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1.1 Problem 1

(a) Solve the integral:

$$I = \int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

Hint: Consider solving the two-dimensional integral $I^2 = \int_{-\infty}^{\infty} dx dy e^{-\alpha(x^2+y^2)}$.

(b) Consider a particle in the state

$$\psi(x) = \langle x | \psi \rangle = e^{-\alpha x^2}$$

Calculate the expectation values $\langle x^2 \rangle$ and $\langle p^2 \rangle$. Take $\hat{p} = -i\hbar\partial_x$.

(c) Calculate the Fourier Transform of $f(x) = e^{-\mu|x|}$ where $\mu = \mu^*$ and $\mu > 0$.

Solution

(a) Convert the two-dimensional integral to polar coordinates.

$$I^2 = \iint_{-\infty}^{\infty} dx dy e^{-\alpha x^2} e^{-\alpha y^2} = \int_{r=0}^{\infty} \int_{\varphi=0}^{2\pi} e^{-\alpha r^2} r dr d\varphi = \frac{\pi}{\alpha} \rightarrow I = \sqrt{\frac{\pi}{\alpha}}$$

(b) Use parametric differentiation.

$$\langle \psi | x^2 | \psi \rangle = \int_{-\infty}^{\infty} dx x^2 e^{-2\alpha x^2} = -\frac{1}{2} \frac{\partial}{\partial \alpha} \int_{-\infty}^{\infty} dx e^{-2\alpha x^2} = \frac{1}{4} \sqrt{\frac{\pi}{2\alpha^3}}$$

Consider what it means for a wavefunction to be “bounded”. (It must vanish at the edges of the region of interest; draw some wavefunctions and consider what must happen for the wavefunction to be normalizable.) This means that $\psi|_{\pm\infty} = 0$. Use integration by parts:

$$\langle \psi | p^2 | \psi \rangle = -\hbar^2 \langle \psi | \partial_x^2 | \psi \rangle = -\hbar^2 \psi \frac{d\psi}{dx} \Big|_{-\infty}^{\infty} + \hbar^2 \int_{-\infty}^{\infty} dx \left| \frac{d\psi}{dx} \right|^2 = \hbar^2 \int_{-\infty}^{\infty} dx \left| \frac{d\psi}{dx} \right|^2$$

Note that for any bounded wavefunction ψ we may apply the above trick (the first term must always go to zero if the wavefunction is bounded). For this particular ψ the result is:

$$\langle p^2 \rangle = \hbar^2 \sqrt{\frac{\pi\alpha}{2}}$$

(c) We deal with the absolute value by splitting the integral into positive and negative components.

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\mu|x|} e^{-ikx} = \frac{1}{\sqrt{2\pi}} \left[\int_{-\infty}^0 dx e^{\mu x} e^{-ikx} + \int_0^{\infty} dx e^{-\mu x} e^{-ikx} \right] \rightarrow = \sqrt{\frac{2}{\pi}} \frac{\mu}{\mu^2 + k^2}$$

1.2 Problem 2

Consider two operators A and B , shown below, where a and b are real constants.

$$A = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \quad B = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & -ib \\ 0 & ib & 0 \end{pmatrix}$$

- (a) Are these operators Hermitian? ($A = A^\dagger$ – Self-adjoint).
 (b) Show that A and B commute.
 (c) Determine the eigenvalues and eigenvectors of A and B .
 (d) If two operators commute, it is always possible to find a set of simultaneous eigenvectors for those operators (ie the operators can be diagonalized in the same basis). Find a set of orthonormal eigenvectors which are simultaneous eigenvectors of both A and B .
 (e) Use the eigenvectors from part (d) to construct a rotation matrix R such that $R^\dagger AR$ and $R^\dagger BR$ are diagonal. Is the rotation matrix R unitary? (For a unitary matrix U , we have $U^\dagger U = U U^\dagger = \mathbb{I}$, where \mathbb{I} is the identity matrix.)

