

**Exercise 8.0.1.** Show that \( \rho^\dagger = \rho \).

**Solution 8.0.1.** Trivial by the definition (8.9).

**Exercise 8.0.2.** Show that \( \text{Tr}(\rho) = 1 \).

**Solution 8.0.2.** Using a complete orthonormal basis \( \sum_m |b_m\rangle \langle b_m| = 1 \) one has
\[
\text{Tr} (\rho) = \sum_m \langle b_m | \left( \sum_i w_i | \alpha^{(i)} \rangle \langle \alpha^{(i)} | \right) | b_m \rangle \\
= \sum_i w_i \langle \alpha^{(i)} | \left( \sum_m | b_m \rangle \langle b_m | \right) | \alpha^{(i)} \rangle \\
= \sum_i w_i \langle \alpha^{(i)} | \bar{\alpha}^{(i)} \rangle \\
= \sum_i w_i \\
= 1.
\]  
(8.12)

**Exercise 8.0.3.** Show that for any normalized state \(|\beta\rangle\) the following holds

\[0 \leq \langle \beta | \rho | \beta \rangle \leq 1.\]  
(8.13)

**Solution 8.0.3.** Clearly, \(0 \leq \langle \beta | \rho | \beta \rangle \) since

\[
\langle \beta | \rho | \beta \rangle = \sum_i w_i \langle \beta | \alpha^{(i)} \rangle \langle \alpha^{(i)} | \beta \rangle = \sum_i w_i \left| \langle \alpha^{(i)} | \beta \rangle \right|^2 \geq 0.
\]  
(8.14)

On the other hand, according to the Schwartz inequality [see Eq. (2.167)], which is given by

\[
|\langle u | v \rangle| \leq \sqrt{\langle u | u \rangle} \sqrt{\langle v | v \rangle},
\]  
(8.15)

one has

\[
\left| \langle \alpha^{(i)} | \beta \rangle \right| \leq \sqrt{\langle \beta | \beta \rangle} \sqrt{\langle \alpha^{(i)} | \alpha^{(i)} \rangle} = 1.
\]  
(8.16)

Moreover, \(\sum_i w_i = 1\), thus

\[
\langle \beta | \rho | \beta \rangle = \sum_i w_i \left| \langle \alpha^{(i)} | \beta \rangle \right|^2 \leq 1.
\]  
(8.17)

**Exercise 8.0.4.** Show that \(\text{Tr} (\rho^2) \leq 1\).

**Solution 8.0.4.** The fact that \(\rho\) is Hermitian (i.e., \(\rho^\dagger = \rho\)) guaranties the existence of a complete orthonormal basis \(\{|q_m\rangle\}\) of eigenvectors of \(\rho\), which satisfy

\[
\langle q_{m'} | q_m \rangle = \delta_{mm'},
\]  
(8.18)

\[
\sum_m |q_m\rangle \langle q_m| = 1,
\]  
(8.19)

and...
\( \rho |q_m\rangle = q_m |q_m\rangle \), \( (8.20) \)

where the eigenvalues \( q_m \) are real. Using this basis one has

\[
\text{Tr} (\rho^2) = \sum_m \langle q_m | \rho^2 | q_m \rangle = \sum_m q_m^2 . \tag{8.21}
\]

According to inequality (8.13)

\[ 0 \leq q_m = \langle q_m | \rho | q_m \rangle \leq 1 , \tag{8.22} \]

thus

\[
\text{Tr} (\rho^2) = \sum_m q_m^2 \leq \left( \sum_m q_m \right)^2 = (\text{Tr} (\rho))^2 = 1 . \tag{8.23}
\]

**Definition 8.0.1.** An ensemble is said to be pure if its density operator can be expressed as

\[ \rho = |\alpha \rangle \langle \alpha | . \]

**Exercise 8.0.5.** Show that \( \text{Tr} (\rho^2) = 1 \) iff \( \rho \) represents a pure ensemble.

**Solution 8.0.5.** (i) Assuming that \( \rho \) represents a pure ensemble, one has \( \rho^2 = \rho \), thus \( \text{Tr} (\rho^2) = \text{Tr} (\rho) = 1 \). (ii) Assume that \( \text{Tr} (\rho^2) = 1 \). Since \( \rho \) is Hermitian (i.e., \( \rho^\dagger = \rho \)), there is a complete orthonormal basis \( \{ |q_m\rangle \} \) of eigenvectors of \( \rho \), such that

\[
\langle q_{m'} | q_m \rangle = \delta_{mm'} , \tag{8.24}
\]

\[
\sum_m |q_m\rangle \langle q_m| = 1 , \tag{8.25}
\]

and

\[ \rho |q_m\rangle = q_m |q_m\rangle \), \( (8.26) \]

where the eigenvalues \( q_m \) are real. Moreover, according to inequality (8.22)

\[ 0 \leq q_m \leq 1 . \tag{8.27} \]

For this basis the assumption \( \text{Tr} (\rho^2) = 1 \) yields

\[ 1 = \text{Tr} (\rho^2) = \sum_m q_m^2 . \tag{8.28} \]

Moreover, also \( \text{Tr} (\rho) = 1 \), thus

\[ 1 = \sum_m q_m . \tag{8.29} \]

Both equalities can be simultaneously satisfied only if

\[ q_m = \begin{cases} 1 & m = m_0 \\ 0 & m \neq m_0 \end{cases} . \tag{8.30} \]

For this case \( \rho = |q_{m_0}\rangle \langle q_{m_0}| \), thus \( \rho \) represents a pure ensemble.
8.1 Time Evolution

Consider a density operator
\[ \rho(t) = \sum_i w_i \alpha_i(t) \alpha_i^*(t) , \]  
where the state vectors \( \{ \alpha_i(t) \} \) evolve in time according to
\[ i\hbar \frac{d}{dt} \alpha_i = \mathcal{H} \alpha_i , \]
\[ -i\hbar \frac{d}{dt} \alpha_i^* = \alpha_i^* \mathcal{H} , \]
where \( \mathcal{H} \) is the Hamiltonian. Taking the time derivative yields
\[ \frac{d\rho}{dt} = -\frac{1}{i\hbar} [\rho, \mathcal{H}] . \]
This result resembles the equation of motion (4.37) of an observable in the Heisenberg representation, however, instead of a minus sign on the right hand side, Eq. (4.37) has a plus sign.

8.2 Quantum Statistical Mechanics

Consider an ensemble of identical copies of a quantum system. Let \( \mathcal{H} \) be the Hamiltonian having a set of eigenenergies \( \{ E_i \} \) and a corresponding set of eigenstates \( \{ |i\rangle \} \), which forms an orthonormal and complete basis
\[ \mathcal{H} |i\rangle = E_i |i\rangle , \]
\[ \sum_i |i\rangle \langle i| = 1 . \]
Consider the case where the ensemble is assumed to be in thermal equilibrium at temperature \( T \). According to the laws of statistical mechanics the probability \( w_i \) to find an arbitrary system in the ensemble in a state vector \( |i\rangle \) having energy \( E_i \) is given by
\[ w_i = \frac{1}{Z} e^{-\beta E_i} , \]
where \( \beta = 1/k_B T \), \( k_B \) is Boltzmann’s constant, and where
\[ Z = \sum_i e^{-\beta E_i} \]
is the partition function.
Exercise 8.2.1. Show that the density operator $\rho$ can be written as

$$\rho = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}.$$  \hfill (8.40)

Solution 8.2.1. According to the definition (8.9) one has

$$\rho = \sum_i w_i |i\rangle \langle i| = \frac{1}{Z} \sum_i e^{-\beta E_i} |i\rangle \langle i|.$$  \hfill (8.41)

Moreover, the following hold

$$Z = \sum_i e^{-\beta E_i} = \sum_i \langle i| e^{-\beta H} |i\rangle = \text{Tr}(e^{-\beta H}),$$  \hfill (8.42)

and

$$\sum_i e^{-\beta E_i} |i\rangle \langle i| = \sum_i e^{-\beta H} |i\rangle \langle i| = e^{-\beta H} \sum_i |i\rangle \langle i| = e^{-\beta H},$$  \hfill (8.43)

thus

$$\rho = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})}.$$  \hfill (8.44)

8.3 Problems

1. Consider a spin 1/2 in a magnetic field $B = B_\hat{z}$ and in thermal equilibrium at temperature $T$. Calculate $\langle \mathbf{S} \cdot \hat{u} \rangle$, where $\mathbf{S}$ is the vector operator of the angular momentum and where $\hat{u}$ is a unit vector, which can be described using the angles $\theta$ and $\phi$

$$\hat{u} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta).$$  \hfill (8.45)

2. A spin 1/2 particle is an eigenstate of the operator $S_y$ with eigenvalue $+\hbar/2$.

   a) Write the density operator in the basis of eigenvectors of the operator $S_z$.
   
   b) Calculate $\rho^n$, where $n$ is integer.
   
   c) Calculate the density operator (in the same basis) of an ensemble of particles, half of them in an eigenstate of $S_y$ with eigenvalue $+\hbar/2$, and half of them in an eigenstate of $S_y$ with eigenvalue $-\hbar/2$.
   
   d) Calculate $\rho^n$ for this case.

3. A spin 1/2 is at time $t = 0$ in an eigenstate of the operator $S_\theta = S_x \sin \theta + S_z \cos \theta$ with an eigenvalue $+\hbar/2$, where $\theta$ is real and $S_x$ and $S_z$ are the $x$ and $z$ components, respectively, of the angular momentum vector operator. A magnetic field $B$ is applied in the $x$ direction between time $t = 0$ and time $t = T$. 

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a) The $z$ component of the angular momentum is measured at time $t > T$. Calculate the probability $P_{+}$ to measure the value $\hbar/2$.
b) Calculate the density operator $\rho$ of the spin at times $t = T$.

4. A spin $1/2$ electron is put in a constant magnetic field given by $\mathbf{B} = B\mathbf{z}$, where $B$ is a constant. The system is in thermal equilibrium at temperature $T$.
a) Calculate the correlation function
$$C_z (t) = \langle S_z (t) S_z (0) \rangle .$$  
(8.46)
b) Calculate the correlation function
$$C_x (t) = \langle S_x (t) S_x (0) \rangle .$$  
(8.47)

5. Consider a harmonic oscillator with frequency $\omega$. Show that the variance of the number operator $\Delta N = \sqrt{\langle N^2 \rangle - \langle N \rangle^2}$ (where $N = a^\dagger a$) is given by
a) $\Delta N = 0$ for energy eigenstates.
b) $\Delta N = \sqrt{\langle N \rangle}$ for coherent states.
c) $\Delta N = \sqrt{\langle N \rangle (\langle N \rangle + 1)}$ for thermal states.

6. Consider a harmonic oscillator having angular resonance frequency $\omega$. The oscillator is in thermal equilibrium at temperature $T$. Calculate the expectation value $\langle x^2 \rangle$.

7. Consider a harmonic oscillator in thermal equilibrium at temperature $T$, whose Hamiltonian is given by
$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2} .$$  
(8.48)

Show that the density operator is given by
$$\rho = \int \int d^2 \alpha |\alpha \rangle \langle \alpha | P (\alpha) ,$$  
(8.49)

where $|\alpha \rangle$ is a coherent state, $d^2 \alpha$ denotes infinitesimal area in the $\alpha$ complex plane,
$$P (\alpha) = \frac{1}{\pi \langle N \rangle} \exp \left( - \frac{|\alpha|^2}{\langle N \rangle} \right) ,$$  
(8.50)

and where $\langle N \rangle$ is the expectation value of the number operator $N$.

8. Consider a harmonic oscillator in thermal equilibrium at temperature $T$, whose Hamiltonian is given by
$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2 \hat{x}^2}{2} .$$  
(8.51)

Calculate the probability density $f (x)$ of the random variable $x$.
9. An LC oscillator (see figure) made of a capacitor \( C \) in parallel with an inductor \( L \), is in thermal equilibrium at temperature \( T \). The charge in the capacitor \( q \) is being measured.

![Diagram of an LC oscillator]

a) Calculate the expectation value \( \langle q \rangle \) of \( q \).

b) Calculate the variance \( \langle (\Delta q)^2 \rangle \).

10. Consider an observable \( A \) having a set of eigenvalues \( \{a_n\} \). Let \( P_n \) be a projector operator onto the eigensubspace corresponding to the eigenvalue \( a_n \). A given physical system is initially described by the density operator \( \rho_0 \). A measurement of the observable \( A \) is then performed. What is the density operator \( \rho_1 \) of the system immediately after the measurement?

11. The model that was proposed by von Neumann describes an indirect measurement process of a given observable \( A \). The observable \( A \) is assumed to be a function of the degrees of freedom of a subsystem, which we refer to as the measured system (MS). The indirect measurement is performed by first letting the MS to interact with a measuring device (MD), having its own degrees of freedom, and then in the final step, performing a quantum measurement on the MD. The MS is assumed to initially be in a pure state \( |\alpha\rangle \) (i.e. its density operator is assumed to initially be given by \( \rho_0 = |\alpha\rangle \langle \alpha| \)). Let \( A \) be an observable operating on the Hilbert space of the MS. The initial state of the MS can be expanded in the basis of eigenvectors \( \{ |a_n\rangle \} \) of the observable \( A \)

\[
|\alpha\rangle = \sum_n c_n |a_n\rangle , \tag{8.52}
\]

where \( c_n = \langle a_n | \alpha \rangle \) and where

\[
A |a_n\rangle = a_n |a_n\rangle . \tag{8.53}
\]

For simplicity, the Hamiltonian of the MS is taken to be zero. The MD is assumed to be a one dimensional free particle, whose Hamiltonian vanishes, and whose initial state is labeled by \( |\psi_i\rangle \). The position wavefunction \( \psi(x^\prime) = \langle x^\prime | \psi_i\rangle \) of this state is taken to be Gaussian having width \( x_0 \)

\[
\psi(x^\prime) = \frac{1}{\sqrt{\pi} x_0^{1/2}} \exp \left( -\frac{1}{2} \left( \frac{x^\prime}{x_0} \right)^2 \right) . \tag{8.54}
\]
The interaction between the MS and the MD is taken to be given by

\[ V(t) = -f(t) x A, \]  

(8.55)

where \( f(t) \) is assumed to have compact support with a peak near the time of the measurement.

a) Express the vector state of the entire system \( |\Psi(t)\rangle \) at time \( t \) in the basis of states \( \{|p\rangle \otimes |a_{n'}\rangle\} \). This basis spans the Hilbert space of the entire system (MS and MD). The \( |p\rangle \otimes |a_{n'}\rangle \) is both, an eigenvector of \( A \) (with eigenvalue \( a_n \)) and of the momentum \( p \) of the MD (with eigenvalue \( p' \)).

b) In what follows the final state of the system after the measurement will be evaluated by taking the limit \( t \to \infty \). The outcome of the measurement of the observable \( A \), which is labeled by \( A \), is determined by performing a measurement of the momentum variable \( p \) of the MD. The outcome, which is labeled by \( P \), is related to \( A \) by

\[ A = \frac{P \cdot p}{p_\text{r}}, \]  

(8.56)

where

\[ p_\text{r} = \int_{-\infty}^{\infty} dt' f(t'). \]  

(8.57)

Calculate the probability distribution \( g(A) \) of the random variable \( A \).

c) Consider another measurement that is performed after the entanglement between the MS and the MD has been fully created. The additional measurement is associated with the observable \( B \), which is assumed to be a function of the degrees of freedom of the MS only. Show that the expectation value \( \bar{B} \) of the observable \( B \) is given by

\[ \bar{B} = \sum_{n'} \langle a_{n'} | B \rho_R | a_{n'} \rangle, \]  

(8.58)

where the operator \( \rho_R \), which is called the reduced density operator, is given by

\[ \rho_R = \sum_{n',n''} c_{n'}^* c_{n''} e^{-\eta^2 \left( \frac{a_{n'} - a_{n''}}{\sqrt{2}} \right)^2} |a_{n'}\rangle \langle a_{n''}|. \]  

(8.59)

12. A particle having mass \( m \) moves in the \( xy \) plane under the influence of a two dimensional potential \( V(x,y) \), which is given by

\[ V(x, y) = \frac{m \omega^2}{2} \left( x^2 + y^2 \right) + \lambda m \omega^2 xy, \]  

(8.60)

where both \( \omega \) and \( \lambda \) are real constants. Calculate in thermal equilibrium at temperature \( T \) the expectation values \( \langle x \rangle, \langle x^2 \rangle \).
8.4 Solutions

1. The Hamiltonian is given by

\[ H = \omega S_z \quad (8.61) \]

where

\[ \omega = \frac{|e| B}{mc} \quad (8.62) \]

is the Larmor frequency. In the basis of the eigenvectors of \( S_z \)

\[ S_z |\pm\rangle = \pm \frac{\hbar}{2} |\pm\rangle \quad (8.63) \]

one has

\[ H |\pm\rangle = \pm \frac{\hbar \omega}{2} |\pm\rangle \quad (8.64) \]

thus

\[ \rho = e^{-H\beta} \frac{\text{Tr}(e^{-H\beta})}{\text{Tr}(e^{-H\beta})} = e^{-\frac{\hbar \omega \beta}{2}} \langle + | + \rangle + e^{\frac{\hbar \omega \beta}{2}} \langle - | - \rangle, \]

\[ (8.65) \]

where \( \beta = 1/k_BT \), and therefore with the help of Eqs. (2.102) and (2.103), which are given by

\[ S_x = \frac{\hbar}{2} (|+\rangle \langle -| + |-\rangle \langle +|) \quad (8.66) \]

\[ S_y = \frac{\hbar}{2} (-i |+\rangle \langle +| - i |-\rangle \langle -|) \quad (8.67) \]

one has

\[ \langle S_x \rangle = \text{Tr}(\rho S_x) = 0 \quad (8.68) \]

\[ \langle S_y \rangle = \text{Tr}(\rho S_y) = 0 \quad (8.69) \]

and with the help of Eq. (2.99), which is given by

\[ S_z = \frac{\hbar}{2} (|+\rangle \langle +| - |-\rangle \langle -|) \quad (8.70) \]

one has
\( \langle S_z \rangle = \text{Tr}(\rho S_z) \)
\[ = \text{Tr} \left( \frac{e^{-\frac{\hbar}{2} \omega \beta}}{e^{-\frac{\hbar}{2} \omega \beta} + e^{\frac{\hbar}{2} \omega \beta}} |+\rangle \langle +| + e^{\frac{\hbar}{2} \omega \beta} |\rangle \langle -| \frac{\hbar}{2} (|+\rangle \langle +| - |\rangle \langle -|) \right) \]
\[ = \hbar e^{-\frac{\hbar}{2} \omega \beta} - e^{\frac{\hbar}{2} \omega \beta} \]
\[ = -\frac{\hbar}{2} \tanh \left( \frac{\hbar \omega \beta}{2} \right), \]

thus
\[ \langle S \cdot \hat{u} \rangle = -\frac{\hbar \cos \theta}{2} \tanh \left( \frac{\hbar \omega \beta}{2} \right). \] (8.71)