Solution

- (a) The matrices A and B are self-adjoint by inspection. ($A_{ij}^* = A_{ji}$ and the same is true of B).
 (b) The commutator $[A, B] = AB - BA$. Do this out to show that $AB - BA = 0$.
 (c) Recall that the eigenvalues α_i and β_j are determined by solving the characteristic equation $\det(A - \alpha\mathbb{I}) = 0$, and the corresponding equation for B . We obtain $\alpha_1 = a$, $\alpha_{2,3} = -a$, and $\beta_1 = -b$, $\beta_{2,3} = b$. Since the matrix A is diagonal writing the eigenvectors of A is trivial:

$$|\alpha_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\alpha_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\alpha_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

For B , we plug in each of the eigenvalues found above into $B|\beta_i\rangle = \beta_i|\beta_i\rangle$ in order to set up a system to solve for the elements of each vector $|\beta_i\rangle$. One orthonormal choice of eigenvectors is:

$$|\beta_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -i \end{pmatrix}, \quad |\beta_2\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad |\beta_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ i \\ -1 \end{pmatrix}$$

(d) Notice that the eigenvectors of A are the standard unit vectors. This makes things easier. We can see right away that the pair of eigenvalues $(\alpha_1, \beta_2) = (a, b)$ share the same eigenvector ($|\alpha_1\rangle = |\beta_2\rangle$). The same logic can be applied to other pairs:

$$(-a, b): \quad |\beta_3\rangle = \frac{i}{\sqrt{2}}|\alpha_2\rangle - \frac{1}{\sqrt{2}}|\alpha_3\rangle \therefore \text{share } |\beta_3\rangle \quad (-a, -b): \quad |\beta_1\rangle = \frac{1}{\sqrt{2}}|\alpha_2\rangle - \frac{i}{\sqrt{2}}|\alpha_3\rangle \therefore \text{share } |\beta_1\rangle$$

(e) The matrix (which must perform a rotation from the original basis into the eigenbasis) is constructed using the shared eigenvectors as columns. Consider:

$$R = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & i & 1 \\ 0 & -1 & -i \end{pmatrix} \rightarrow R^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & -i & -1 \\ 0 & 1 & i \end{pmatrix}$$

Evaluating with the original matrices gives the desired the result (simply perform the matrix multiplication):

$$R^\dagger AR = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & -a \end{pmatrix} \quad R^\dagger BR = \begin{pmatrix} b & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -b \end{pmatrix}$$

Such a rotation matrix must always be Unitary, and performing the matrix multiplication for $R^\dagger R$ we find that this is indeed the case.

1.3 Problem 3

Consider a Hamiltonian represented by the matrix shown below, in a state $|\psi\rangle$.

$$H = \begin{pmatrix} 1 & 0 & \sqrt{3} \\ 0 & 2 & 0 \\ \sqrt{3} & 0 & 3 \end{pmatrix} \quad |\psi\rangle = \begin{pmatrix} 1 \\ 2i \\ -1 \end{pmatrix}$$

- (a) Which eigenvalue of H is most likely to emerge from a measurement?
 (b) What is the average value of H in this state?

Solution

Applying the same process as in the preceding problem, we obtain the eigenvalues $(0, 2, 4)$, and their corresponding eigenvectors:

$$|0\rangle = \frac{1}{2} \begin{pmatrix} -\sqrt{3} \\ 0 \\ 1 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |4\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ \sqrt{3} \end{pmatrix}$$

(a) The probabilities for each eigenvalue occurring are given by:

$$P(0) = \frac{|\langle 0|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{(1+\sqrt{3})^2}{24}, \quad P(2) = \frac{|\langle 2|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{2}{3}, \quad P(4) = \frac{|\langle 4|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{(1-\sqrt{3})^2}{24}$$

By inspection of the above results, $P(2)$ is the most probable.

(b) Two ways of calculating this result:

$$\langle H \rangle = 0 \cdot P(0) + 2 \cdot P(2) + 4 \cdot P(4) = 2 - \frac{1}{\sqrt{3}}$$

or

$$\langle H \rangle = \langle \psi | H | \psi \rangle = \frac{1}{6} (1, -2i, -1) \begin{pmatrix} 1 & 0 & \sqrt{3} \\ 0 & 2 & 0 \\ \sqrt{3} & 0 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 2i \\ -1 \end{pmatrix} = 2 - \frac{1}{\sqrt{3}}$$

1.4 Problem 4

Consider a particle in a 1-dimensional infinite square well, described by the potential

$$V(x) = \begin{cases} 0 & x \in [0, L] \\ \infty & \text{else} \end{cases}$$

(a) Determine the normalized eigenfunctions of the Hamiltonian $\psi_n(x)$

(b) Determine the probability of finding the particle in the range $0 < x < \frac{L}{a}$. Show that the classical result is obtained as $n \rightarrow \infty$.