2. Recall that
\[ |\pm; \hat{y} \rangle = \frac{1}{\sqrt{2}} (|+\rangle \pm i |\rangle \langle -|) \],

a) thus
\[ \rho = \frac{1}{2} \left( \begin{array}{cc} 1 & i \\ i & -1 \end{array} \right) = \frac{1}{2} \left( \begin{array}{cc} 1 & i \\ -i & 1 \end{array} \right). \] (8.74)

b) For a pure state \( \rho^n = \rho \).

c) For this case
\[ \rho = \frac{1}{2} \left( \begin{array}{cc} |+; \hat{y} \rangle \langle +; \hat{y}| & |+; \hat{y} \rangle \langle -; \hat{y}| \\ |+; \hat{y} \rangle \langle -; \hat{y}| & |\rangle \langle +| \end{array} \right) = \frac{1}{2} \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \] (8.75)

d) and
\[ \rho^n = \frac{1}{2^n} \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right). \] (8.76)

3. The state at time \( t = 0 \) is given by
\[ |\psi(t = 0)\rangle \equiv \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{pmatrix}, \] (8.77)

and the one at time \( t = T \) is
\[ |\psi(t = T)\rangle = \exp \left( \frac{\hbar T \sigma_x}{2} \right) |\psi(t = 0)\rangle, \] (8.78)

where \( \sigma_x \) is a Pauli matrix, and
\[ \omega = \frac{eB}{m_e c}, \]  
\hline
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\[ \exp \left( -\frac{i\sigma \cdot \hat{n}\phi}{2} \right) = \cos \frac{\phi}{2} - i\sigma \cdot \hat{n} \sin \frac{\phi}{2}, \]  
(8.80)
one finds
\[ \exp \left( -\frac{i\sigma \cdot \hat{n}\phi}{2} \right) = \cos \frac{\omega T}{2} + i\sigma_x \sin \frac{\omega T}{2} \left( \cos \frac{\omega T}{2} \frac{i \sin \omega T}{2} \cos \frac{\omega T}{2} \right), \]  
(8.81)
thus
\[ |\psi(t = T)\rangle \equiv \begin{pmatrix} \cos \frac{\omega T}{2} \frac{i \sin \omega T}{2} \\ i \sin \frac{\omega T}{2} \cos \frac{\omega T}{2} \end{pmatrix} \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} \]
\[ = \begin{pmatrix} \cos \frac{\omega T}{2} \cos \theta + i \sin \frac{\omega T}{2} \sin \theta \\ i \sin \frac{\omega T}{2} \cos \theta + \cos \frac{\omega T}{2} \sin \theta \end{pmatrix}. \]  
(8.82)
a) The probabilities to measured \( \pm h/2 \) are thus given by
\[ P_+ = \cos^2 \frac{\omega T}{2} \cos^2 \frac{\theta}{2} + \sin^2 \frac{\omega T}{2} \cos^2 \frac{\theta}{2} \]
\[ = 1 + \cos (\omega T) \cos \theta, \]  
(8.83)
and
\[ P_- = \cos^2 \frac{\omega T}{2} \sin^2 \frac{\theta}{2} + \sin^2 \frac{\omega T}{2} \cos^2 \frac{\theta}{2} \]
\[ = 1 - \cos (\omega T) \cos \theta. \]  
(8.84)
b) The density operator is given by
\[ \rho_{11} = P_+, \]
\[ \rho_{22} = P_-, \]
\[ \rho_{21} = \left( \cos \frac{\omega T}{2} \cos \frac{\theta}{2} + i \sin \frac{\omega T}{2} \sin \frac{\theta}{2} \right) \left( -i \sin \frac{\omega T}{2} \cos \frac{\theta}{2} + \cos \frac{\omega T}{2} \sin \frac{\theta}{2} \right) \]
\[ = \sin \frac{\theta}{2} - i \frac{1}{2} \sin \omega T \cos \theta, \]
\[ \rho_{12} = \rho_{21}^*. \]
4. The Hamiltonian is given by
\[ H = -\omega S_z, \]  
(8.85)
where
\[ \omega = \frac{eB}{m_e c}, \]  
(8.86)
\hline
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thus, the density operator is given by

\[ \rho = \frac{1}{Z} \begin{pmatrix} \exp \left( \frac{\hbar \omega}{2k_B T} \right) & 0 \\ 0 & \exp \left( -\frac{\hbar \omega}{2k_B T} \right) \end{pmatrix}, \quad (8.87) \]

where

\[ Z = \exp \left( \frac{\hbar \omega}{2k_B T} \right) + \exp \left( -\frac{\hbar \omega}{2k_B T} \right). \quad (8.88) \]

a) Using

\[ S_z(t) = \exp \left( \frac{iHt}{\hbar} \right) S_z(0) \exp \left( -\frac{iHt}{\hbar} \right) = S_z(0), \quad (8.89) \]

one finds

\[ C_z(t) = \langle S_z^2(0) \rangle = \text{Tr} \left( \rho S_z^2(0) \right) = \frac{\hbar^2}{4}. \quad (8.90) \]

b) The following holds

\[ S_x(t) = \exp \left( -\frac{i\omega S_z t}{\hbar} \right) S_x(0) \exp \left( \frac{i\omega S_z t}{\hbar} \right) = S_x \cos(\omega t) + S_y \sin(\omega t), \quad (8.91) \]

thus

\[ C_x(t) = \cos(\omega t) \langle S_x^2(0) \rangle + \sin(\omega t) \langle S_y(0) S_x(0) \rangle \]

\[ = \frac{\cos(\omega t) \hbar^2}{4} + \sin(\omega t) \langle S_y(0) S_x(0) \rangle. \quad (8.92) \]

In terms of Pauli matrices

\[ \langle S_y(0) S_x(0) \rangle = \frac{\hbar^2}{4Z} \text{Tr} \left( \begin{pmatrix} \exp \left( \frac{\hbar \omega}{2k_B T} \right) & 0 \\ 0 & \exp \left( -\frac{\hbar \omega}{2k_B T} \right) \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \]

\[ = \frac{\hbar^2}{4Z} \text{Tr} \left( \begin{pmatrix} -i \exp \left( \frac{\hbar \omega}{2k_B T} \right) & 0 \\ 0 & i \exp \left( -\frac{\hbar \omega}{2k_B T} \right) \end{pmatrix} \right) \]

\[ = -\frac{i\hbar^2}{4} \tanh \left( \frac{\hbar \omega}{2k_B T} \right), \quad (8.93) \]

thus

\[ C_x(t) = \frac{\hbar^2}{4} \left[ \cos(\omega t) - i \sin(\omega t) \tanh \left( \frac{\hbar \omega}{2k_B T} \right) \right]. \quad (8.94) \]

5. The variance \( \Delta N \) is given by
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a) For an energy eigenstate $|n\rangle$ one has

$$N |n\rangle = n |n\rangle ,$$  \hspace{1cm} (8.95)

thus

$$\langle N \rangle = \langle n | N | n \rangle = n ,$$  \hspace{1cm} (8.96)

and

$$\langle N^2 \rangle = \langle n | N^2 | n \rangle = n^2 ,$$  \hspace{1cm} (8.97)

therefore

$$\Delta N = 0 .$$  \hspace{1cm} (8.98)

b) For a coherent state $|\alpha\rangle$ one has

$$a |\alpha\rangle = \alpha |\alpha\rangle ,$$  \hspace{1cm} (8.99)

thus

$$\langle N \rangle = \langle \alpha | N | \alpha \rangle = \langle \alpha | a^\dagger a | \alpha \rangle = |\alpha|^2 ,$$  \hspace{1cm} (8.100)

and

$$\langle N^2 \rangle = \langle \alpha | a^\dagger a a^\dagger a | \alpha \rangle = \langle \alpha | a^\dagger \left(\begin{bmatrix} a^\dagger a & a^\dagger a \\ a^\dagger a & a^\dagger a \end{bmatrix} \right) a | \alpha \rangle = |\alpha|^2 + |\alpha|^4 ,$$  \hspace{1cm} (8.101)

therefore

$$\Delta N = \sqrt{\langle N \rangle} .$$  \hspace{1cm} (8.102)

c) In general, for a thermal state one has

$$\langle O \rangle = \text{Tr} (\rho O) ,$$  \hspace{1cm} (8.103)

where $O$ is an operator,

$$\rho = \frac{1}{Z} e^{-\mathcal{H} \beta} ,$$  \hspace{1cm} (8.104)

$$Z = \text{Tr} (e^{-\mathcal{H} \beta}) ,$$  \hspace{1cm} (8.105)

and $\beta = 1/k_B T$ and $\mathcal{H}$ is the Hamiltonian. For the present case

$$\mathcal{H} = \hbar \omega \left( N + \frac{1}{2} \right) ,$$  \hspace{1cm} (8.106)
thus

\[ \langle N \rangle = \text{Tr} (\rho N) = \sum_{n=0}^{\infty} \langle n | e^{-\beta H} N | n \rangle = \sum_{n=0}^{\infty} \langle n | e^{-\beta H} | n \rangle \sum_{n=0}^{\infty} n e^{-n\hbar \omega \beta} = \sum_{n=0}^{\infty} e^{-n\hbar \omega \beta} = -\frac{1}{\hbar \omega} \partial \log \left( \sum_{n=0}^{\infty} e^{-n\hbar \omega \beta} \right) \frac{\partial}{\partial \beta} = \frac{e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}, \]

and therefore

\[ \langle N^2 \rangle = \text{Tr}(\rho N^2) = \sum_{n=0}^{\infty} \langle n | e^{-\beta H} N^2 | n \rangle = \sum_{n=0}^{\infty} \langle n | e^{-\beta H} | n \rangle \sum_{n=0}^{\infty} n^2 e^{-n\hbar \omega \beta} = \sum_{n=0}^{\infty} e^{-n\hbar \omega \beta} \left( \frac{1}{\hbar \omega} \right)^2 \frac{\partial^2}{\partial \beta^2} \sum_{n=0}^{\infty} e^{-n\hbar \omega \beta} = \left( e^{-\beta \hbar \omega} + 1 \right) e^{-\beta \hbar \omega} \left( 1 - e^{-\beta \hbar \omega} \right)^2, \]

and therefore

\[ (\Delta N)^2 = \langle N^2 \rangle - \langle N \rangle^2 = \frac{e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} = \langle N \rangle \left( \langle N \rangle + 1 \right). \]

6. The density operator is given by

\[ \rho = \frac{1}{Z} e^{-\beta H}. \]
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where

\[
Z = \text{tr} \left( e^{-\beta H} \right) = \sum_{n=0}^{\infty} e^{-\beta \omega (n + \frac{1}{2})} = \frac{e^{-\frac{\hbar \omega}{2}}}{1 - e^{-\hbar \omega}} = \frac{1}{2 \sinh \left( \frac{\hbar \omega \beta}{2} \right)} ,
\]  

(8.111)

and \( \beta = 1/k_B T \). Thus using

\[
x^2 = \frac{\hbar}{2m\omega} \left( a^2 + (a^\dagger)^2 + 2a^\dagger a + 1 \right) ,
\]

(8.112)

one finds

\[
\langle x^2 \rangle = \text{Tr} \left( x^2 \rho \right) \\
= \frac{1}{Z} \sum_{n=0}^{\infty} \langle n | x^2 e^{-H \beta} | n \rangle \\
= \frac{1}{Z} \sum_{n=0}^{\infty} e^{-\hbar \omega (n + \frac{1}{2}) \beta} \langle n | x^2 | n \rangle \\
= \frac{\hbar}{m\omega Z} \sum_{n=0}^{\infty} \left( n + \frac{1}{2} \right) e^{-\hbar \omega (n + \frac{1}{2}) \beta} \\
= \frac{\hbar}{m\omega Z} \left( -1 + \frac{1}{\hbar \omega} \right) \frac{d}{d\beta} \sum_{n=0}^{\infty} e^{-\hbar \omega (n + \frac{1}{2}) \beta} .
\]

(8.113)

However

\[
\sum_{n=0}^{\infty} e^{-\hbar \omega (n + \frac{1}{2}) \beta} = Z ,
\]

(8.114)

thus

\[
\langle x^2 \rangle = \frac{1}{m\omega^2} \frac{d}{d\beta} \log Z^{-1} \\
= \frac{1}{m\omega^2} \frac{d}{d\beta} \sinh \left( \frac{\hbar \omega \beta}{2} \right) \\
= \frac{1}{m\omega^2} \frac{\hbar \omega}{2} \coth \left( \frac{\hbar \omega \beta}{2} \right) .
\]

(8.115)

Note that at high temperatures \( \hbar \omega \beta \ll 1 \)

\[
\langle x^2 \rangle \simeq \frac{k_B T}{m\omega^2} ,
\]

(8.116)

as is required by the equipartition theorem of classical statistical mechanics.
7. In the basis of number states the density operator is given by

\[
\rho = \frac{e^{-\mathcal{H}\beta}}{\text{Tr}(e^{-\mathcal{H}\beta})} = \frac{\sum_{n=0}^{\infty} e^{-\mathcal{H}\beta} |n\rangle \langle n|}{\sum_{n=0}^{\infty} (n|e^{-\mathcal{H}\beta} |n\rangle}
\]

\[
= \sum_{n=0}^{\infty} e^{-\beta \omega (N+\frac{1}{2})} |n\rangle \langle n|
\]

\[
= \sum_{n=0}^{\infty} e^{-n\beta \omega} |n\rangle \langle n|
\]

\[
= (1 - e^{-\beta \omega}) \sum_{n=0}^{\infty} e^{-n\beta \omega} |n\rangle \langle n|,
\]

(8.117)

where \( \beta = 1/k_B T \). Thus, \( \langle N \rangle \) is given by

\[
\langle N \rangle = \text{Tr}(\rho N)
\]

\[
= (1 - e^{-\beta \omega}) \sum_{n=0}^{\infty} ne^{-n\beta \omega}
\]

\[
= -\hbar \omega (1 - e^{-\beta \omega}) \frac{\partial}{\partial \beta} \sum_{n=0}^{\infty} e^{-n\beta \omega}
\]

\[
= -\hbar \omega (1 - e^{-\beta \omega}) \frac{1}{\partial \beta} \frac{1}{1 - e^{-\beta \omega}}
\]

\[
= \frac{e^{-\beta \omega}}{1 - e^{-\beta \omega}}.
\]

(8.118)

Moreover, the following holds

\[
\langle N \rangle + 1 = \frac{1}{1 - e^{-\beta \omega}},
\]

(8.119)

\[
\frac{\langle N \rangle}{\langle N \rangle + 1} = e^{-\beta \omega},
\]

(8.120)

thus, \( \rho \) can be rewritten as
\[ \rho = (1 - e^{-\beta \hbar \omega}) \sum_{n=0}^{\infty} e^{-n \beta \hbar \omega} |n\rangle \langle n| \]
\[ = \frac{1}{\langle N \rangle + 1} \sum_{n=0}^{\infty} \left( \frac{\langle N \rangle}{\langle N \rangle + 1} \right)^n |n\rangle \langle n| . \]  
(8.121)

To verify the validity of Eq. (8.49) we calculate
\[ \langle n | \rho | m \rangle = \int \int d^2 \alpha P (\alpha) \langle n | \langle \alpha | \langle m | \rangle \]. 
(8.122)

With the help of Eq. (5.42), which is given by
\[ |\alpha\rangle = e^{-|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle , \]  
(8.123)
one finds that
\[ \langle n | \rho | m \rangle = \frac{1}{\pi \langle N \rangle} \sqrt{n! m!} \int_0^{\infty} dr e^{-\left(1 + \frac{1}{\langle N \rangle}\right)r^2} r^{n+m+1} \int_0^{2\pi} d\theta e^{i(\theta(n-m)-\frac{\pi}{2})} \]  
\[ = \frac{2\delta_{nm}}{\langle N \rangle n!} \int_0^{\infty} dr e^{-\left(1 + \frac{1}{\langle N \rangle}\right)r^2} r^{2n+1} , \]  
(8.125)

and the transformation of the integration variable
\[ t = \left(1 + \frac{1}{\langle N \rangle}\right) r^2 , \]  
(8.126)
\[ dt = \left(1 + \frac{1}{\langle N \rangle}\right) 2r dr , \]  
(8.127)
lead to
8.4. Solutions

\[ \langle n | \rho | m \rangle = \frac{\delta_{nm}}{\langle N \rangle (1 + \frac{1}{\langle N \rangle})^{n+1}} \int_0^\infty dt e^{-t} t^n \frac{\Gamma(n+1)=n!}{\Gamma(n+1)=n!} \]

\[ = \frac{\delta_{nm}}{\langle N \rangle (1 + \frac{1}{\langle N \rangle})^{n+1}} \]

\[ = \frac{\langle N \rangle^n \delta_{nm}}{(1 + \langle N \rangle)^{n+1}}, \]

(8.128)
in agreement with Eq. (8.121).