(c) Determine $\langle E \rangle$ of a particle the the state $|\phi\rangle$:

$$|\phi\rangle = \frac{1}{\sqrt{3}} |\psi_1\rangle + \sqrt{\frac{2}{3}} |\psi_3\rangle$$

(d) Compute $\langle p \rangle_t$.

Solution

(a) Set up the Schrödinger equation and the boundary conditions $\psi(0) = 0 = \psi(L)$.

$$H|\psi_n\rangle = E_n|\psi_n\rangle \quad \rightarrow \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi_n}{\partial x^2} = E_n \psi_n(x) \quad \rightarrow \quad \sin \left[\sqrt{\frac{2mE_n}{\hbar^2}} L \right] = 0 \quad \rightarrow \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$\text{and } \psi_n(x) = \langle x | \psi_n \rangle = \sqrt{\frac{2}{L}} \sin \left(\frac{n\pi x}{L} \right)$$

(b)

$$\int_0^{\frac{L}{a}} \langle \psi_n | x \rangle \langle x | \psi_n \rangle dx = \int_0^{\frac{L}{a}} \psi_n^*(x) \psi_n(x) dx = \frac{1}{2} \left[\frac{2}{a} - \frac{1}{n\pi} \sin \left(\frac{2\pi n}{a} \right) \right] \quad \text{for } n \rightarrow \infty, \quad \text{Solution} \rightarrow \frac{1}{a}$$

(c) The average energy $\langle E \rangle$ in the state $|\phi\rangle$ is given by $\langle \phi | H | \phi \rangle$. (Notice that each ψ is an eigenstate of H , so we can throw out the cross terms right away.)

$$\langle \phi | H | \phi \rangle = \frac{1}{3} \langle \psi_1 | H | \psi_1 \rangle + \frac{2}{3} \langle \psi_3 | H | \psi_3 \rangle = \frac{E_1}{3} \langle \psi_1 | \psi_1 \rangle + \frac{2E_3}{3} \langle \psi_3 | \psi_3 \rangle = \frac{19\pi^2 \hbar^2}{6mL^2}$$

This can also be calculated by evaluating:

$$\langle \phi | H | \phi \rangle = \frac{\hbar^2}{2m} \int_0^L \left| \frac{\partial \phi}{\partial x} \right|^2 dx$$

(d) Let $|\Phi\rangle$ be the time dependent version of $|\phi\rangle$.

$$\langle \Phi | p | \Phi \rangle = \int_0^L \left(\frac{1}{\sqrt{3}} \psi_1^* e^{\frac{iE_1 t}{\hbar}} + \sqrt{\frac{2}{3}} \psi_3^* e^{\frac{iE_3 t}{\hbar}} \right) \left(-i\hbar \frac{\partial}{\partial x} \right) \left(\frac{1}{\sqrt{3}} \psi_1 e^{-\frac{iE_1 t}{\hbar}} + \sqrt{\frac{2}{3}} \psi_3 e^{-\frac{iE_3 t}{\hbar}} \right) dx = 0$$

This occurs because:

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0$$

for $n = m$, and $(n = 1, m = 3)$, and $(n = 3, m = 1)$.

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2.1 Problem 5

Solve the integral using residue theory for $n = 2$ and $n = 3$:

$$\int_{-\infty}^{\infty} dx \frac{1}{(x^2 + 1)^n}$$

Solution

The integrand has n^{th} -order poles at $z = \pm i$. Since the integrand goes to zero faster than $|z|^{-1}$ we can close a semi-circular contour at infinity without changing the value of the integral (the added part goes to zero), and use residue theory. We choose to close this contour in the upper half of the complex plane, and call this contour C . (The residues are then evaluated as positive since we circle the poles counter-clockwise.) Then:

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{dx}{(x+i)^n(x-i)^n} &= \oint_C \frac{dz}{(z^2+1)^n} = 2\pi i \operatorname{Res} \left[\frac{1}{(z^2+1)^n}, z=i \right] = \frac{2\pi i}{(n-1)!} \lim_{z \rightarrow i} \frac{d^{n-1}}{dz^{n-1}} \frac{(z-i)^n}{(z^2+1)^n} \\ &= \frac{2\pi i}{(n-1)!} \lim_{z \rightarrow i} \frac{d^{n-1}}{dz^{n-1}} \frac{1}{(z+i)^n} \end{aligned}$$

We evaluate this expression to obtain:

$$n = 2 : \quad \frac{\pi}{2} \qquad n = 3 : \quad \frac{3\pi}{8}$$

2.2 Problem 6

We can see by dimensional analysis that the solution of the integral below will be of the form shown (for some constant λ):

$$\int_{-\infty}^{\infty} dx \frac{1}{(x^2 + a^2)^3} = \frac{\lambda}{a^5}$$

Given this result, compute the following in terms of a and λ *without integrating*.

(a)

$$\int_{-\infty}^{\infty} dx \frac{1}{(x^2 + a^2)^4}$$

(b)

$$\int_{-\infty}^{\infty} dx \frac{x^2}{(x^2 + a^2)^4}$$

Solution

(a)

$$\frac{d}{db^2} \int_{-\infty}^{\infty} dx (x^2 + b^2)^{-3} = -3 \int_{-\infty}^{\infty} dx (x^2 + b^2)^{-4} \rightarrow \int_{-\infty}^{\infty} dx (x^2 + b^2)^{-4} = -\frac{1}{3} \frac{d}{db^2} \frac{\lambda}{(b^2)^{\frac{5}{2}}} = \frac{5\lambda}{6b^7}$$

(b) Let $x \rightarrow cx$. Then:

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{cdx}{(c^2x^2 + b^2)^3} &= \frac{\lambda}{b^5} \rightarrow \int_{-\infty}^{\infty} \frac{dx}{(c^2x^2 + b^2)^3} = \frac{\lambda}{cb^5} \\ \frac{d}{dc^2} \int_{-\infty}^{\infty} dx (c^2x^2 + b^2)^{-3} &= -3 \int_{-\infty}^{\infty} \frac{x^2 dx}{(c^2x^2 + b^2)^4} \rightarrow \int_{-\infty}^{\infty} \frac{x^2 dx}{(c^2x^2 + b^2)^4} \Big|_{c=1} = -\frac{1}{3} \frac{d}{dc^2} \left(\frac{\lambda}{(c^2)^{\frac{1}{2}} b^5} \right) \Big|_{c=1} = \frac{\lambda}{6b^5} \end{aligned}$$

2.3 Problem 7

Parts (a) - (d) show some familiar objects, properties, and operations from linear algebra expressed over a discrete basis, in Dirac notation. Write the analogous statements for a continuous basis.

(a) Kronecker Delta δ_{ij} .

(b) Inner Product / Projection operator: $\langle a|b\rangle = \sum_i a_i^* b_i = \sum_i \langle a|i\rangle \langle i|b\rangle$. (Note $\sum_i |i\rangle \langle i| = \mathbb{I}$).

(c) Matrix transformations: $|a'\rangle = M|a\rangle \rightarrow a'_i = \sum_j M_{ij} a_j \leftrightarrow \langle i|a'\rangle = \sum_j \langle i|M|j\rangle \langle j|a\rangle$.

(d) Unitary transformations: $U^\dagger U = \mathbb{I} \rightarrow \sum_i U_{ij}^* U_{ik} = \delta_{jk}$. Make sure you can derive the second expression shown before writing the continuous form of this relationship. (Note that when this is true, for $|a'\rangle = U|a\rangle$ and $|b'\rangle = U|b\rangle$ we have $\langle a'|b'\rangle = \langle a|U^\dagger U|b\rangle = \langle a|b\rangle$.)

(e) Consider how the Fourier Series and Fourier Transform relate to the ideas above. What property of the Fourier Transform is suggested by Parseval's theorem?