8. The density operator [see Eq. (8.49)] is given by

\[ \rho = \int \int d^2 \alpha |\alpha\rangle \langle \alpha| P(\alpha), \]

(8.129)

where \(|\alpha\rangle\) is a coherent state, \(d^2 \alpha\) denotes infinitesimal area in the \(\alpha\) complex plane,

\[ P(\alpha) = \frac{1}{\pi \langle N \rangle} \exp \left( -\frac{|\alpha|^2}{\langle N \rangle} \right), \]

(8.130)

and where

\[ \langle N \rangle = \frac{e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} \]

(8.131)
is the expectation value of the number operator \(N\). Thus,

\[ f(x') = \langle x'| \rho |x'\rangle = \int \int d^2 \alpha P(\alpha) \langle x'| \alpha\rangle \langle \alpha |x'\rangle. \]

By employing the expression for the wave function \(\psi_\alpha(x') = \langle x'| \alpha\rangle\) of a coherent state which is given by [see Eq. (5.51)]

\[ \psi_\alpha(x') = \langle x'| \alpha\rangle = \exp \left( \frac{\alpha^2 - \alpha^2}{4} \frac{m \omega}{\hbar} \right)^{1/4} \exp \left[ -\left( \frac{x' - \langle x \rangle_\alpha}{2 \Delta x_\alpha} \right)^2 + i \langle p \rangle_\alpha \frac{x'}{\hbar} \right], \]

(8.132)

where

\[ \langle x \rangle_\alpha = \langle \alpha | x | \alpha \rangle = \sqrt{\frac{2 \hbar}{m \omega}} \text{Re}(\alpha), \]

(8.133)

\[ \Delta x_\alpha = \sqrt{\langle \alpha | (\Delta x)^2 | \alpha \rangle} = \sqrt{\frac{\hbar}{2 m \omega}}, \]

(8.134)
one finds that
\[
f(x') = (x' \rho | x') = \frac{1}{\pi \langle N \rangle} \left( \frac{m \omega}{\pi \hbar} \right)^{1/2} \times \int \int d^2 \alpha \exp \left( -\frac{|\alpha|^2}{\langle N \rangle} \right) \exp \left[ -2 \left( \frac{x' - \langle x \rangle_\alpha}{2 \Delta x_\alpha} \right)^2 \right] \\
= \frac{1}{\pi \langle N \rangle} \left( \frac{m \omega}{\pi \hbar} \right)^{1/2} \times \int \int d^2 \alpha \exp \left( -\frac{|\alpha|^2}{\langle N \rangle} \right) \exp \left( -2 \left( \frac{x'}{\sqrt{\frac{2 \hbar}{m \omega}}} - \operatorname{Re} \alpha \right)^2 \right) \\
= \frac{\left( \frac{m \omega}{\pi \hbar} \right)^{1/2}}{\sqrt{1 + 2 \langle N \rangle}} e^{-2 \left( \frac{x'}{\sqrt{\frac{2 \hbar}{m \omega}}} \right)^2} \\
= \frac{1}{\sqrt{\pi}} \sqrt{\frac{1}{\frac{h}{m \omega} (1 + 2 \langle N \rangle)}} e^{-2 \left( \frac{x'}{\sqrt{\frac{2 \hbar}{m \omega}}} \right)^2} \\
= \frac{1}{\xi \sqrt{\pi}} e^{-\left( \frac{x'}{\xi} \right)^2},
\]

where
\[
\xi = \sqrt{\frac{h}{m \omega} (1 + 2 \langle N \rangle)},
\]

and where
\[
1 + 2 \langle N \rangle = 1 + 2 \frac{e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} = \coth \left( \frac{\beta \hbar \omega}{2} \right).
\] 

9. Recall that the LC circuit is a harmonic oscillator.

a) In terms of the annihilation and creation operators
\[
a = \sqrt{\frac{L \omega}{2 \hbar}} \left( q + \frac{ip}{L \omega} \right), \quad (8.136)
\]
\[
a^\dagger = \sqrt{\frac{L \omega}{2 \hbar}} \left( q - \frac{ip}{L \omega} \right), \quad (8.137)
\]

one has
\[
q = \sqrt{\frac{h}{2L \omega}} (a + a^\dagger), \quad (8.138)
\]
\[
\mathcal{H} = \hbar \omega \left( a^\dagger a + \frac{1}{2} \right). \quad (8.139)
\]
8.4. Solutions

The density operator is given by

$$\rho = \frac{1}{Z} e^{-\beta H}, \quad (8.140)$$

where

$$\beta = \frac{1}{k_B T}, \quad (8.141)$$

and

$$Z = \text{Tr} e^{-\beta H} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega(n + \frac{1}{2})} = \frac{\frac{\hbar \omega}{2}}{1 - e^{-\beta \hbar \omega}} = \frac{1}{2 \sinh \frac{\beta \hbar \omega}{2}}, \quad (8.142)$$

thus

$$\langle q \rangle = \text{Tr} (q \rho) = \frac{1}{Z} \sqrt{\frac{h}{2 L \omega}} \sum_{n=0}^{\infty} \langle n \rangle (a + a^\dagger)^2 e^{-\beta H} |n\rangle = 0. \quad (8.143)$$

b) Similarly

$$\langle q^2 \rangle = \text{Tr} (q^2 \rho)$$

$$= \frac{h}{2 L \omega} Z \sum_{n=0}^{\infty} \langle n \rangle (a + a^\dagger)^2 e^{-\beta H} |n\rangle$$

$$= \frac{1}{L \omega^2} \frac{1}{Z} \sum_{n=0}^{\infty} \hbar \omega \left( n + \frac{1}{2} \right) e^{-\beta \hbar \omega(n + \frac{1}{2})}$$

$$= -\frac{1}{L \omega^2} \frac{1}{Z} \frac{dZ}{d\beta}$$

$$= \frac{\hbar \omega}{2} \coth \frac{\hbar \omega}{2 k_B T}. \quad (8.144)$$

10. In general, $\rho_0$ can be expressed as

$$\rho_0 = \sum_i w_i |\alpha^{(i)}\rangle \langle \alpha^{(i)}|, \quad (8.145)$$

where $0 \leq w_i \leq 1$, $\sum_i w_i = 1$, and where $\langle \alpha^{(i)} | \alpha^{(i)} \rangle = 1$. Assume first that the system is initially in the state $|\alpha^{(i)}\rangle$. The probability for this to be the case is $w_i$. In general, the possible results of a measurement of the observable $A$ are the eigenvalues $\{a_n\}$. The probability $p_n$ to measure the eigenvalue $a_n$ given that the system is initially in state $|\alpha^{(i)}\rangle$ is given by

$$p_n = \langle \alpha^{(i)} | P_n | \alpha^{(i)} \rangle. \quad (8.146)$$

After a measurement of $A$ with an outcome $a_n$, the state vector collapses onto the corresponding eigensubspace and becomes
Chapter 8. Density Operator

\[ |\alpha^{(i)}\rangle \rightarrow \frac{P_n |\alpha^{(i)}\rangle}{\sqrt{\langle \alpha^{(i)} | P_n |\alpha^{(i)}\rangle}}. \] (8.147)

Thus, given that the system is initially in state \( |\alpha^{(i)}\rangle \) the final density operator is given by

\[
\rho_1^{(i)} = \sum_n \frac{P_n |\alpha^{(i)}\rangle \langle \alpha^{(i)}| P_n}{\sqrt{\langle \alpha^{(i)} | P_n |\alpha^{(i)}\rangle}} = \sum_n P_n |\alpha^{(i)}\rangle \langle \alpha^{(i)}| P_n.
\] (8.148)

Averaging over all possible initial states thus yields

\[
\rho_1 = \sum_i w_i \rho_1^{(i)} = \sum_n P_n \sum_i w_i |\alpha^{(i)}\rangle \langle \alpha^{(i)}| P_n = \sum_n P_n \rho_0 P_n. \tag{8.149}
\]

11. Since \([V (t), V (t')] = 0\) the time evolution operator from initial time \(t_0\) to time \(t\) is given by

\[
u (t, t_0) = \exp \left( \frac{i}{\hbar} \int_{t_0}^{t} dt' \, V (t') \right) = \exp \left( \frac{ip_i x}{\hbar} \right), \tag{8.150}
\]

where

\[
p_i = \int_{t_0}^{t} dt' f (t'). \tag{8.151}
\]

While the initial state of the entire system at time \(t_0\) is given by \(|\Psi (t_0)\rangle = |\psi_i\rangle \otimes |\alpha\rangle\), the final state at time \(t\) is given by

\[
|\Psi (t)\rangle = \nu (t, t_0) |\Psi (t_0)\rangle = \sum_n c_n J_n |\psi_i\rangle \otimes |\alpha_n\rangle,
\] (8.152)

where the operator \(J_n\) is given by

\[
J_n = \exp \left( \frac{i p_i a_n x}{\hbar} \right). \tag{8.153}
\]
8.4. Solutions

a) By introducing the identity operator \( \int dp' |p'| \langle p'| = 1_{MD} \) on the Hilbert space of the MD, where \( |p'| \) are eigenvectors of the momentum operator \( p \), which is canonically conjugate to \( x \), the state \( |\Psi(t)\rangle \) can be expressed as

\[
|\Psi(t)\rangle = \sum_n c_n \int dp' \langle p'| J_n |\psi_i\rangle |p'| \otimes |a_n\rangle .
\] (8.154)

With the help of the general identity (3.75), which is given by

\[
[p, A(x)] = -i\hbar \frac{dA}{dx} ,
\] (8.155)

where \( A(x) \) is a function of the operator \( x \), one finds that

\[
pJ_n |p'\rangle = ([p, J_n] + J_n p) |p'\rangle = (p a_n + p') J_n |p'\rangle ,
\] (8.156)

thus the vector \( J_n |p'\rangle \) is an eigenvector of \( p \) with eigenvalue \( p a_n + p' \). Moreover, note that this vector, which is labeled as \( |p' + p a_n\rangle \equiv J_n |p'\rangle \), is normalized, provided that \( |p'\rangle \) is normalized, since \( J_n \) is unitary. The momentum wavefunction \( \phi (p') = \langle p' | \psi_i \rangle \) of the state \( |\psi_i\rangle \) is related to the position wavefunction \( \langle x' | \psi_i \rangle \) by a Fourier transform [see Eq. (3.59)]

\[
\phi (p') = \frac{1}{\sqrt{2\pi \hbar}} \int -\infty \rightarrow \infty dx' e^{-i\frac{\hbar}{\pi} x' p'} \langle x' | \psi_i \rangle \\
= \frac{1}{\pi^{1/2}} \frac{\pi^{1/2}}{p_0^{1/2}} \exp \left( -\frac{1}{2} \left( \frac{p'}{p_0} \right)^2 \right)
\] (8.157)

where

\[
p_0 = \frac{\hbar}{x_0} .
\] (8.158)

In terms of \( \phi (p') \) the state \( |\Psi(t)\rangle \) thus can be expressed as

\[
|\Psi(t)\rangle = \sum_n c_n \int dp' \langle p' - p a_n |\psi_i\rangle |p'\rangle \otimes |a_n\rangle \\
= \sum_n c_n \int dp' \phi (p' - p a_n) |p'\rangle \otimes |a_n\rangle .
\] (8.159)
b) The probability distribution \( g(A) \) of the random variable \( A \) can be calculated using Eq. (8.159)

\[
g(A) = p_i \sum_{n'} |(a_{n'} | \otimes | p_i A_i | \Psi(t))|^2
= p_i \sum_{n'} |c_{n'}|^2 \phi(p_i (A - a_{n'}))|^2
= \frac{\eta}{\pi^{1/2}} \sum_{n'} |c_{n'}|^2 e^{-\eta^2(A - a_{n'})^2},
\]

where

\[
\eta = \frac{p_i}{p_0} = \frac{x_0}{\pi} \int^\infty_{-\infty} dt' f(t') .
\]

The expectation value of \( A \) is given by

\[
\langle A \rangle = \int_{-\infty}^{\infty} dA' g(A') A'
= \sum_{n'} |c_{n'}|^2 \frac{\eta}{\pi^{1/2}} \int_{-\infty}^{\infty} dA'' e^{-(\eta A'' - a_{n'}^2)}(A'' + a_{n'})
= \sum_{n'} |c_{n'}|^2 a_{n'} .
\]

(8.162)

c) The density operator of the entire system is taken to be given by \( \rho_f = |\Psi(\infty)\rangle \langle \Psi(\infty)| \) for this case. The additional measurement is associated with the observable \( B \), which is assumed to be a function of the degrees of freedom of the MS only. This assumption allows expressing the expectation value \( \bar{B} \) of the observable \( B \) as

\[
\bar{B} = Tr(B\rho_f)
= \sum_{n'} \int dp' \langle a_{n'} | \otimes | p' \rangle B\rho_f | p' \rangle \otimes | a_{n'} \rangle
= \sum_{n'} \langle a_{n'} | B\rho_R | a_{n'} \rangle ,
\]

(8.163)

where \( \rho_R \), which is given by

\[
\rho_R = \int dp' \langle p' | \rho_t | p' \rangle ,
\]

(8.164)
8.4. Solutions

is called the reduced density operator. Note that $\rho_R$ is an operator on the Hilbert space of the MS. With the help of the expressions

$$|\Psi(\infty)\rangle = \sum_n c_{n'} \int dp'' \phi(p'' - p_1 a_{n'}) |p''\rangle \otimes |a_{n'}\rangle ,$$  
(8.165)

$$\langle \Psi(\infty) | = \sum_{n'} c_{n''}^* \int dp''' \phi^*(p''' - p_1 a_{n''}) \langle a_{n''}| \otimes \langle p''' | ,$$  
(8.166)

one finds that

$$\rho_R = \sum_{n', n''} c_{n'} c_{n''}^* \int dp' \times \phi(p' - p_1 a_{n'}) \phi^*(p' - p_1 a_{n''}) \langle a_{n'}| \langle a_{n''} | .$$  
(8.167)

Employing the transformation of integration variable

$$x = \frac{2p' - p_1 (a_{n'} + a_{n''})}{2p_0} ,$$  
(8.168)

and its inverse

$$p' = p_0 \left( x + \frac{p_1 (a_{n'} + a_{n''})}{p_0} \right) ,$$  
(8.169)

one finds that

$$\int dp' \phi(p' - p_1 a_{n'}) \phi^*(p' - p_1 a_{n''}) = e^{-\eta^2 \left( \frac{a_{n'} - a_{n''}}{2} \right)^2} ,$$  
(8.170)

thus

$$\rho_R = \sum_{n', n''} c_{n'} c_{n''}^* e^{-\eta^2 \left( \frac{a_{n'} - a_{n''}}{2} \right)^2} |a_{n'}\rangle \langle a_{n''} | .$$  
(8.171)

12. It is convenient to employ the coordinate transformation

$$x' = \frac{x + y}{\sqrt{2}} ,$$  
(8.172)

$$y' = \frac{x - y}{\sqrt{2}} .$$  
(8.173)

The Lagrangian of the system can be written using these coordinates [see Eq. (9.167)] as

$$\mathcal{L} = \mathcal{L}_+ + \mathcal{L}_- ,$$  
(8.174)

where
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\[ \mathcal{L}_+ = \frac{m \dot{x}^2}{2} - \frac{m \omega^2}{2} (1 + \lambda) x^2, \]

(8.175)

and

\[ \mathcal{L}_- = \frac{m \dot{y}^2}{2} - \frac{m \omega^2}{2} (1 - \lambda) y^2. \]

(8.176)

Thus, the system is composed of two decoupled harmonic oscillators with angular resonance frequencies \( \omega \sqrt{1 + \lambda} \) (for \( x_0^2 \)) and \( \omega \sqrt{1 - \lambda} \) (for \( y_0^2 \)). In thermal equilibrium according to Eq. (8.115) one has

\[ \langle x^2 \rangle = \frac{\hbar}{2m \omega \sqrt{1 + \lambda}} \coth \left( \frac{\hbar \omega \sqrt{1 + \lambda^2}}{2} \right), \]

(8.177)

\[ \langle y^2 \rangle = \frac{\hbar}{2m \omega \sqrt{1 - \lambda}} \coth \left( \frac{\hbar \omega \sqrt{1 - \lambda^2}}{2} \right), \]

(8.178)

where \( \beta = 1/k_B T \). Moreover, due to symmetry, the following holds

\[ \langle x' \rangle = \langle y' \rangle = 0, \]

(8.179)

\[ \langle x'y' \rangle = 0. \]

(8.180)

With the help of the inverse transformation, which is given by

\[ x = \frac{x' + y'}{\sqrt{2}}, \]

(8.181)

\[ y = \frac{x' - y'}{\sqrt{2}}, \]

(8.182)

one thus finds

\[ \langle x \rangle = 0, \]

(8.183)

and

\[ \langle x^2 \rangle = \frac{1}{2} \left( \langle x'^2 \rangle + \langle y'^2 \rangle \right) = \frac{\hbar}{4m \omega} \left[ \frac{\coth \left( \frac{\hbar \omega \sqrt{1 + \lambda^2}}{2} \right)}{\sqrt{1 + \lambda}} + \frac{\coth \left( \frac{\hbar \omega \sqrt{1 - \lambda^2}}{2} \right)}{\sqrt{1 - \lambda}} \right]. \]

(8.184)
9. Time Independent Perturbation Theory

Consider a Hamiltonian \( \mathcal{H}_0 \) having a set of eigenenergies \( \{ E_k \} \). Let \( g_k \) be the degree of degeneracy of eigenenergy \( E_k \), namely \( g_k \) is the dimension of the corresponding eigensubspace, which is denoted by \( \mathcal{F}_k \). The set \( \{|k, i\} \) of eigenvectors of \( \mathcal{H}_0 \) is assumed to form an orthonormal basis for the vector space, namely

\[
\mathcal{H}_0 |k, i\rangle = E_k |k, i\rangle ,
\]  
(9.1)

and

\[
\langle k', i' | k, i \rangle = \delta_{k k'} \delta_{i i'} .
\]  
(9.2)

For a given \( k \) the degeneracy index \( i \) can take the values \( 1, 2, \ldots, g_k \). The set of vectors \( \{|k, 1\}, |k, 2\}, \ldots, |k, g_k\} \) forms an orthonormal basis for the eigensubspace \( \mathcal{F}_k \). The closure relation can be written as

\[
1 = \sum_k g_k \sum_{i=1}^{g_k} |k, i\rangle \langle k, i| = \sum_k P_k ,
\]  
(9.3)

where

\[
P_k = \sum_{i=1}^{g_k} |k, i\rangle \langle k, i|
\]  
(9.4)

is a projector onto eigen subspace \( \mathcal{F}_k \). The orthogonality condition (9.2) implies that

\[
P_k P_{k'} = P_k \delta_{kk'} .
\]  
(9.5)

A perturbation \( V = \lambda \tilde{V} \) is being added to the Hamiltonian

\[
\mathcal{H} = \mathcal{H}_0 + \lambda \tilde{V} ,
\]  
(9.6)

where \( \lambda \in \mathcal{R} \). We wish to find the eigenvalues and the eigenvectors of the Hamiltonian \( \mathcal{H} \)

\[
\mathcal{H} |\alpha\rangle = E |\alpha\rangle .
\]  
(9.7)
In many cases finding an analytical solution to the above equation is either very hard or impossible. In such cases one possibility is to employ numerical methods. However, another possibility arises provided that the eigenvalues and eigenvectors of $H_0$ are known and provided that the perturbation $\tilde{\lambda}V$ can be considered as small, namely, provided the eigenvalues and eigenvectors of $H$ do not significantly differ from those of $H_0$. In such a case an approximate solution can be obtained by the time independent perturbation theory.

**9.1 The Level $E_n$**

Consider the level $E_n$ of the unperturbed Hamiltonian $H_0$. Let $P_n$ be the projector onto the eigensubspace $F_n$, and let

$$Q_n = 1 - P_n = \sum_{k \neq n} P_k . \quad (9.8)$$

Equation (9.7) reads

$$\tilde{\lambda} \tilde{V} |\alpha\rangle = (E - H_0) |\alpha\rangle . \quad (9.9)$$

It is useful to introduce the operator $R$, which is defined as

$$R = \sum_{k \neq n} \frac{P_k}{E - E_k} . \quad (9.10)$$

**Claim.** The eigenvector $|\alpha\rangle$ of the Hamiltonian $H$ is given by

$$|\alpha\rangle = \left(1 - \lambda R \tilde{V}\right)^{-1} P_n |\alpha\rangle . \quad (9.11)$$

**Proof.** Using Eq. (9.5) it is easy to show that

$$P_n R = R P_n = 0 . \quad (9.12)$$

Moreover, the following hold

$$Q_n R = \sum_{k \neq n} \sum_{k' \neq n} \frac{P_k P_{k'}}{E - E_{k'}} = \sum_{k \neq n} \frac{P_k}{E - E_k} = R , \quad (9.13)$$

and similarly

$$R Q_n = R . \quad (9.14)$$

Furthermore, by expressing $H_0$ as

$$H_0 = \sum_{k} \sum_{i=1}^{g_k} E_k |k, i\rangle \langle k, i| = E_n P_n + \sum_{k \neq n} E_k P_k , \quad (9.15)$$
one finds that
\[
R(E - \mathcal{H}_0) = \sum_{k \neq n} P_k \left( \frac{E - E_n P_n - \sum_{k' \neq n} E_{k'} P_{k'}}{E - E_k} \right)
\]
\[
= \sum_{k \neq n} P_k \frac{E - E_k}{E - E_k}
\]
\[
= Q_n,
\]
(9.16)
and similarly
\[
(E - \mathcal{H}_0) R = Q_n.
\]
(9.17)
The last two results suggest that the operator \( R \) can be considered as the inverse of \( E - \mathcal{H}_0 \) in the subspace of eigenvalue zero of the projector \( P_n \) (which is the subspace of eigenvalue unity of the projector \( Q_n \)).

Multiplying Eq. (9.9) from the left by \( R \) yields
\[
\lambda R \tilde{V} |\alpha_i\rangle = R(E - \mathcal{H}_0)|\alpha_i\rangle.
\]
(9.18)
With the help of Eq. (9.16) one finds that
\[
\lambda R \tilde{V} |\alpha_i\rangle = Q_n |\alpha_i\rangle.
\]
(9.19)
Since \( P_n = 1 - Q_n \) [see Eq. (9.8)] the last result implies that
\[
P_n |\alpha\rangle = |\alpha\rangle - \lambda R \tilde{V} |\alpha\rangle = \left(1 - \lambda R \tilde{V}\right) |\alpha\rangle,
\]
(9.20)
which leads to Eq. (9.11)
\[
|\alpha\rangle = \left(1 - \lambda R \tilde{V}\right)^{-1} P_n |\alpha\rangle.
\]
(9.21)
Note that Eq. (9.11) can be expanded as power series in \( \lambda \)
\[
|\alpha\rangle = \left(1 + \lambda R \tilde{V} + \lambda^2 R \tilde{V} R \tilde{V} + \cdots\right) P_n |\alpha\rangle.
\]
(9.22)

### 9.1.1 Nondegenerate Case

In this case \( g_n = 1 \) and
\[
P_n = |n\rangle \langle n|.
\]
(9.23)
In general the eigenvector \( |\alpha\rangle \) is determined up to multiplication by a constant. For simplicity we choose that constant to be such that
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\[ P_n |\alpha\rangle = |n\rangle , \quad (9.24) \]

namely

\[ \langle n |\alpha\rangle = 1 . \quad (9.25) \]

Multiplying Eq. (9.9), which is given by

\[ \lambda \tilde{V} |\alpha\rangle = (E - \mathbf{H}_0) |\alpha\rangle , \quad (9.26) \]

from the left by \( |n\rangle \) yields

\[ \langle n | \lambda \tilde{V} |\alpha\rangle = \langle n | (E - \mathbf{H}_0) |\alpha\rangle , \quad (9.27) \]

or

\[ \langle n | E |\alpha\rangle = \langle n | \mathbf{H}_0 |\alpha\rangle + \langle n | \lambda \tilde{V} |\alpha\rangle , \quad (9.28) \]

thus

\[ E = E_n + \langle n | \lambda \tilde{V} |\alpha\rangle . \quad (9.29) \]

Equation (9.22) together with Eq. (9.24) yield

\[
|\alpha\rangle = \left( 1 + \lambda R\tilde{V} + \lambda^2 R\tilde{V}R\tilde{V} + \cdots \right) |n\rangle \\
= |n\rangle + \lambda \sum_{k \neq n} \frac{|k,i\rangle \langle k,i| \tilde{V} |n\rangle}{E - E_k} \\
+ \lambda^2 \sum_{k \neq n} \sum_{k' \neq n} \frac{|k,i\rangle \langle k,i| \tilde{V} |k',i\rangle \langle k',i| \tilde{V} |n\rangle}{(E - E_k)(E - E_{k'})} + \cdots . \quad (9.30)
\]

Substituting Eq. (9.30) into Eq. (9.29) yields

\[
E = E_n + \lambda \langle n | \tilde{V} |n\rangle \\
+ \lambda^2 \sum_{k \neq n} \frac{\langle n | \tilde{V} |k,i\rangle \langle k,i| \tilde{V} |n\rangle}{E - E_k} \\
+ \lambda^3 \sum_{k \neq n} \sum_{k' \neq n} \frac{\langle n | \tilde{V} |k,i\rangle \langle k,i| \tilde{V} |k',i\rangle \langle k',i| \tilde{V} |n\rangle}{(E - E_k)(E - E_{k'})} + \cdots . \quad (9.31)
\]
Note that the right hand side of Eq. (9.31) contains terms that depend on $E$. To second order in $\lambda$ one finds

$$E = E_n + \langle n | V | n \rangle + \sum_{k \neq i} \frac{|\langle k, i | V | n \rangle|^2}{E_n - E_k} + O(\lambda^3) .$$

(9.32)

Furthermore, to first order in $\lambda$ Eq. (9.30) yields

$$|\alpha\rangle = |n\rangle + \sum_{k \neq i} \frac{|\langle k, i | V | n \rangle|}{E_n - E_k} + O(\lambda^2) .$$

(9.33)

**9.1.2 Degenerate Case**

The set of vectors $\{|n, 1\rangle, |n, 2\rangle, \ldots, |n, g_n\rangle\}$ forms an orthonormal basis for the eigensubspace $F_n$. Multiplying Eq. (9.9) from the left by $P_n$ yields

$$P_n \lambda \tilde{V} |\alpha\rangle = P_n \left( E - H_0 \right) |\alpha\rangle ,$$

(9.34)

thus with the help of Eq. (9.15) one has

$$P_n \lambda \tilde{V} |\alpha\rangle = (E - E_n) P_n |\alpha\rangle .$$

(9.35)

Substituting Eq. (9.22), which is given by

$$|\alpha\rangle = \left( P_n + \lambda \tilde{V} P_n + \lambda^2 \tilde{V} \tilde{R} \tilde{V} P_n + \cdots \right) |\alpha\rangle ,$$

(9.36)

into this and noting that $P_n R = 0$ and $P_n^2 = P_n$ yield

$$P_n \lambda \tilde{V} P_n |\alpha\rangle + \lambda^2 P_n \tilde{V} \tilde{R} \tilde{V} P_n |\alpha\rangle + \cdots = (E - E_n) P_n |\alpha\rangle .$$

(9.37)

Thus, to first order in $\lambda$ the energy correction $E - E_n$ is found by solving

$$P_n \tilde{V} P_n |\alpha\rangle = (E - E_n) P_n |\alpha\rangle .$$

(9.38)

The solutions are the eigenvalues of the $g_n \times g_n$ matrix representation of the operator $\tilde{V}$ in the subspace $F_n$.

**9.2 Example**

Consider a point particle having mass $m$ whose Hamiltonian is given by

$$\mathcal{H} = H_0 + V ,$$

(9.39)

where
Chapter 9. Time Independent Perturbation Theory

\[ H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \].

(9.40)

and where

\[ V = \lambda \hbar \omega \sqrt{\frac{m\omega}{\hbar}} \).

(9.41)

The eigenvectors and eigenvalues of the Hamiltonian \( H_0 \), which describes a one dimensional harmonic oscillator, are given by

\[ H_0 |n\rangle = E_n |n\rangle \),

(9.42)

where \( n = 0, 1, 2 \cdots \), and where

\[ E_n (\lambda = 0) = \sqrt{\frac{m\omega}{\hbar}} \left( n + \frac{1}{2} \right) \).

(9.43)

Note that, as was shown in chapter 5 [see Eq. (5.144)], the eigenvectors and eigenvalues of \( H \) can be found analytically for this particular case. For the sake of comparison we first derive this exact solution. Writing \( H \) as

\[ H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} + \hbar \omega \sqrt{\frac{m\omega}{\hbar}} x + \lambda \sqrt{\frac{m\omega}{\hbar}} x \)

(9.44)

one sees that \( H \) describes a one dimensional harmonic oscillator (as \( H_0 \) also does). The exact eigenenergies are given by

\[ E_n (\lambda) = E_n (\lambda = 0) - \frac{1}{2} \hbar \omega \lambda^2 \),

(9.45)

and the corresponding exact wavefunctions are

\[ \langle x' | n (\lambda) \rangle = \left( x' + \lambda \sqrt{\frac{\hbar}{m\omega}} |n\rangle \right) \).

(9.46)

Using identity (3.19), which is given by

\[ J (\Delta x) |x'\rangle = |x' + \Delta x\rangle \),

(9.47)

where \( J (\Delta x) \) is the translation operator, the exact solution (9.46) can be rewritten as

\[ \langle x' | n (\lambda) \rangle = \langle x'| J \left( -\lambda \sqrt{\frac{\hbar}{m\omega}} \right) |n\rangle \),

(9.48)
or simply as

\[ |n(\lambda)\rangle = J \left( -\lambda \sqrt{\frac{\hbar}{m\omega}} \right) |n\rangle . \]

(9.49)

Next we calculate an approximate eigenvalues and eigenvectors using perturbation theory. Using the identity

\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger) , \]

(9.50)

one has

\[ V = \frac{\lambda \hbar \omega}{\sqrt{2}} (a + a^\dagger) . \]

(9.51)

Furthermore, using the identities

\[ a |n\rangle = \sqrt{n} |n-1\rangle , \]

\[ a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle , \]

(9.52)

(9.53)

one has

\[ \langle m| V |n\rangle = \frac{\lambda \hbar \omega}{\sqrt{2}} \left( \langle m| a |n\rangle + \langle m| a^\dagger |n\rangle \right) \]

\[ = \frac{\lambda \hbar \omega}{\sqrt{2}} \left( \sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1} \right) . \]

(9.54)

Thus \( E_n(\lambda) \) can be expanded using Eq. (9.32) as

\[ E_n(\lambda) = E_n + \langle n| V |n\rangle + \sum_{i \neq n} \frac{|\langle k,i| V |n\rangle|^2}{E_n - E_k} + O(\lambda^3) \]

\[ = E_n + \frac{|\langle n-1| V |n\rangle|^2}{E_n - E_{n-1}} + \frac{|\langle n+1| V |n\rangle|^2}{E_n - E_{n+1}} + O(\lambda^3) \]

\[ = \hbar \omega \left( n + \frac{1}{2} \right) + \hbar \omega \frac{n\lambda^2}{2} - \hbar \omega \frac{(n+1)\lambda^2}{2} + O(\lambda^3) \]

\[ = \hbar \omega \left( n + \frac{1}{2} \right) - \hbar \omega \frac{\lambda^2}{2} + O(\lambda^3) , \]

(9.55)

in agreement (to second order) with the exact result (9.45), and \( |n(\lambda)\rangle \) can be expanded using Eq. (9.30) as
\[ |n(\lambda)\rangle = |n\rangle + \sum_{k \neq n} \frac{|k, i\rangle \langle k, i| V |n\rangle}{E_n - E_k} + O(\lambda^2) \]

\[ = |n\rangle + \frac{|n - 1\rangle \langle n - 1| V |n\rangle}{E_n - E_{n-1}} + \frac{|n + 1\rangle \langle n + 1| V |n\rangle}{E_n - E_{n+1}} + O(\lambda^2) \]

\[ = |n\rangle + \frac{|n - 1\rangle \frac{\hbar \omega}{\sqrt{2}} \sqrt{n}}{\hbar \omega} - \frac{|n + 1\rangle \frac{\hbar \omega}{\sqrt{2}} \sqrt{n + 1}}{\hbar \omega} + O(\lambda^2) \]

\[ = |n\rangle + \frac{\lambda}{\sqrt{2}} |n\rangle - \frac{\lambda}{\sqrt{2}} a|n\rangle + O(\lambda^2) \, . \]

(9.56)

Note that with the help of the following identify

\[ p = i \sqrt{\frac{m \hbar \omega}{2}} (-a + a^\dagger) \, , \]

(9.57)

the last result can be written as

\[ |n(\lambda)\rangle = \left( 1 + \lambda \sqrt{\frac{\hbar}{m \omega}} \frac{ip}{\hbar} \right) |n\rangle + O(\lambda^2) \, . \]

(9.58)

Alternatively, in terms of the translation operator \( J(\Delta x) \), which is given by

\[ J(\Delta x) = \exp \left( -\frac{ip\Delta x}{\hbar} \right) \, , \]

(9.59)

one has

\[ |n(\lambda)\rangle = J \left( -\lambda \sqrt{\frac{\hbar}{m \omega}} \right) |n\rangle + O(\lambda^2) \, , \]

(9.60)

in agreement (to second order) with the exact result (9.49).

9.3 Problems

1. The volume effect: The energy spectrum of the hydrogen atom was calculated in chapter 8 by considering the proton to be a point particle. Consider a model in which the proton is instead assumed to be a sphere of radius \( \rho_0 \) where \( \rho_0 << a_0 \) (\( a_0 \) is Bohr’s radius), and the charge of the proton +e is assumed to be uniformly distributed in that sphere. Show that the energy shift due to such perturbation to lowest order in perturbation theory is given by

\[ \Delta E_{n,l} = \frac{\epsilon^2}{10\rho_0^2} (R_{n,l}(0))^2 \, , \]

(9.61)

where \( R_{n,l}(r) \) is the radial wave function.
2. Consider an Hydrogen atom. A perturbation given by

\[ V = A r, \]  
(9.62)

where \( r = \sqrt{x^2 + y^2 + z^2} \) is the radial coordinate and \( A \) is a constant is added.

a) Calculate to first order in \( A \) the energy of the ground state.

b) Calculate to first order in \( A \) the energy of the first excited state.

3. A weak uniform electric field \( E = E \hat{z} \), where \( E \) is a constant, is applied to a hydrogen atom. Calculate to 1st order in perturbation theory the correction to the energy of the

a) level \( n = 1 \) (\( n \) is the principle quantum number).

b) level \( n = 2 \).

4. Consider two particles, both having the same mass \( m \), moving in a one-dimensional potential with coordinates \( x_1 \) and \( x_2 \) respectively. The potential energy is given by

\[ V (x_1, x_2) = \frac{1}{2} m \omega^2 (x_1 - a)^2 + \frac{1}{2} m \omega^2 (x_2 + a)^2 + \lambda m \omega^2 (x_1 - x_2)^2, \]  
(9.63)

where \( \lambda \) is real. Find the energy of the ground state to lowest non-vanishing order in \( \lambda \).