Solution

(Introduction to the Problem)

Finite-Dimensional / Discrete Expressions	Infinite-Dimensional / Continuous Expressions
Kronecker Delta function for two indices i, j $\langle i j\rangle = \delta_{ij}$	Dirac Delta function for two quantities over continuous variables. $\langle t_2 t_1\rangle = \delta(t_2 - t_1)$
Inner/Dot Product generalized to complex vectors: $\langle a b\rangle = \mathbf{a}^\dagger \cdot \mathbf{b} \rightarrow \sum_i \langle a i\rangle \langle i b\rangle = \sum_i a_i^* b_i$	Inner Product for complex functions: $\langle f g\rangle = \int dt \langle f t\rangle \langle t g\rangle = \int dt f^*(t)g(t)$
Matrix transformations: $ a'\rangle = M a\rangle$ $a'_i = \sum_j M_{ij} a_j \leftrightarrow \langle i a'\rangle = \sum_j \langle i M j\rangle \langle j a\rangle$	Integral Transformations: $ \tilde{f}\rangle = M f\rangle$ ($M \rightarrow$ Kernel) $\tilde{f}(\tau) = \langle \tau \tilde{f}\rangle = \int dt \langle \tau M t\rangle \langle t f\rangle = \int dt M(\tau, t)f(t)$
Unitary Transformations: $\langle a b\rangle = \langle a U^\dagger U b\rangle = \langle a' b'\rangle$ True iff $\sum_i U_{ij}^* U_{ik} = \delta_{jk}$ $\langle a' b'\rangle = \sum_i \langle a U^\dagger i\rangle \langle i U b\rangle$ $= \sum_i \left(\sum_j \langle a j\rangle \langle j U^\dagger i\rangle \right) \left(\sum_k \langle i U k\rangle \langle k b\rangle \right)$ $= \sum_i a_i'^* b_i' = \sum_i \left(\sum_j (U_{ij} a_j)^* \sum_k (U_{ik} b_k) \right)$ $= \sum_{jk} a_j^* b_k \sum_i U_{ij}^* U_{ik} = \langle a b\rangle$ iff U is Unitary.	Unitary Transformations: $\langle f g\rangle = \langle f U^\dagger U g\rangle = \langle \tilde{f} \tilde{g}\rangle$ True iff $\int d\tau U(\tau, t_1)^* U(\tau, t_2) = \delta(t_2 - t_1)$ $\langle \tilde{f} \tilde{g}\rangle = \int d\tau \langle f U^\dagger \tau\rangle \langle \tau U g\rangle$ $= \int d\tau \left(\int dt_1 \langle f t_1\rangle \langle t_1 U^\dagger \tau\rangle \right) \left(\int dt_2 \langle \tau U t_2\rangle \langle t_2 g\rangle \right)$ $= \int d\tau \left(\int dt_1 (U(\tau, t_1)f(t_1))^* \right) \left(\int dt_2 U(\tau, t_2)g(t_2) \right)$ $= \int dt_1 dt_2 f^*(t_1)g(t_2) \int d\tau U^*(\tau, t_1)U(\tau, t_2)$ $= \langle f g\rangle$ iff U is Unitary.

(e) Consider the following series and inverse Fourier Transform ($\tilde{g}(k)$ is the Fourier Transform of $g(x)$):

$$\text{Fourier Series: } f(x) = \sum_{n=-\infty}^{\infty} C_n e^{2\pi i n x/L} \quad \text{Inverse Transform: } g(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{g}(k) e^{ikx} dk$$

In each expression C_n and $\tilde{g}(k)$ represent the "amount" of a given frequency needed to construct some function $f(x)$ or $g(x)$. The constraint on x being finite for the series, however, makes the frequency space discrete, whereas in the unbound case for the transform all frequencies are allowed. This is stated by the nature of C_n being dependent on an integer n , whereas k is a continuous variable. If we consider $k \leftrightarrow \frac{2\pi n}{L}$ we see that the two expressions are related in a fashion very similar to all of the expressions considered in the previous parts of this problem. If we notate $C_n = \langle n|C\rangle$ and $\tilde{g}(k) = \langle k|g\rangle$ this relationship is clearer. The Kernel for the Fourier transform is $M(x, k) = e^{-ikx}/\sqrt{2\pi}$ for $\tilde{g}(k) = \int dx M(x, k)g(x)$.

Parseval's Theorem states that for Fourier Transform $\langle \tilde{f} | \tilde{g} \rangle = \langle f | g \rangle$. The theorem is thereby essentially a statement that the Fourier Transform is Unitary. (This can be shown using some integration tricks directly from the Kernel / definition of the transform.)

2.4 Problem 8

In this problem we will show that in one dimension, bound states cannot be degenerate.

(a) Consider two degenerate states $\psi_1(x)$ and $\psi_2(x)$. Evaluate the quantity $\psi_1(x)H\psi_2(x) - \psi_2(x)H\psi_1(x)$ using the Schrödinger equation.

(b) Use the result from above to determine the relation between ψ_1 and ψ_2 . (What do you expect if there is no degeneracy?)

Solution

Solution from Prof. Das' PHY 407 course. Since we are positing two degenerate states, they must have the same energy, by definition. This means $H\psi_1 = E\psi_1$ and $H\psi_2 = E\psi_2$. This implies:

$$\psi_1 H \psi_2 - \psi_2 H \psi_1 = E(\psi_1 \psi_2 - \psi_2 \psi_1) = 0$$

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad \rightarrow \quad -\frac{\hbar^2}{2m} \left[\psi_1 \frac{d^2 \psi_2}{dx^2} - \psi_2 \frac{d^2 \psi_1}{dx^2} \right] + V(x) \psi_1 \psi_2 - V(x) \psi_2 \psi_1 = 0 \quad \rightarrow \quad \psi_1 \frac{d^2 \psi_2}{dx^2} - \psi_2 \frac{d^2 \psi_1}{dx^2} = 0$$

This last expression can be reduced to (where the prime is differentiation with respect to x):

$$\frac{d}{dx}(\psi_1 \psi_2' - \psi_2 \psi_1') = 0 \quad \rightarrow \quad \psi_1 \psi_2' - \psi_2 \psi_1' = W = \text{constant}$$

Note that W is the Wronskian. We now apply the assumption that the states are bound. For a bound state, we must have $\psi_1, \psi_2 \rightarrow 0$ as $x \rightarrow \pm\infty$. But if W is a constant and that constant is zero at $\pm\infty$, then that constant is zero everywhere. Therefore $W = 0$. If the Wronskian is zero however, that implies that $\psi_1 = \lambda\psi_2$ for some constant λ (i.e. ψ_1 and ψ_2 are linearly dependent for all x). If that is the case, then ψ_1 and ψ_2 , in fact, represent the same state. Therefore the solution is unique and there is no degeneracy.

2.5 Problem 9

Consider the Hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2m} + V(x, y) \quad \rightarrow \quad V(x, y) = \begin{cases} 0 & |x| < \frac{L}{2}, 0 < y < L \\ \infty & \text{else} \end{cases}$$

- (a) Determine the eigenvalues and normalized eigenfunctions of the system.
- (b) Set up an equation describing the degenerate states of the system.
- (c) Find some degenerate states.

Solution

- (a) We can write down the answer based on previous derivations from workshop 1.

$$E = E_x + E_y = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2)$$

The wavefunction (*not* normalized) is given by:

$$\psi(x, y) = \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_x \pi x}{L}\right) \quad \text{for } n_x \text{ even} \quad , \quad \psi(x, y) = \sin\left(\frac{n_y \pi y}{L}\right) \cos\left(\frac{n_x \pi x}{L}\right) \quad \text{for } n_x \text{ odd}$$

We may take the product of the x and y parts of the function because the Schrödinger equation can be solved by separation of variables in this case. The energies add cleanly because the Hamiltonian can be broken into $H = H_x + H_y$, where H_x contains all the x dependence in the Hamiltonian, and H_y all the y , and $[H_x, H_y] = 0$. This separation of the Schrödinger equation as a differential equation, and ability to factor the Hamiltonian into commuting terms are, in fact, equivalent statements.

The normalization condition can be expressed by:

$$\int_{-L/2}^{L/2} dx \int_0^L dy |A|^2 \psi^*(x, y) \psi(x, y) = 1$$

Note that the integrals each in x and in y evaluate are the same as those for the one-dimensional box:

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2} \quad \rightarrow \quad \int_{-L/2}^{L/2} dx \int_0^L dy \psi^*(x, y) \psi(x, y) = \frac{L^2}{4} \quad \rightarrow \quad A = \frac{2}{L}$$

$$\psi(x, y) = \frac{2}{L} \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_x \pi x}{L}\right) \quad \text{for } n_x \text{ even} \quad , \quad \psi(x, y) = \frac{2}{L} \sin\left(\frac{n_y \pi y}{L}\right) \cos\left(\frac{n_x \pi x}{L}\right) \quad \text{for } n_x \text{ odd}$$

(b) Degeneracy occurs when $E_{n_x, n_y} = E_{n'_x, n'_y}$. Since $E \propto (n_x^2 + n_y^2)$, degeneracy arises when multiple integer coordinates are on the circumference of a circle with radius proportional to \sqrt{E} .