5. A particle having mass \( m \) is confined in a potential well of width \( l \), which is given by

\[ V (x) = \begin{cases} 
0 & \text{for} \ 0 \leq x \leq l, \\
+\infty & \text{elsewhere}.
\end{cases} \]  
(9.64)

Find to lowest order in perturbation theory the correction to the ground state energy due to a perturbation given by

\[ W (x) = w_0 \delta \left(x - \frac{l}{2}\right), \]  
(9.65)

where \( w_0 \) is a real constant.

6. Consider a particle having mass \( m \) in a two dimensional potential well of width \( a \) that is given by

\[ V (x, y) = \begin{cases} 
0 & \text{if} \ 0 \leq x \leq a \text{ and } 0 \leq y \leq a, \\
+\infty & \text{elsewhere}.
\end{cases} \]  
(9.66)

A perturbation given by

\[ W (x, y) = \begin{cases} 
w_0 & \text{if} \ 0 \leq x \leq \frac{a}{2} \text{ and } 0 \leq y \leq \frac{a}{2}, \\
0 & \text{elsewhere}
\end{cases} \]  
(9.67)

is added.
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a) Calculate to lowest non-vanishing order in $w_0$ the energy of the ground state.

b) The same for the first excite state.

7. Consider a particle having mass $m$ moving in a potential energy given by

$$V(x, y) = \frac{m\omega^2}{2} (x^2 + y^2) + \beta m\omega^2 xy,$$

(9.68)

where the angular frequency $\omega$ is a constant and where the dimensionless real constant $\beta$ is assumed to be small.

a) Calculate to first order in $\beta$ the energy of the ground state.

b) Calculate to first order in $\beta$ the energy of the first excited state.

8. Consider an harmonic oscillator having angular resonance frequency $\omega_r$. A perturbation given by

$$V = \beta (a^\dagger a^\dagger + aa)$$

(9.69)

is added, where $a$ is the annihilation operator and $\beta$ is a real constant. Calculate the energies of the system to second order in $\beta$.

9. The Hamiltonian of a spin $S = 1$ is given by

$$\mathcal{H} = \alpha S_z^2 + \beta (S_x^2 - S_y^2),$$

(9.70)

where $\alpha$ and $\beta$ are both constants.

a) Write the matrix representation of $\mathcal{H}$ in the basis $\{|S = 1, m = -1\}, |S = 1, m = 0\rangle |S = 1, m = 1\rangle$.

b) Calculate (exactly) the eigenenergies and the corresponding eigenvectors.

c) For the case $\beta \ll \alpha$ use perturbation theory to calculate to lowest order in $\alpha$ and $\beta$ the eigen energies of the system.

10. Consider a system composed of an harmonic oscillator having angular resonance frequency $\omega_r > 0$ and a two-level system. The Hamiltonian of the system is given by

$$\mathcal{H} = \mathcal{H}_r + \mathcal{H}_a + V.$$

(9.71)

The term $\mathcal{H}_r$ is the Hamiltonian for the harmonic oscillator

$$\mathcal{H}_r = \hbar \omega_r \left(a^\dagger a + \frac{1}{2}\right),$$

(9.72)

where $a$ and $a^\dagger$ are annihilation and creation operators respectively. The term $\mathcal{H}_a$ is the Hamiltonian for the two-level system

$$\mathcal{H}_a = \frac{\hbar \omega_a}{2} (|+\rangle \langle +| - |-\rangle \langle -|),$$

(9.73)

where the ket vectors $|\pm\rangle$ represent the two levels and where $\omega_a > 0$. The coupling term between the oscillator and the two-level system is given by
9.3. Problems

\[ V = \hbar g (a^+ | - \left.<+| + a | +\right> <|-|) . \]  
(9.74)

Assume the case where \(|g| \ll \omega_r\) and where \(|g| \ll \omega_n\). Calculate to lowest non-vanishing order in \(g\) the eigen energies of the system for the following cases: (a) \(\omega_r \neq \omega_n\); (b) \(\omega_r = \omega_n\).

11. Consider a particle having mass \(m\) in a two-dimensional potential given by

\[ V_0 = \frac{1}{2} m \omega^2 (x^2 + y^2) . \]  
(9.75)

The following perturbation is added

\[ V_1 = \frac{\beta \omega}{R} L_z^2 , \]  
(9.76)

where \(L_z\) is the \(z\) component of the angular momentum operator.

a) Find to second orders in \(\beta\) the energy of the ground state.

b) Find to first order in \(\beta\) the energy of the first excited level.

12. A particle having mass \(m\) moves in a one dimensional potential\n
\[ V_0 = \begin{cases} V_0 \sin \frac{2\pi x}{L} & 0 \leq x \leq L \\ \infty & \text{else} \end{cases} . \]  
(9.77)

Consider the constant \(V_0\) to be small. Calculate the system’s eigenenergies \(E_n\) to first order in \(V_0\).

13. Consider a particle having mass \(m\) confines by the one-dimensional potential well, which is given by

\[ V(x) = \begin{cases} \infty & x < 0 \\ \frac{\epsilon}{L} & 0 \leq x \leq L \\ \infty & x > L \end{cases} . \]  

Find to first order in \(\epsilon\) the energy of the ground state.

14. A particle of mass \(m\) is trapped in an infinite 2 dimensional well of width \(l\)

\[ V(x, y) = \begin{cases} 0 & 0 \leq x \leq l \text{ and } 0 \leq y \leq l \\ \infty & \text{else} \end{cases} . \]  
(9.78)

A perturbation given by

\[ W(x, y) = \frac{\lambda h^2 \pi^2}{m} \delta(x - l_x) \delta(y - l_y) . \]  
(9.79)

is added, where

\[ 0 \leq l_x \leq l , \]  
(9.80)
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and

\[ 0 \leq l_y \leq l. \quad (9.81) \]

Calculate to 1st order in perturbation theory the correction to the energy of the:

a) ground state.

b) first excited state.

15. Consider a rigid rotator whose Hamiltonian is given by

\[ H = \frac{L_x^2 + L_y^2}{2I_{xy}} + \frac{L_z^2 - L_y^2}{2I_{xy}}, \quad (9.82) \]

where \( L \) is the angular momentum vector operator. Use perturbation theory to calculate the energy of the ground state to second order in \( \lambda \).

16. Consider two particles having the same mass \( m \) moving along the \( x \) axis.

The Hamiltonian of the system is given by

\[ H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \alpha \delta (x_1) - \alpha \delta (x_2) + \lambda \delta (x_1 - x_2), \quad (9.83) \]

where \( x_1 \) and \( x_2 \) are the coordinates of the first and second particle respectively, \( p_1 \) and \( p_2 \) are the corresponding canonically conjugate momentums, \( \alpha \) and \( \lambda \) are both real positive constants and \( \delta () \) denotes the delta function. Calculate to first order in \( \lambda \) the energy of the ground state of the system.

17. In this problem the main results of time independent perturbation theory are derived using an alternative approach. Consider a general square matrix

\[ W = D + \Omega V, \quad (9.84) \]

where \( \Omega \in \mathbb{R} \), \( D \) is diagonal

\[ D |n_0\rangle = \lambda_{n_0} |n_0\rangle, \quad (9.85a) \]

\[ \langle n_0 | D = \lambda_{n_0} \langle n_0 |, \quad (9.85b) \]

and we assume that none of the eigenvalues of \( D \) is degenerate. The set of eigenvectors of \( D \) is assumed to be orthonormal

\[ \langle n_0 | n_0 \rangle = \delta_{nn}, \quad (9.86) \]

and complete (the dimensionality is assumed to be finite)

\[ 1 = \sum_n |n_0 \rangle \langle n_0 |. \quad (9.87) \]

Calculate the eigenvalues of \( W \)

\[ W |n\rangle = \lambda |n\rangle \quad (9.88) \]

to second order in \( \Omega \).
9.4 Solutions

1. The radial force acting on the electron is found using Gauss’ theorem

\[
F_r (r) = \begin{cases} 
\frac{e^2}{r^2} \left( \frac{r}{\rho_0} \right) r > \rho_0 \\
\frac{e^2}{r^2} \left( \frac{r}{\rho_0} \right)^2 - 3 r \leq \rho_0 
\end{cases}
\]  

(9.89)

The potential energy \( V (r) \) is found by integrating \( F_r (r) \) and by requiring that \( V (r) \) is continuous at \( r = \rho_0 \)

\[
V (r) = \begin{cases} 
-\frac{e^2}{r} r > \rho_0 \\
\frac{e^2}{2\rho_0} \left( \frac{r}{\rho_0} \right)^2 - 3 r \leq \rho_0 
\end{cases}
\]  

(9.90)

Thus, the perturbation term in the Hamiltonian is given by

\[
V_p (r) = V (r) - \left( -\frac{e^2}{r} \right) = \begin{cases} 
0 r > \rho_0 \\
\frac{e^2}{2\rho_0} \left( \frac{r}{\rho_0} \right)^2 + \frac{2\rho_0}{r} - 3 r \leq \rho_0 
\end{cases}
\]  

(9.91)

To first order one has

\[
\Delta E_{n,l} = \langle nlm | V_p | nlm \rangle \, .
\]  

(9.92)

The wavefunctions for the unperturbed case are given by

\[
\psi_{nlm} (r, \theta, \phi) = R_{nl} (r) Y^m_l (\theta, \phi) \, ,
\]  

(9.93)

Since \( V_p \) depends on \( r \) only, one finds that

\[
\Delta E_{n,l} = \int_0^\infty dr \int_0^{\rho_0} r^2 |R_{nl} (r)|^2 V_p (r)
\]

\[
= \int_0^{\rho_0} |R_{nl} (r)|^2 \frac{e^2}{2\rho_0} \left( \frac{r}{\rho_0} \right)^2 + \frac{2\rho_0}{r} - 3 \, .
\]  

(9.94)

In the limit where \( \rho_0 \ll a_0 \) the term \( |R_{nl} (r)|^2 \) can approximately be replaced by \( |R_{nl} (0)|^2 \), thus

\[
\Delta E_{n,l} = |R_{nl} (0)|^2 \int_0^{\rho_0} dr \int_0^{\rho_0} r^2 \frac{e^2}{2\rho_0} \left( \frac{r}{\rho_0} \right)^2 + \frac{2\rho_0}{r} - 3
\]

\[
= \frac{e^2 \rho_0^2}{10} |R_{nl} (0)|^2 \, .
\]  

(9.95)
2. The wavefunctions for the unperturbed case are given by
\[ \psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_{lm}^m(\theta, \phi), \]  
(9.96)
where for the states relevant to this problem
\[ R_{10}(r) = 2 \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0}, \]  
(9.97a)
\[ R_{20}(r) = (2 - r/a_0) \left( \frac{1}{2a_0} \right)^{3/2} e^{-r/a_0}, \]  
(9.97b)
\[ R_{21}(r) = \left( \frac{1}{2a_0} \right)^{3/2} \frac{r}{\sqrt{3a_0}} e^{-r/2a_0}, \]  
(9.97c)
\[ Y_{00}^0(\theta, \phi) = \sqrt{\frac{1}{4\pi}}, \]  
(9.97d)
\[ Y_{-11}^{-1}(\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-i\phi}, \]  
(9.97e)
\[ Y_{10}^0(\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta, \]  
(9.97f)
\[ Y_{11}^1(\theta, \phi) = -\frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{i\phi}, \]  
(9.97g)
and the corresponding eigenenergies are given by
\[ E_n^{(0)} = \frac{E_1}{n^2}, \]  
(9.98)
where
\[ E_1 = \frac{m_e e^4}{2\hbar^2}. \]  
(9.99)

The perturbation term \( V \) in the Hamiltonian is given by \( V = Ar \). The matrix elements of \( V \) are expressed as
\[ \langle n'l'm' | V | nlm \rangle = A \int_0^\infty \int_{-1}^1 \int_0^{2\pi} r^3 R_{nl'} R_{ml'} d(\cos \theta) d\phi \left( Y_{l'm'}^m \right)^* Y_{lm}^m \]  
\[ = A \delta_{l,l'} \delta_{m,m'} \int_0^\infty r^3 R_{nl'} R_{ml'} dr. \]  
(9.100)
a) Thus, to first order
\[ E_1 = E_1^{(0)} + \langle 100 | V | 100 \rangle + O(A^2), \]  
(9.101)
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where

\[ |100\rangle \langle 100| = A \int_0^\infty dr \ r^3 R_{10}^2 (r) = \frac{3Aa_0}{2}. \quad (9.102) \]

b) The first excited state is degenerate, however, as can be seen from Eq. (9.100) all off-diagonal elements are zero. The diagonal elements are given by

\[ |200\rangle \langle 200| = A \int_0^\infty dr \ r^3 R_{20}^2 = 6Aa_0, \quad (9.103a) \]

\[ |21m\rangle \langle 21m| = A \int_0^\infty dr \ r^3 R_{21} = 5Aa_0. \quad (9.103b) \]

Thus, the degeneracy is lifted

\[ E_{2,l=0} = E^{(0)}_2 + 6Aa_0 + O(A^2), \quad (9.104) \]

\[ E_{2,l=1} = E^{(0)}_2 + 5Aa_0 + O(A^2). \quad (9.105) \]

3. The wavefunctions for the unperturbed case are given by

\[ \psi_{nlm} (r, \theta, \phi) = R_{nl}(r) Y_{lm} (\theta, \phi), \quad (9.106) \]

where for the states relevant to this problem

\[ R_{10}(r) = 2 \left( \frac{1}{a_0} \right)^{3/2} e^{-r/a_0}, \quad (9.107) \]

\[ R_{20}(r) = (2 - r/a_0) \left( \frac{1}{2a_0} \right)^{3/2} e^{-\frac{r}{2a_0}}, \quad (9.108) \]

\[ R_{21}(r) = \left( \frac{1}{2a_0} \right)^{3/2} \frac{r}{\sqrt{3}a_0} e^{-\frac{r}{2a_0}}, \quad (9.109) \]

\[ Y_0^0 (\theta, \phi) = \frac{1}{\sqrt{4\pi}}, \quad (9.110) \]

\[ Y_1^{-1} (\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{-i\phi}, \quad (9.111) \]

\[ Y_1^0 (\theta, \phi) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos \theta, \quad (9.112) \]

\[ Y_1^1 (\theta, \phi) = -\frac{1}{2} \sqrt{\frac{3}{2\pi}} \sin \theta e^{i\phi}, \quad (9.113) \]

and the corresponding eigenenergies are given by

\[ E_n^{(0)} = \frac{E_1}{n^2}, \quad (9.114) \]
where

\[ E_1 = \frac{m_e e^4}{2h^2}. \]  

(9.115)

The perturbation term \( V \) in the Hamiltonian is given by

\[ V = eEz = eEr \cos \theta. \]  

(9.116)

The matrix elements of \( V \) are expressed as

\[ \langle n'l'm' | V | nlm \rangle = eE \int_0^{\infty} dr^3 r^3 R_{n'l'} R_{nl} \int_{-1}^{1} d(\cos \theta) \int_0^{2\pi} d\phi \cos \theta \left( Y_{l'm'}^{m'} \right)^* Y_{l''}^m. \]  

(9.117)

a) Disregarding spin this level is non degenerate. To 1st order

\[ E_1 = E_1^{(0)} + \langle 1, 0, 0 | V | 1, 0, 0 \rangle = E_1^{(0)}, \]

since

\[ \int_{-1}^{1} d(\cos \theta) \cos \theta = 0, \]

thus the energy of the ground state is unchanged to 1st order.

b) The level \( n = 2 \) has degeneracy 4. The matrix of the perturbation \( V \) in the degenerate subspace is given by

\[ M = \begin{pmatrix}
\langle 2, 0, 0 | V | 2, 0, 0 \rangle & \langle 2, 0, 0 | V | 2, 1, -1 \rangle & \langle 2, 0, 0 | V | 2, 1, 0 \rangle & \langle 2, 0, 0 | V | 2, 1, 1 \rangle \\
\langle 2, 1, -1 | V | 2, 0, 0 \rangle & \langle 2, 1, -1 | V | 2, 1, -1 \rangle & \langle 2, 1, -1 | V | 2, 1, 0 \rangle & \langle 2, 1, -1 | V | 2, 1, 1 \rangle \\
\langle 2, 1, 0 | V | 2, 0, 0 \rangle & \langle 2, 1, 0 | V | 2, 1, -1 \rangle & \langle 2, 1, 0 | V | 2, 1, 0 \rangle & \langle 2, 1, 0 | V | 2, 1, 1 \rangle \\
\langle 2, 1, 1 | V | 2, 0, 0 \rangle & \langle 2, 1, 1 | V | 2, 1, -1 \rangle & \langle 2, 1, 1 | V | 2, 1, 0 \rangle & \langle 2, 1, 1 | V | 2, 1, 1 \rangle
\end{pmatrix}. \]  

(9.118)
\[ \int_{-1}^{1} d(\cos \theta) \cos \theta = 0 , \]  
\[ (9.119) \]
\[ \int_{-1}^{1} d(\cos \theta) \cos \theta \sin \theta = 0 , \]  
\[ (9.120) \]
\[ \int_{-1}^{1} d(\cos \theta) \cos \theta \sin^2 \theta = 0 , \]  
\[ (9.121) \]
\[ \int_{-1}^{1} d(\cos \theta) \cos^3 \theta = 0 , \]  
\[ (9.122) \]
\[ \int_{0}^{2\pi} d\phi e^{\pm i\phi} = 0 , \]  
\[ (9.123) \]

one finds

\[ M = \begin{pmatrix} 0 & 0 & \gamma & 0 \\ 0 & 0 & 0 & 0 \\ \gamma^* & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} , \]  
\[ (9.124) \]

where

\[ \gamma = \langle 2, 0, 0 | V | 2, 1, 0 \rangle \]
\[ = eE \int_{0}^{\infty} dr r^3 R_{2,0}R_{2,1} \int_{-1}^{1} d(\cos \theta) \int_{0}^{2\pi} d\phi \cos \theta (Y_0^0)^* Y_1^0 \]
\[ = eE \int_{0}^{\infty} dr \left( 2 - \frac{r}{a_0} \right) \left( \frac{r}{a_0} \right)^4 e^{-\frac{r}{a_0}} \]
\[ \times \frac{1}{4\pi} \int_{-1}^{1} d(\cos \theta) \cos^2 \theta \int_{0}^{2\pi} d\phi . \]  
\[ (9.125) \]

Using

\[ \int_{-1}^{1} d(\cos \theta) \cos^2 \theta = \frac{2}{3} , \]  
\[ (9.126) \]

and
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\[ \int_{0}^{\infty} x^4 e^{-x} \, dx = 24 \]  
(9.127)

\[ \int_{0}^{\infty} x^5 e^{-x} \, dx = 120 \]  
(9.128)

one finds

\[ \gamma = \langle 2, 0, 0 | V | 2, 1, 0 \rangle \]

\[ = e E \frac{e}{24} \int_{0}^{\infty} dr \left( 2 - \frac{r}{a_0} \right) \left( \frac{r}{a_0} \right)^4 e^{-\frac{r}{a_0}} \]

\[ = \frac{a_0 e E}{24} \int_{0}^{\infty} dx \left( 2 - x \right) x^4 e^{-x} \]

\[ = -3a_0 e E . \]  
(9.129)

The eigenvalues of the matrix \( M \) are 0, 0, 3\( a_0 e E \) and \( -3a_0 e E \). Thus to 1st order the degeneracy is partially lifted with subspace of dimension 2 having energy \( E^{(0)}_2 \), and another 2 nondegenerate subspaces having energies \( E^{(0)}_2 \pm 3a_0 e E \).