(c) The following pair of coordinates (n_x, n_y) satisfy the relationship (there are many more): (5, 5) and (7, 1).

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3.1 Problem 10

Show the following using Dirac Notation, where Ω and Λ are some operators.

- (a) $Tr(\Omega\Lambda) = Tr(\Lambda\Omega)$.
 (b) $(\Omega\Lambda)^\dagger = \Lambda^\dagger\Omega^\dagger$. What happens if one takes the adjoint of 3 operators?

Solution

(a)

$$Tr(\Omega\Lambda) = \sum_i \langle i | \Omega\Lambda | i \rangle = \sum_i \sum_j \langle i | \Omega | j \rangle \langle j | \Lambda | i \rangle = \sum_{ij} \langle j | \Lambda | i \rangle \langle i | \Omega | j \rangle = \sum_j \langle j | \Lambda\Omega | j \rangle = Tr(\Lambda\Omega)$$

(b) Method 1 (more formal):

$$\langle i | (\Omega\Lambda)^\dagger | j \rangle = (\langle j | \Omega\Lambda | i \rangle)^\dagger = \sum_k (\langle j | \Omega | k \rangle \langle k | \Lambda | i \rangle)^\dagger = \sum_k (\langle k | \Lambda | i \rangle \langle j | \Omega | k \rangle)^\dagger = \sum_k \langle i | \Lambda^\dagger | k \rangle \langle k | \Omega^\dagger | j \rangle = \langle i | \Lambda^\dagger \Omega^\dagger | j \rangle$$

Method 2:

$$\langle i | (\Omega\Lambda)^\dagger | j \rangle = \langle \Omega\Lambda i | j \rangle = \langle \Lambda i | \Omega^\dagger | j \rangle = \langle i | \Lambda^\dagger \Omega^\dagger | j \rangle$$

Method two makes it clearer that $(ABC)^\dagger = C^\dagger B^\dagger A^\dagger$, and so forth for more operators.

3.2 Problem 11

We apply a variational approach to a known problem. Consider the Hamiltonian for the one-dimensional SHO, and the trial wavefunction ψ .

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} \quad \psi(x) = x e^{-\alpha|x|}$$

- (a) Compute $\langle H \rangle$ as a function of α .
 (b) Minimize $\langle H \rangle$.
 (c) Which energy eigenstate of H most closely resembles the trial wavefunction?

Solution

(a)

$$\begin{aligned} \langle H \rangle &= \frac{\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(x e^{-\alpha|x|} \frac{d^2}{dx^2} x e^{-\alpha|x|} \right) + \frac{m\omega^2}{2} \int_{-\infty}^{\infty} dx x^4 e^{-2\alpha|x|}}{\int_{-\infty}^{\infty} dx e^{-2\alpha|x|} x^2} \\ &= \frac{\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left[x e^{-\alpha|x|} \left(-\frac{\alpha x}{|x|} \right) + e^{-\alpha|x|} \right]^2 + \frac{m\omega^2}{2} \int_{-\infty}^{\infty} dx x^4 e^{-2\alpha|x|}}{\int_{-\infty}^{\infty} dx e^{-2\alpha|x|} x^2} \\ &= \left[\int_0^{\infty} e^{-2\alpha x} dx \right]^{-1} \times \left[\frac{\hbar^2}{2m} \int_0^{\infty} (\alpha^2 x^2 - 2\alpha x + 1) e^{-2\alpha x} dx + \frac{m\omega^2}{2} \int_0^{\infty} x^4 e^{-2\alpha x} dx \right] \\ &= \left[\left(\frac{\partial}{\partial(-2\alpha)} \right)^2 \frac{1}{2\alpha} \right]^{-1} \times \left[\frac{\hbar^2}{2m} \left(\alpha^2 \left(\frac{\partial}{\partial(-2\alpha)} \right)^2 - 2\alpha \left(\frac{\partial}{\partial(-2\alpha)} \right) + 1 \right) \frac{1}{2\alpha} + \frac{m\omega^2}{2} \left(\frac{\partial}{\partial(-2\alpha)} \right)^4 \frac{1}{2\alpha} \right] \\ &= \left[\frac{2}{(2\alpha)^3} \right]^{-1} \times \left[\frac{\hbar^2}{2m} \left(\alpha^2 \frac{2}{(2\alpha)^3} - \frac{2\alpha}{(2\alpha)^2} + \frac{1}{2\alpha} \right) + \frac{1}{2} m\omega^2 \frac{24}{(2\alpha)^5} \frac{12}{(2\alpha)^2} \right] = \frac{\hbar^2 \alpha^2}{2m} + \frac{3}{2} \frac{m\omega^2}{\alpha^2} \end{aligned}$$