4. To lowest order in perturbation theory the ground state energy is given by

\[ E_{gs} = \hbar \omega + \lambda m \omega^2 \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \varphi_0^2 (x_1 - a) \varphi_0^2 (x_2 + a) (x_1 - x_2)^2 + O (\lambda^2) , \]

(9.130)

where \( \varphi_0 (x) \) is the ground state wavefunction of a particle having mass \( m \) confined by a potential \( (1/2) m \omega^2 x^2 \) centered at \( x = 0 \). Employing the transformation

\[ x_1' = x_1 - a , \]  
(9.131)

\[ x_2' = x_2 + a , \]  
(9.132)

and Eq. (5.116) one finds that
\[ E_{gs} = \hbar \omega \]
\[ + \lambda m \omega^2 \int_{-\infty}^{\infty} dx' \varphi_0^2 (x' \varphi_0 (x'_1 + a)^2 \]
\[ + \lambda m \omega^2 \int_{-\infty}^{\infty} dx' \varphi_0^2 (x' \varphi_0 (x'_2 + a)^2 \]
\[ - 2\lambda m \omega^2 \int_{-\infty}^{\infty} dx' \varphi_0^2 (x' \varphi_0 (x'_1 + a) \int_{-\infty}^{\infty} dx' \varphi_0^2 (x' \varphi_0 (x'_2 - a) \]
\[ + O (\lambda^2) \]
\[ = \hbar \omega + 2\lambda m \omega^2 \left( \frac{\hbar}{2m \omega} + a^2 \right) + 2\lambda m \omega^2 a^2 + O (\lambda^2) \]
\[ = \hbar \omega + \lambda (\hbar \omega + 4m \omega^2 a^2) + O (\lambda^2) . \] (9.133)

Note that this problem can be also solved exactly by employing the co-
ordinate transformation
\[ x_+ = \frac{x_1 + x_2}{\sqrt{2}} , \] (9.134)
\[ x_- = \frac{x_1 - x_2}{\sqrt{2}} . \] (9.135)

The inverse transformation is given by
\[ x_1 = \frac{x_+ + x_-}{\sqrt{2}} , \] (9.136)
\[ x_2 = \frac{x_+ - x_-}{\sqrt{2}} . \] (9.137)

The following holds
\[ x_1^2 + x_2^2 = x_+^2 + x_-^2 . \] (9.138)

and
\[ \dot{x}_1^2 + \dot{x}_2^2 = \dot{x}_+^2 + \dot{x}_-^2 . \] (9.139)

Thus, the Lagrangian of the system can be written as
\[ \mathcal{L} = \frac{m}{2} \left( \dot{x}_1^2 + \dot{x}_2^2 \right) - V (x_1, x_2) \]
\[ = \frac{m}{2} \left( \dot{x}_1^2 + \dot{x}_2^2 \right) - \frac{1}{2} m \omega^2 \left( x_+^2 + x_-^2 - 2a \sqrt{2} x_- + 2a^2 + 4\lambda x_-^2 \right) \]
\[ = \mathcal{L}_+ + \mathcal{L}_- . \] (9.140)
where
\[ \mathcal{L}_+ = \frac{m \dot{x}_+^2}{2} - \frac{1}{2} m \omega^2 x_+^2, \quad (9.141) \]
and
\[ \mathcal{L}_- = \frac{m \dot{x}_-^2}{2} - \frac{1}{2} m \omega^2 \left[ (1 + 4\lambda) \left( x_- - \frac{a \sqrt{2}}{1 + 4\lambda} \right)^2 + \frac{8\lambda a^2}{1 + 4\lambda} \right]. \quad (9.142) \]

Thus, the system is composed of two decoupled harmonic oscillators, and therefore, the exact eigenenergies are given by
\[ E_{n_+, n_-} = \hbar \omega \left( n_+ + \frac{1}{2} \right) + \hbar \omega \sqrt{1 + 4\lambda} \left( n_- + \frac{1}{2} \right) + \frac{4\lambda m \omega^2 a^2}{1 + 4\lambda}, \quad (9.143) \]
where \( n_+, n_- = 0, 1, 2, \cdots \). To first order in \( \lambda \) one thus has
\[ E_{n_+, n_-} = \hbar \omega \left( n_+ + \frac{1}{2} \right) + \hbar \omega \left( n_- + \frac{1}{2} \right) + \lambda \left[ \hbar \omega (2n_+ + 1) + 4m \omega^2 a^2 \right] + O(\lambda^2). \quad (9.144) \]

5. For \( w_0 = 0 \) the normalized wavefunctions \( \psi^{(0)}_n(x) \) are given by
\[ \psi^{(0)}_n(x) = \langle x | n \rangle = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}, \quad (9.145) \]
and the corresponding eigenenergies are
\[ E^{(0)}_n = \frac{\hbar^2 \pi^2 n^2}{2ml^2}. \quad (9.146) \]
The matrix elements of the perturbation are given by
\[ \langle n | W | m \rangle = \frac{2w_0}{l} \int_0^l \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l} \delta \left( x - \frac{l}{2} \right) dx \]
\[ = \frac{2w_0}{l} \sin \frac{n\pi}{2} \sin \frac{m\pi}{2}. \quad (9.147) \]

For the ground state
\[ \langle 1 | V | 1 \rangle = \frac{2w_0}{l}, \quad (9.148) \]
thus
\[ E_1 = \frac{\hbar^2 \pi^2}{2ml^2} + \frac{2w_0}{l} + O(w_0^2). \quad (9.149) \]
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6. For \( w_0 = 0 \) the normalized wavefunctions \( \psi_{n_x, n_y}^{(0)} (x', y') \) are given by

\[
\psi_{n_x, n_y}^{(0)} (x', y') = \langle x', y' | n_x, n_y \rangle = \frac{2}{a} \sin \left( \frac{n_x \pi x'}{a} \right) \sin \left( \frac{n_y \pi y'}{a} \right),
\]

and the corresponding eigenenergies are

\[
E_{n_x, n_y}^{(0)} = \frac{\hbar^2 \pi^2 \left( n_x^2 + n_y^2 \right)}{2ma^2},
\]

where \( n_x = 1, 2, \ldots \) and \( n_y = 1, 2, \ldots \).

a) The ground state \( \left( n_x, n_y \right) = (1, 1) \) is nondegenerate, thus to first order in \( w_0 \)

\[
E_0 = \frac{\hbar^2 \pi^2}{ma^2} + \langle 1, 1 | W | 1, 1 \rangle
\]

\[= \frac{\hbar^2 \pi^2}{ma^2} + \frac{4w_0}{a^2} \int_0^{a/2} \sin^2 \left( \frac{n \pi x}{a} \right) dx \int_0^{a/2} \sin^2 \left( \frac{n \pi y}{a} \right) dy \]

\[= \frac{\hbar^2 \pi^2}{ma^2} + \frac{w_0}{4},\]

(9.152)

b) The first excite state is doubly degenerate. The matrix of the perturbation in the corresponding subspace is given by

\[
\mu = \frac{4w_0}{a^2} \begin{pmatrix}
\int_0^{a/2} \sin^2 \frac{n \pi x}{a} dx \int_0^{a/2} \sin^2 \frac{n \pi y}{a} dy & \int_0^{a/2} \sin \frac{n \pi x}{a} \sin \frac{2n \pi y}{a} dx \int_0^{a/2} \sin \frac{2n \pi x}{a} \sin \frac{2n \pi y}{a} dy \\
\int_0^{a/2} \sin \frac{2n \pi x}{a} \sin \frac{n \pi y}{a} dx \int_0^{a/2} \sin \frac{n \pi x}{a} \sin \frac{2n \pi y}{a} dy & \int_0^{a/2} \sin^2 \frac{n \pi x}{a} dx \int_0^{a/2} \sin^2 \frac{n \pi y}{a} dy
\end{pmatrix}
\]

\[= w_0 \left( \begin{pmatrix}
\frac{16}{\pi^2} & \frac{16}{9\pi^2} \\
\frac{16}{9\pi^2} & \frac{16}{\pi^2}
\end{pmatrix}
\right),
\]

(9.153)

To first order in perturbation theory the eigenenergies are found by adding the eigenvalues of the above matrix to the unperturbed eigenenergy \( E_{1,2}^{(0)} = E_{2,1}^{(0)} \). Thus, to first order in \( w_0 \)

\[
E_{1, \pm} = \frac{5\hbar^2 \pi^2}{2ma^2} + \frac{w_0}{4} \pm \frac{16w_0}{9\pi^2} + O \left( w_0^2 \right).
\]

(9.154)

7. For the unperturbed case \( \beta = 0 \) one has

\[
H_0 |n_x, n_y\rangle = \hbar \omega (n_x + n_y + 1) |n_x, n_y\rangle,
\]

(9.155)

where \( n_x, n_y = 0, 1, 2, \ldots \). Using the identities
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\[ x = \sqrt{\frac{\hbar}{2m\omega}} (a_x + a_x^\dagger), \quad (9.156) \]

\[ y = \sqrt{\frac{\hbar}{2m\omega}} (a_y + a_y^\dagger), \quad (9.157) \]

the perturbation term \( V_1 = \beta m \omega^2 xy \) can be expressed as

\[ V_1 = \beta \frac{\hbar \omega}{2} (a_x + a_x^\dagger) (a_y + a_y^\dagger). \]

a) For the ground state \( |0, 0\rangle \), which is nondegenerate, one has

\[ E_{0,0} (\beta) = \hbar \omega + \langle 0, 0 | V_1 | 0, 0 \rangle + \sum_{n_x, n_y \neq 0, 0} \left| \langle n_x, n_y | V_1 | 0, 0 \rangle \right|^2 \]

\[ = \hbar \omega + \frac{\left| \langle 1, 1 | V_1 | 0, 0 \rangle \right|^2}{2\hbar \omega} \]

\[ = \hbar \omega - \frac{(\hbar \beta)^2}{2\hbar \omega} \]

\[ = \hbar \omega \left( 1 - \frac{\beta^2}{8} \right). \quad (9.158) \]

b) The first excited state is doubly degenerate, thus the eigenenergies are found by diagonalizing the matrix of \( V_1 \) in the corresponding subspace

\[ \begin{pmatrix} \langle 1, 0 | V_1 | 1, 0 \rangle & \langle 1, 0 | V_1 | 0, 1 \rangle \\ \langle 0, 1 | V_1 | 1, 0 \rangle & \langle 0, 1 | V_1 | 0, 1 \rangle \end{pmatrix} = \frac{\hbar \omega \beta}{2} \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \quad (9.159) \]

Thus the degeneracy is lifted and the energies are given by \( 2\hbar \omega \left( 1 \pm \beta/4 \right) \).

Note that this problem can be also solved exactly by employing the coordinate transformation

\[ x' = \frac{x + y}{\sqrt{2}}, \quad (9.160) \]

\[ y' = \frac{x - y}{\sqrt{2}}. \quad (9.161) \]

The inverse transformation is given by

\[ x = \frac{x' + y'}{\sqrt{2}}, \quad (9.162) \]

\[ y = \frac{x' - y'}{\sqrt{2}}. \quad (9.163) \]

The following hold

\[ x^2 + y^2 = x'^2 + y'^2, \quad (9.164) \]

\[ \dot{x}^2 + \dot{y}^2 = \dot{x}'^2 + \dot{y}'^2, \quad (9.165) \]

\[ xy = \frac{1}{2} (x'^2 - y'^2). \quad (9.166) \]
Thus, the Lagrangian of the system can be written as
\[
\mathcal{L} = \frac{m}{2} (\dot{x}^2 + \dot{y}^2) - \frac{m\omega^2}{2} (x'^2 + y'^2) - \frac{\beta m\omega^2}{2} (x'^2 - y'^2) - V(x_1, x_2)
\]
where
\[
\mathcal{L}_+ = \frac{m\dot{x}^2}{2} - \frac{m\omega^2}{2} (1 + \beta) x'^2,
\]
and
\[
\mathcal{L}_- = \frac{m\dot{y}^2}{2} - \frac{m\omega^2}{2} (1 - \beta) y'^2.
\]
Thus, the system is composed of two decoupled harmonic oscillators, and therefore, the exact eigenenergies are given by
\[
E_{n_+, n_-} = \hbar \omega \left( n_x + \frac{1}{2} \right) + \beta \hbar \omega \left( n_y + \frac{1}{2} \right),
\]
where \(n_x, n_y = 0, 1, 2, \cdots\). To second order in \(\beta\) one thus has
\[
E_{n_+, n_-} = \hbar \omega (n_x + n_y + 1 + \frac{n_x - n_y}{2} \beta - \frac{n_x + n_y + 1}{8} \beta^2) + O(\beta^3).
\]

8. Using Eqs. (5.28) and (5.29) one finds that
\[
\langle m | V | n \rangle = \beta \sqrt{n(n-1)} \delta_{m,n-2} + \beta \sqrt{(n+1)(n+2)} \delta_{m,n+2},
\]
thus
\[
E_n(\beta) = \hbar \omega \left( n + \frac{1}{2} \right) + \frac{\langle m | V | n \rangle}{E_m(0)} + \sum_{m \neq n} \frac{|\langle m | V | n \rangle|^2}{E_n(0) - E_m(0)} + O(\beta^3)
\]
\[
= \hbar \omega \left( n + \frac{1}{2} \right) + \frac{\beta^2}{2\hbar\omega} [n(n-1) - (n+1)(n+2)] + O(\beta^3)
\]
\[
= \hbar \omega \left( n + \frac{1}{2} \right) \left[ 1 - 2 \left( \frac{\beta}{\hbar\omega} \right)^2 \right] + O(\beta^3).
\]

9. In general the subspace of angular momentum states with \(J = 1\) is spanned by the basis
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\[ \{|j = 1, m = -1\}, |j = 1, m = 0\}, |j = 1, m = 1\} , \quad (9.174) \]

and the following holds

\[ \langle j', m' | J_z | j, m \rangle = m \hbar \delta_{j', j} \delta_{m', m} , \quad (9.175) \]
\[ \langle j', m' | J^2 | j, m \rangle = j (j + 1) \hbar^2 \delta_{j', j} \delta_{m', m} , \quad (9.176) \]
\[ \langle j', m' | J_{\pm} | j, m \rangle = \hbar \sqrt{(j \mp m)} (j \pm m + 1) \delta_{j', j} \delta_{m', m \pm 1} , \quad (9.177) \]
\[ J_{\pm} = J_x \pm i J_y . \quad (9.178) \]

In matrix form

\[ J_z \dot{=} \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} , \quad (9.179) \]
\[ J^2 \dot{=} 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad (9.180) \]
\[ J_+ \dot{=} \hbar \sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} , \quad (9.181) \]
\[ J_- \dot{=} \hbar \sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} . \quad (9.182) \]

a) The Hamiltonian is given by

\[ \mathcal{H} = \alpha S_z^2 + \beta (S_x^2 - S_y^2) \]
\[ = \alpha S_z^2 + \beta \left[ (S_+ + S_-)^2 + (S_+ - S_-)^2 \right] \]
\[ = \alpha S_z^2 + \beta \frac{1}{2} (S_+^2 + S_-^2) . \quad (9.183) \]

Thus, in matrix form

\[ \mathcal{H} \dot{=} \alpha \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \beta \hbar^2 \left( \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right) \]
\[ = \hbar^2 \begin{pmatrix} \alpha & 0 & \beta \\ 0 & \beta & 0 \\ \beta & 0 & \alpha \end{pmatrix} . \quad (9.184) \]

b) The eigenvalues and eigenvectors are given by

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\[
\begin{align*}
\hbar^2 \begin{pmatrix}
\alpha & 0 & \beta \\
0 & 0 & 0 \\
\beta & 0 & \alpha
\end{pmatrix}
\begin{pmatrix}
1 \\
0 \\
1
\end{pmatrix}
&= \hbar^2 \begin{pmatrix}
\alpha + \beta \\
0 \\
1
\end{pmatrix}, \quad (9.185) \\
\hbar^2 \begin{pmatrix}
\alpha & 0 & \beta \\
0 & 0 & 0 \\
\beta & 0 & \alpha
\end{pmatrix}
\begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix}
&= \hbar^2 \begin{pmatrix}
\alpha - \beta \\
0 \\
1
\end{pmatrix}, \quad (9.186) \\
\hbar^2 \begin{pmatrix}
\alpha & 0 & \beta \\
0 & 0 & 0 \\
\beta & 0 & \alpha
\end{pmatrix}
\begin{pmatrix}
1 \\
0 \\
0
\end{pmatrix}
&= \hbar^2 \times 0 \begin{pmatrix}
0 \\
1 \\
0
\end{pmatrix}. \quad (9.187)
\end{align*}
\]

c) The Hamiltonian is written as \( \mathcal{H} = \mathcal{H}_0 + V \) where in matrix form

\[
\begin{align*}
\mathcal{H}_0 & \doteq \hbar^2 \alpha \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix}, \quad (9.188) \\
V & \doteq \hbar^2 \beta \begin{pmatrix}
0 & 0 & 1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{pmatrix}. \quad (9.189)
\end{align*}
\]

For the nondegenerate eigenenergy \( E_{m=0}^0 = 0 \) on has to second order in perturbation expansion

\[
E_{m=0} = E_{m=0}^0 + \langle 1, 0 | V | 1, 0 \rangle + \sum_{m'=\pm 1} \frac{\langle 1, m'| V | 1, 0 \rangle^2}{E_{m=0}^0 - E_{m=0}^{m'}} = 0. \quad (9.190)
\]

For the degenerate eigenenergy \( E_{m=\pm 1}^0 = \hbar^2 \alpha \) the perturbation in the subspace spanned by \( \{|1, -1\}, |1, 1\}\) is given in matrix form by

\[
V_{m=\pm 1} \doteq \hbar^2 \beta \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}, \quad (9.191)
\]

thus to first order in perturbation expansion

\[
E_{m=\pm 1} = \hbar^2 (\alpha \pm \beta). \quad (9.192)
\]

10. For the unperturbed case \( V = 0 \), the eigenvectors and eigenenergies are related by

\[
(\mathcal{H}_r + \mathcal{H}_a) |n, \sigma\rangle = E_{n,\sigma}^0 |n, \sigma\rangle, \quad (9.193)
\]

where \( n = 0, 1, 2, \cdots \) is the quantum number of the harmonic oscillator, and \( \sigma \in \{-1, +1\} \) is the quantum number associated with the two-level particle, and

\[
E_{n,\sigma}^0 = \hbar \omega_r \left( n + \frac{1}{2} \right) + \sigma \hbar \omega_a \frac{1}{2}. \quad (9.194)
\]

Consider first the nondegenerate case where \( \omega_r \neq \omega_a \). To second order in perturbation theorem
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\[ E_{n,\sigma} = E_{n,\sigma}^0 + \langle n, \sigma | V | n, \sigma \rangle + \sum_{n', \sigma' \neq n, \sigma} \frac{|\langle n', \sigma' | V | n, \sigma \rangle|^2}{E_{n,\sigma}^0 - E_{n',\sigma'}^0}. \]  

(9.195)

Using

\[
V |n, +\rangle = \hbar g \sqrt{n+1} |n+1, -\rangle, \quad (9.196)
\]

\[
V |n, -\rangle = \hbar g |n, +\rangle = \hbar g \sqrt{n-1} |n-1, +\rangle, \quad (9.197)
\]

one finds for \( \sigma = +1 \)

\[ E_{n,+1} = \hbar \omega_r \left( n + \frac{1}{2} \right) + \frac{\hbar \omega_a}{2} + \frac{\hbar g^2 (n+1)}{\omega_a - \omega_r}, \quad (9.198) \]

and for \( \sigma = -1 \)

\[ E_{n,-1} = \hbar \omega_r \left( n + \frac{1}{2} \right) - \frac{\hbar \omega_a}{2} - \frac{\hbar g^2 n}{\omega_a - \omega_r}. \quad (9.199) \]

For the general case this can be written as

\[ E_{n,\sigma} = \hbar \left( \omega_r + \frac{\sigma g^2}{\omega_a - \omega_r} \right) \left( n + \frac{1}{2} \right) + \frac{\sigma \hbar \omega_a}{2} + \frac{1}{2} \frac{\hbar g^2}{\omega_a - \omega_r}. \quad (9.200) \]

In the degenerate case \( \omega_r = \omega_a \equiv \omega \) the eigenenergies for the case \( V = 0 \) are given by

\[ E_{n,\sigma}^0 = \hbar \left( n + \frac{1}{2} + \frac{\sigma}{2} \right), \quad (9.201) \]

thus the pairs of states \( |n, +\rangle \) and \( |n+1, -\rangle \) are degenerate. In the subset of such a pair the perturbation is given by

\[
\begin{pmatrix}
\langle n, + | V | n, + \rangle & \langle n, + | V | n+1, - \rangle \\
\langle n+1, - | V | n, + \rangle & \langle n+1, - | V | n+1, - \rangle
\end{pmatrix} = \begin{pmatrix}
0 & \hbar g \sqrt{n+1} \\
\hbar g \sqrt{n+1} & 0
\end{pmatrix},
\]

(9.202)

thus to first order in \( g \) the eigenenergies are given by

\[ E = \hbar \left[ \omega (n + 1) \pm g \sqrt{n+1} \right]. \quad (9.203) \]

11. Using creation and annihilation operators one has

\[ \mathcal{H}_0 = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2} m \omega^2 \left( x^2 + y^2 \right) = \hbar \omega (N_x + N_y + 1), \quad (9.204) \]

where \( N_x = a_x^+ a_x, \ N_y = a_y^+ a_y \), and
\[ V = \frac{\beta \omega}{\hbar} L_z^2 \]
\[ = \frac{\beta \omega}{\hbar} (xp_y - yp_x)^2 \]
\[ = \frac{\beta \omega}{\hbar} \left[ \hbar \left( a_x a_y^\dagger - a_y a_x^\dagger \right) \right]^2 \]
\[ = -\beta \omega \left[ a_x^2 (a_y^\dagger)^2 + (a_x^\dagger)^2 a_y^2 - a_x a_y a_y^\dagger a_x^\dagger - a_y a_x a_x^\dagger a_y^\dagger \right] \]
\[ = -\beta \omega \left[ a_x^2 (a_y^\dagger)^2 + (a_x^\dagger)^2 a_y^2 - (1 + N_x) N_y - N_x (1 + N_y) \right].\]

(9.205)

a) For the case \( \beta = 0 \) the ground state \( |0,0\rangle \) is nondegenerate and has energy \( E_{0,0} = \hbar \omega \). Since \( V|0,0\rangle = 0 \) one finds to second order in \( \beta \)
\[ E_{0,0} = \hbar \omega + \langle 0,0 | V |0,0\rangle - \frac{1}{\hbar \omega} \sum_{n_x,n_y \neq 0,0} \frac{|\langle n_x,n_y | V |0,0\rangle|^2}{n_x + n_y} = \hbar \omega + O(\beta^3).\]

(9.206)

b) For the case \( \beta = 0 \) the first excited state is doubly degenerate
\[ \mathcal{H}_0 |1,0\rangle = 2 \hbar \omega |1,0\rangle, \]
\[ \mathcal{H}_0 |0,1\rangle = 2 \hbar \omega |0,1\rangle. \]

The matrix of \( V \) in the basis \( \{|1,0\rangle, |0,1\rangle\} \) is given by
\[ \left( \begin{array}{cc}
(1,0) V |1,0\rangle & (1,0) V |0,1\rangle \\
(0,1) V |1,0\rangle & (0,1) V |0,1\rangle
\end{array} \right) \]
\[ \begin{array}{c}
\beta \hbar \omega \left( (1,0) \left( (1 + N_x) N_y + N_x (1 + N_y) \right) |1,0\rangle \right) \\
\left( 0,1 \right) \left( (1 + N_x) N_y + N_x (1 + N_y) \right) |0,1\rangle
\end{array} \]
\[ = \beta \hbar \omega \left( \begin{array}{cc}
1 & 0 \\
0 & 1
\end{array} \right). \]

(9.209)

Thus to first order in \( \beta \) the first excited state remains doubly degenerate with energy \( 2 \hbar \omega (1 + \beta) \). Note - The exact solution can be found using the transformation
\[ a_d = \frac{1}{\sqrt{2}} \left( a_x - ia_y \right), \]
\[ a_g = \frac{1}{\sqrt{2}} \left( a_x + ia_y \right). \]

(9.210)

The following holds
\[ [a_d, a_d^\dagger] = [a_g, a_g^\dagger] = 1, \]
\[ a_d^\dagger a_d + a_g^\dagger a_g = \frac{1}{2} (a_x^+ + ia_y^+) (a_x - ia_y) + \frac{1}{2} (a_x^+ - ia_y^+) (a_x + ia_y) \]
\[ = a_d^\dagger a_d + a_g a_g. \]

(9.212)
and
\[ a_d^+a_d - a_g^+a_g = \frac{1}{2} \left( a_x^+ + ia_y^+ \right) \left( a_x - ia_y \right) - \frac{1}{2} \left( a_x^+ - ia_y^+ \right) \left( a_x + ia_y \right) \]
\[ = i \left( a_xa_y^+ - a_x^+a_y \right), \]
thus
\[ \mathcal{H}_0 = \hbar \omega (N_d + N_g + 1), \]
\[ V = \beta \hbar \omega (N_d - N_g)^2, \]
and the exact eigen vectors and eigen energies are given by
\[ (\mathcal{H}_0 + V) |n_d, n_g\rangle = \hbar \omega \left[ n_d + n_g + 1 + \beta (n_d - n_g)^2 \right] |n_d, n_g\rangle. \]

12. For \( V_0 = 0 \) the wavefunctions \( \psi_n^{(0)}(x) \) are given by
\[ \psi_n^{(0)}(x) = \langle x' | n \rangle = \sqrt{\frac{2}{l}} \sin \frac{n\pi x'}{l}, \]
and the corresponding eigenenergies are
\[ E_n^{(0)} = \frac{\hbar^2 \pi^2 n^2}{2ml^2}. \]
The matrix elements of the perturbation are given by
\[ \langle n|V|m\rangle = \frac{2V_0}{l} \int_0^l \sin \frac{n\pi x}{l} \sin \frac{m\pi x}{l} \sin \frac{2\pi x}{l} dx. \]

For the diagonal case \( n = m \)
\[ \langle n|V|n\rangle = \frac{2V_0}{l} \int_0^l \sin^2 \frac{n\pi x}{l} - \sin \frac{2\pi x}{l} dx \]
\[ = \frac{2V_0}{l} \int_{-l/2}^{l/2} \sin^2 \left( \frac{n\pi y}{l} + \frac{n\pi}{2} \right) \sin \left( \frac{2\pi y}{l} + \pi \right) dy \]
\[ = -2V_0 \int_{-l/2}^{l/2} 1 - \cos \left( \frac{2n\pi y}{l} + n\pi \right) \sin \frac{2\pi y}{l} dy \]
\[ = 0, \]
since the integrand is clearly an odd function of \( y \). Thus to first order in \( V_0 \) the energies are unchanged.
9.4. Solutions

\[ E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + O \left( V_0^2 \right) . \]  

(9.225)

13. For the case \( \varepsilon = 0 \) the exact wave functions are given by

\[ \psi_n^{(0)}(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n \pi x}{L} \right) , \]  

(9.226)

and the corresponding eigen energies are

\[ E_n^{(0)} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} , \]  

(9.227)

where \( n \) is integer. To first order in \( \varepsilon \) the energy of the ground state \( n = 1 \) is given by

\[ E_1 = E_1^{(0)} + \frac{\varepsilon L}{L} \int_0^L dx \left( \psi_1^{(0)}(x) \right)^2 x + O (\varepsilon^2) \]
\[ = E_1^{(0)} + \frac{2 \varepsilon}{L^2} \int_0^L dx \sin^2 \left( \frac{\pi x}{L} \right) x + O (\varepsilon^2) \]
\[ = E_1^{(0)} + \frac{\varepsilon}{2} + O (\varepsilon^2) \]  

(9.228)

14. For the case \( \lambda = 0 \) the exact wave functions of the eigenstates are given by

\[ \psi_{n_x, n_y}^{(0)}(x, y) = \frac{2}{l} \sin \frac{n_x \pi x}{l} \sin \frac{n_y \pi y}{l} , \]  

(9.229)

and the corresponding eigen energies are

\[ E_{n_x, n_y}^{(0)} = \frac{\hbar^2 \pi^2 (n_x^2 + n_y^2)}{2ml^2} , \]  

(9.230)

where \( n_x \) and \( n_y \) are non-zero integers.

a) The ground state is non-degenerate thus to 1st order the energy is given by

\[ E_0 = E_1^{(0)} + \int_0^l \int_0^l \left( \psi_{1,1}^{(0)} \right)^2 W \, dx \, dy \]
\[ = \frac{\hbar^2 \pi^2}{ml^2} \]
\[ + \frac{\hbar^2 \pi^2}{ml^2} 4\lambda \int_0^l \int_0^l \sin^2 \frac{\pi x}{l} \sin^2 \frac{\pi y}{l} \delta (x - l_x) \delta (y - l_y) \, dx \, dy \]
\[ = \frac{\hbar^2 \pi^2}{ml^2} \left( 1 + 4\lambda \sin^2 \frac{\pi l_x}{l} \sin^2 \frac{\pi l_y}{l} \right) . \]  

(9.231)
b) The first excited state is doubly degenerate. The matrix of the perturbation $W$ in the eigen subspace is given by

\[
W = \begin{pmatrix}
\langle 2, 1 | W | 2, 1 \rangle & \langle 2, 1 | W | 1, 2 \rangle \\
\langle 1, 2 | W | 2, 1 \rangle & \langle 1, 2 | W | 1, 2 \rangle
\end{pmatrix}
\]

\[
= 4\lambda \frac{\hbar^2 \pi^2}{ml^2} \begin{pmatrix}
\sin^2 \frac{2\pi l_x}{l} & \sin \frac{2\pi l_x}{l} \sin \frac{\pi l_y}{l} & \sin \frac{2\pi l_x}{l} \sin \frac{\pi l_y}{l} \\
\sin \frac{2\pi l_x}{l} \sin \frac{2\pi l_y}{l} & \sin^2 \frac{2\pi l_y}{l} & \sin \frac{2\pi l_x}{l} \sin \frac{2\pi l_y}{l} \\
\sin \frac{2\pi l_x}{l} \sin \frac{2\pi l_y}{l} & \sin \frac{2\pi l_x}{l} \sin \frac{2\pi l_y}{l} & \sin^2 \frac{2\pi l_y}{l}
\end{pmatrix}
\]

\[
= 4\lambda \frac{\hbar^2 \pi^2}{ml^2} \begin{pmatrix}
4 \sin^2 \frac{\pi l_x}{l} \cos^2 \frac{\pi l_y}{l} & \sin^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & 4 \cos \frac{\pi l_x}{l} \sin^2 \frac{\pi l_y}{l} \\
4 \cos \frac{\pi l_x}{l} \sin^2 \frac{\pi l_y}{l} & \cos^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & 4 \sin^2 \frac{\pi l_x}{l} \sin \frac{\pi l_y}{l} \\
4 \sin^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & 4 \cos \frac{\pi l_x}{l} \sin \frac{\pi l_y}{l} & \sin^2 \frac{\pi l_y}{l}
\end{pmatrix}
\]

\[
= \frac{16\lambda \hbar^2 \pi^2 \sin^2 \frac{\pi l_x}{l} \sin^2 \frac{\pi l_y}{l}}{ml^2} \begin{pmatrix}
\cos^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} \\
\cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} \\
\cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} & \cos^2 \frac{\pi l_y}{l}
\end{pmatrix}
\]

The eigenvalues of $W$ are

\[
w_1 = 0 ,
\]

and

\[
w_2 = \frac{16\lambda \hbar^2 \pi^2 \sin^2 \frac{\pi l_x}{l} \sin^2 \frac{\pi l_y}{l}}{ml^2} \left( \cos^2 \frac{\pi l_x}{l} \cos \frac{\pi l_y}{l} + \cos^2 \frac{\pi l_y}{l} \right).
\]

15. The unperturbed Hamiltonian ($\lambda = 0$) can be written as

\[
\mathcal{H} = \frac{L_x^2}{2I_{xy}} + \frac{L_z^2}{2I_z} + \frac{L_x^2}{2I_{xy}} + \left( \frac{1}{2I_z} - \frac{1}{2I_{xy}} \right) L_z,
\]

thus the states $|l, m\rangle$ (the standard eigenstates of $L^2$ and $L_z$) are eigenstates of $\mathcal{H}$ and the following holds

\[
\mathcal{H} |l, m\rangle = E_{l,m} |l, m\rangle ,
\]

where

\[
E_{l,m} = \hbar^2 \left[ \frac{l(l+1)}{2I_{xy}} + \left( \frac{1}{2I_z} - \frac{1}{2I_{xy}} \right) m^2 \right] .
\]

Since the unperturbed Hamiltonian is positive-definite, it is clear that the state $|l = 0, m = 0\rangle$ is the (nondegenerate) ground state of the system since its energy vanishes $E_{0,0} = 0$. Using

\[
L_x = \frac{L_+ + L_-}{2},
\]

\[
L_y = \frac{L_+ - L_-}{2i},
\]
9.4. Solutions

one finds that the perturbation term $V$ can be written as

$$V = \lambda \frac{L_x^2 + L_y^2}{4I_{xy}}. \quad (9.240)$$

To second order in $\lambda$ the energy of the ground state is found using Eq. (9.32)

$$E_0 = E_{0,0} + \langle 0, 0 | V | 0, 0 \rangle + \sum_{l', m' \neq 0, 0} \frac{|\langle 0, 0 | V | l', m' \rangle|^2}{E_{0,0} - E_{l', m'}} + O(\lambda^3). \quad (9.241)$$

Using the relations

$$L_+ | l, m \rangle = \sqrt{l(l+1) - m(m+1)} \hbar | l, m + 1 \rangle, \quad (9.242)$$
$$L_- | l, m \rangle = \sqrt{l(l+1) - m(m-1)} \hbar | l, m - 1 \rangle, \quad (9.243)$$

it is easy to see that all terms to second order in $\lambda$ vanish, thus

$$E_0 = 0 + O(\lambda^3). \quad (9.244)$$

16. The Hamiltonian can be written as

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2 + V, \quad (9.245)$$

where

$$\mathcal{H}_1 = \frac{p_1^2}{2m} - \alpha \delta(x_1), \quad (9.246)$$
$$\mathcal{H}_2 = \frac{p_2^2}{2m} - \alpha \delta(x_2), \quad (9.247)$$

and

$$V = \lambda \delta(x_1 - x_2). \quad (9.248)$$

First consider $\mathcal{H}_1$ only. A wavefunction $\psi^{(1)}(x_1)$ of an eigenstate of $\mathcal{H}_1$ must satisfy the following Schrödinger equation

$$\left[ \frac{d^2}{dx_1^2} + \frac{2m}{\hbar^2} (E + \alpha \delta(x_1)) \right] \psi^{(1)}(x_1) = 0. \quad (9.249)$$

Integrating around $x_1 = 0$ yields the condition

$$\frac{d\psi^{(1)}(0^+)}{dx_1} - \frac{d\psi^{(1)}(0^-)}{dx_1} + \frac{2m\alpha}{\hbar^2} \psi^{(1)}(0) = 0. \quad (9.250)$$

Requiring also that the wavefunction is normalizable leads to

$$\psi^{(1)}(x_1) = \sqrt{\frac{m\alpha}{\hbar^2}} \exp \left( \frac{m\alpha}{\hbar^2} |x_1| \right).$$
The corresponding eigenenergy is
\[ E^{(1)}_0 = -\frac{m\alpha^2}{2\hbar^2}. \]

The ground state of \( H_2 \) can be found in a similar way. Thus, the normalized wavefunction of the only bound state of \( H_1 + H_2 \), which is obviously the ground state, is given by
\[ \psi_0(x_1, x_2) = \frac{m\alpha}{\hbar^2} \exp\left(-\frac{m\alpha}{\hbar^2}|x_1|\right) \exp\left(-\frac{m\alpha}{\hbar^2}|x_2|\right), \tag{9.251} \]
and the corresponding energy is given by
\[ E_0 = -\frac{m\alpha^2}{\hbar^2}. \tag{9.252} \]

Therefore, to first order in \( \lambda \) the energy of the ground state of \( H \) is given by Eq. (9.32)
\[ E_{gs} = -\frac{m\alpha^2}{\hbar^2} + \lambda \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \psi_0^*(x_1, x_2) \delta(x_1 - x_2) \psi_0(x_1, x_2) + O(\lambda^2) \]
\[ = -\frac{m\alpha^2}{\hbar^2} + \lambda \left(\frac{m\alpha}{\hbar^2}\right)^2 \int_{-\infty}^{\infty} dx_1 \exp\left(-\frac{4m\alpha}{\hbar^2}|x_1|\right) + O(\lambda^2) \]
\[ = -\frac{m\alpha^2}{\hbar^2} + \frac{\lambda m\alpha}{2\hbar^2} + O(\lambda^2). \tag{9.253} \]

17. Substituting the expansions
\[ |n\rangle = |n_0\rangle + \Omega |n_1\rangle + \Omega^2 |n_2\rangle + O(\Omega^3), \tag{9.254} \]
and
\[ \lambda = \lambda_{n_0} + \Omega \lambda_{n_1} + \Omega^2 \lambda_{n_2} + O(\Omega^3), \tag{9.255} \]
into Eq. (9.88) and collecting terms having the same order in \( \Omega \) (up to second order) yield
\[ (D - \lambda_{n_0}) |n_0\rangle = 0, \tag{9.256} \]
\[ (D - \lambda_{n_0}) |n_1\rangle + (V - \lambda_{n_1}) |n_0\rangle = 0, \tag{9.257} \]
\[ (D - \lambda_{n_0}) |n_2\rangle + (V - \lambda_{n_1}) |n_1\rangle - \lambda_{n_2} |n_0\rangle = 0. \tag{9.258} \]
We further require normalization
9.4. Solutions

\[ \langle n|n \rangle = 1 , \]  
\[ \text{and choose the phase of } \langle n_0|n \rangle \text{ such that} \]
\[ \langle n_0|n_0 \rangle \in \mathbb{R} . \]

Expressing the normalization condition using Eq. (9.254) and collecting terms having the same order in \( \Omega \) yield
\[ \langle n_0|n_0 \rangle = 1 , \]  
\[ \langle n_0|n_1 \rangle + \langle n_1|n_0 \rangle = 0 , \]
\[ \langle n_0|n_2 \rangle + \langle n_2|n_0 \rangle + \langle n_1|n_1 \rangle = 0 . \]

These results together with Eq. (9.260) yield
\[ \langle n_0|n_1 \rangle = \langle n_1|n_0 \rangle = 0 , \]  
\[ \langle n_0|n_2 \rangle = \langle n_2|n_0 \rangle = - \frac{1}{2} \langle n_1|n_1 \rangle . \]

Multiplying Eq. (9.257) by \( \langle m_0 \rangle \) yields
\[ \lambda_n \langle m_0|n_0 \rangle = (\lambda_m - \lambda_n) \langle m_0|n_1 \rangle + \langle m_0|V|n_0 \rangle , \]
thus for \( m = n \)
\[ \lambda_n = \langle n_0|V|n_0 \rangle . \]
Using this result for \( m \neq n \) yields
\[ \langle m_0|n_1 \rangle = \frac{\langle m_0|V|n_0 \rangle}{\lambda_m - \lambda_n} , \]
thus with the help of Eq. (9.87) one has
\[ |n_1 \rangle = \sum_m \frac{\langle m_0|V|n_0 \rangle}{\lambda_n - \lambda_m} |m_0 \rangle . \]

Multiplying Eq. (9.258) by \( \langle n_0 \rangle \) yields
\[ \lambda_n = \langle n_0|V|n_1 \rangle - \lambda_n \langle n_0|n_1 \rangle , \]
or using Eq. (9.269)
\[ \lambda_n = \frac{\langle n_0|V|n_0 \rangle \langle n_0|V|n_0 \rangle}{\lambda_n - \lambda_m} . \]

Thus, using this result together with Eq. (9.267) one finds
\[ \lambda = \lambda_n + \Omega \langle n_0|V|n_0 \rangle \]
\[ + \Omega^2 \sum_m \frac{\langle n_0|V|n_0 \rangle \langle n_0|V|n_0 \rangle}{\lambda_n - \lambda_m} + O(\Omega^3) . \]
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10.1 Problems

1. Consider a harmonic oscillator having angular resonance frequency $\omega$ and mass $m$. The oscillator is in thermal equilibrium at temperature $T$. Calculate the correlation function $G(t) = \langle x_{(H)}(t)x_{(H)}(0) \rangle$, where $x_{(H)}(t)$ is the Heisenberg representation of the position operator.

2. The operator $D$ is defined by

$$D = \int_{-\infty}^{\infty} dx' |x'\rangle \langle -x'|,$$  \hspace{1cm} (10.1)

where $|x'\rangle$ is an eigenvector of the position operator $x$ having eigenvalue $x'$, i.e. $x|x'\rangle = x'|x'\rangle$. Express the operator $D$ as a function of the number operator $N = a^\dagger a$.

3. In general, the Wigner function of a point particle moving in one dimension is given by

$$W(x', p') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp \left( i \frac{p' x''}{\hbar} \right) \left( x' - \frac{x''}{2} \right) \rho \left( x' + \frac{x''}{2} \right) dx'', \hspace{1cm} (10.2)$$

where $\rho$ is the density operator of the system, and where $|x'\rangle$ represents an eigenvector of the position operator $x$ having eigenvalue $x'$, i.e. $x|x'\rangle = x'|x'\rangle$. Consider the case of a point particle having mass $m$ in a potential of a harmonic oscillator having angular frequency $\omega$. Calculate the Wigner function $W(x', p')$ for the case where the system is in a coherent state $|\alpha\rangle$.

4. Consider the $2 \times 2$ matrix $\rho$, which is given by

$$\rho = \frac{1}{2} (1 + \mathbf{k} \cdot \mathbf{\sigma}), \hspace{1cm} (10.3)$$

where $\mathbf{k} = (k_x, k_y, k_z)$ is a three dimensional vector of complex numbers and where $\mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix vector.
a) Under what conditions on $k$ the matrix $\rho$ can represent a valid density operator of a spin 1/2 particle?

b) Under what conditions on $k$ the matrix $\rho$ can represent a valid density operator of a spin 1/2 particle in a pure state?

c) Calculate the term $\text{Tr} \left( \hat{\mathbf{u}} \cdot \mathbf{\sigma} \rho \right)$, where $\hat{\mathbf{u}}$ is a unit vector, i.e. $\hat{\mathbf{u}} \cdot \hat{\mathbf{u}} = 1$.

### 10.2 Solutions

1. Using Eq. (5.126), which is given by

$$x_{(H)}(t) = x_{(H)}(0) \cos (\omega t) + \frac{p_{(H)}(0)}{m\omega} \sin (\omega t), \quad (10.4)$$

one finds that

$$G(t) = \cos (\omega t) \left< x_{(H)}^2(0) \right> + \frac{\sin (\omega t)}{m\omega} \left< p_{(H)}(0) x_{(H)}(0) \right>. \quad (10.5)$$

Using the relations

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^\dagger), \quad (10.6)$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (-a + a^\dagger), \quad (10.7)$$

$$[a, a^\dagger] = 1, \quad (10.8)$$

one finds that

$$x^2 = \frac{\hbar}{2m\omega} \left( a^2 + (a^\dagger)^2 + 2a^\dagger a + 1 \right), \quad (10.9)$$

$$\frac{px}{m\omega} = i\frac{\hbar}{2m\omega} \left( -a^2 + (a^\dagger)^2 - 1 \right). \quad (10.10)$$

The density operator $\rho$ is given by Eq. (8.121)

$$\rho = \frac{1}{\langle N \rangle + 1} \sum_{n=0}^{\infty} \left( \frac{\langle N \rangle}{\langle N \rangle + 1} \right)^n |n\rangle \langle n|, \quad (10.11)$$

where

$$\langle N \rangle = \text{Tr} \left( \rho N \right) = \frac{e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}}, \quad (10.12)$$

$N = a^\dagger a$, and where $\beta = 1/k_B T$. Using the fact that $\rho$ is diagonal in the basis of number states one finds that $\langle a^2 \rangle = \left< (a^\dagger)^2 \right> = 0$. Combining all these results leads to
\[ G(t) = \frac{\hbar}{2m\omega} [(2\langle N \rangle + 1)\cos(\omega t) - i\sin(\omega t)] \]
\[ = \frac{\hbar}{2m\omega} \left[ \coth \frac{\beta\hbar\omega}{2} \cos(\omega t) - i\sin(\omega t) \right]. \]

(10.13)

2. As can be seen from the definition of \( D \), the following holds
\[ \langle x' | D | \psi \rangle = \int_{-\infty}^{\infty} dx'' \langle x' | x'' \rangle \langle -x'' | \psi \rangle \]
\[ = \langle -x' | \psi \rangle, \]

(10.14)
thus the wave function of \( D | \psi \rangle \) is \( \psi(-x') \) given that the wave function of \( |\psi\rangle \) is \( \psi(x') \). For the wavefunctions \( \varphi_n(x') = \langle x' | n \rangle \) of the number states \( |n\rangle \), which satisfy \( N |n\rangle = n |n\rangle \), the following holds
\[ \varphi_n(-x') = \begin{cases} -\varphi_n(x') & n \text{ odd} \\ \varphi_n(x') & n \text{ even} \end{cases}, \]

(10.15)
thus
\[ D | n \rangle = \begin{cases} - |n\rangle & n \text{ odd} \\ |n\rangle & n \text{ even} \end{cases}, \]

(10.16)
or \( D | n \rangle = (-1)^n | n \rangle \), thus, the operator \( D \) can be expressed as a function of \( N \)
\[ D = e^{i\pi N}. \]

(10.17)

3. The wave function of the coherent state \( |\alpha\rangle \) is given by Eq. (5.51)
\[ \psi_\alpha(x') = \langle x' |\alpha\rangle \]
\[ = \exp \left( \frac{\alpha^* - \alpha^2}{4} \right) \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \exp \left[ -\left( x' - \langle x \rangle_\alpha \right)^2 + i \langle p \rangle_\alpha \frac{x'}{\hbar} \right]. \]

(10.18)
where
\[ \langle x \rangle_\alpha = \langle \alpha | x | \alpha \rangle = \sqrt{\frac{2\hbar}{m\omega}} \alpha', \]

(10.19)
\[ \langle p \rangle_\alpha = \langle \alpha | p | \alpha \rangle = \sqrt{2m\omega}\alpha'', \]

(10.20)
\[ \alpha' = \text{Re} (\alpha), \]

(10.21)
\[ \alpha'' = \text{Im} (\alpha), \]

(10.22)
\[ \Delta x_\alpha = \sqrt{\langle \alpha | (\Delta x)^2 | \alpha \rangle} = \sqrt{\frac{\hbar}{2m\omega}}, \]

(10.23)
Using the definition (10.2) and the identity

$$\int_{-\infty}^{\infty} \exp \left( -ax^2 + bx + c \right) dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2 - 4ac}{4a}}$$, \hspace{1cm} (10.24)$$

one has

$$W(x', p') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp \left( \frac{ip' x''}{\hbar} \right) \left| x' - \frac{x''}{2} \right| \alpha \left| x' + \frac{x''}{2} \right| \alpha \ d x''$$

$$= \left( \frac{\hbar \omega}{\pi} \right)^{1/2} 2\pi \int_{-\infty}^{\infty} d x''$$

$$\times e \left( \frac{x' - \frac{x''}{2} + (\psi_{\alpha})}{2\Delta x_{\alpha}} \right)^2 - \left( \frac{x' + \frac{x''}{2} - (\psi_{\alpha})}{2\Delta x_{\alpha}} \right)^2 + i \left( \frac{p' - (\psi_{\alpha})}{\hbar} \right) x''$$

$$= \left( \frac{\hbar \omega}{\pi} \right)^{1/2} 2\pi \int_{-\infty}^{\infty} d x''$$

$$\times e \frac{(x' - (\psi_{\alpha}))^2 + (\psi_{\alpha})^2}{2\Delta x_{\alpha}^2} + i \left( \frac{p' - (\psi_{\alpha})}{\hbar} \right) x''$$,

\hspace{1cm} (10.25)

thus

$$W(x', p') = \frac{1}{\pi} e^{-\frac{1}{2}\left( \frac{x' - (\psi_{\alpha})}{2\Delta x_{\alpha}} \right)^2 - \frac{1}{2}\left( \frac{p' - (\psi_{\alpha})}{\hbar} \right)^2}$$,

\hspace{1cm} (10.26)

where [see Eq. (5.49)]

$$\Delta p_{\alpha} = \sqrt{\langle \alpha | (\Delta p)^2 | \alpha \rangle} = \sqrt{\frac{\hbar m \omega}{2}} = \frac{\hbar \omega}{2\Delta x_{\alpha}}$$.

\hspace{1cm} (10.27)

4. Using the definition of the Pauli matrices (6.135) one finds that

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + k_z & k_x - ik_y \\ k_x + ik_y & 1 - k_z \end{pmatrix}$$,

\hspace{1cm} (10.28)

and

$$\rho^2 = \frac{1}{4} \begin{pmatrix} 1 + 2k_z + k_x^2 & 2(k_x - ik_y) \\ 2(k_x + ik_y) & 1 - 2k_z + k_x^2 \end{pmatrix}$$,

\hspace{1cm} (10.29)

where $k^2 = k_x^2 + k_y^2 + k_z^2$.

a) Note that for any $k$ the following holds $\text{Tr} (\rho) = 1$. The requirement that $\rho$ is Hermitian, i.e. the requirement that $\rho^\dagger = \rho$, implies that $k_z^2 = k_z$ and $k_x - k_x^2 + i(k_y - k_y^2) = 0$, thus $k_x$, $k_y$ and $k_z$ are all real. Moreover, the the requirement that $\text{Tr} (\rho^2) = (1 + k^2)/2 \leq 1$ implies that $k^2 \leq 1$. 

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b) For this case $\text{Tr} (\rho^2) = 1$, thus $k^2 = 1$.

c) With the help of Eq. (6.136), which is given by

$$\mathbf{\sigma} \cdot \mathbf{a} (\mathbf{\sigma} \cdot \mathbf{b}) = \mathbf{a} \cdot \mathbf{b} + i \mathbf{\sigma} \cdot (\mathbf{a} \times \mathbf{b}) ,$$

and the fact that all three Pauli matrices have a vanishing trace, one finds that

$$\text{Tr} (\mathbf{\hat{u}} \cdot \mathbf{\sigma} \rho) = \frac{1}{2} \text{Tr} (\mathbf{\hat{u}} \cdot \mathbf{\sigma}) + \frac{1}{2} \text{Tr} ([\mathbf{\hat{u}} \cdot \mathbf{\sigma}] (\mathbf{k} \cdot \mathbf{\sigma}))$$

$$= \frac{1}{2} \text{Tr} (\mathbf{\hat{u}} \cdot \mathbf{\sigma} (\mathbf{k} \cdot \mathbf{\sigma}))$$

$$= \frac{1}{2} \text{Tr} (\mathbf{\hat{u}} \cdot \mathbf{k}) + \frac{i}{2} \text{Tr} (\mathbf{\sigma} \cdot (\mathbf{\hat{u}} \times \mathbf{k}))$$

$$= \frac{1}{2} \text{Tr} (\mathbf{\hat{u}} \cdot \mathbf{k})$$

$$= \mathbf{\hat{u}} \cdot \mathbf{k} .$$

(10.30)
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