(b) Minimize:

$$\frac{d\langle H \rangle}{d\alpha} = 0 \quad \rightarrow \quad \alpha = \left(\frac{3m^2\omega^2}{\hbar^2} \right)^{\frac{1}{4}}$$

Plug that value in to get a measurement for the energy.

$$\langle H \rangle = \frac{\hbar^2}{2m} \left(\frac{3m^2\omega^2}{\hbar^2} \right)^{\frac{1}{2}} + \frac{3}{2}m\omega^2 \left(\frac{\hbar^2}{3m^2\omega^2} \right)^{\frac{1}{2}} = \sqrt{3}\hbar\omega \approx 1.73\hbar\omega$$

(c) This result is closest to the energy associated with the first excited state of the SHO, so we conclude that the trial wavefunction resembles that one the most.

3.3 Problem 12

Recall the following properties of a Dirac delta function, and a generalized form of a Fourier Transform:

$$\delta(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dx e^{-ikx} \quad f(x) = \int dx' f(x') \delta(x-x') \quad \tilde{f}(k) = \sqrt{\frac{|\eta|}{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx\eta} dx$$

(a) Evaluate the expression $\int dx' [\partial_{x'} \delta(x-x')] f(x')$.

(b) Consider an operator D which differentiates a function, (i.e. $\langle x|D|f \rangle = \partial_x f(x)$). If this were written as an integral transformation, what is the Kernel $D(x, x')$? (The Kernel in an integral transformation is analogous to the matrix element in a transformation.)

(c) Can we say anything about whether D is Hermitian? What about an operator $P = -i\hbar D$?

(d) What are the eigenfunctions of the operator P ? (Let the eigenvalue be p . Find $\langle x|p \rangle$ such that $P|p \rangle = p|p \rangle$.)

(e) Write the quantity $\langle p|\psi \rangle$ using an integral over x . What do you notice about the relationship between $\langle x|\psi \rangle$ and $\langle p|\psi \rangle$? Can you use this to say something about the normalization of $\langle x|p \rangle$?

(f) Evaluate $\langle x|[x, P]|\psi \rangle$ for some $|\psi \rangle$, for the definition of P above. Do you get the expected result? Discuss.

Solution

(a) Assume $a < x < b$.

$$\int_a^b dx' f(x') \frac{d}{dx'} \delta(x-x') = f(x') \delta(x-x') \Big|_a^b - \int_a^b dx' \delta(x-x') f'(x') = -\frac{df}{dx}$$

(b) Notice that $\partial_{x'} \delta(x-x') = -\partial_x \delta(x-x')$, and compare the following expansion with the result of part (a):

$$\frac{df}{dx} = \langle x|D|f \rangle = \int dx' \langle x|D|x' \rangle \langle x'|f \rangle \quad \rightarrow \quad \langle x|D|x' \rangle = D(x, x') = \frac{d}{dx} \delta(x-x') = \delta'(x-x')$$

(c)

$$D^\dagger(x, x') = \langle x|D^\dagger|x' \rangle = \langle x'|D|x \rangle^* = D^*(x', x) = \delta'(x'-x) = -D(x, x')$$

D is naively anti-Hermitian. (There are some further restrictions on the normalizability of the wavefunctions this acts on for this to work a Hilbert Space, as we are interested in doing. Please ask questions in the event you would like further clarification on this point. Shankar's "Principles of Quantum Mechanics", on reserve at the POA, contains the more complete proof.)

$$P^\dagger(x, x') = i\hbar D^\dagger(x, x') = -i\hbar D(x, x') = P(x, x')$$

It is therefore reasonable to treat P as Hermitian (again given suitable functions consistent with a Hilbert space).

(d)

$$\langle x|P|p \rangle = p \langle x|p \rangle \quad \rightarrow \quad -i\hbar \frac{dp(x)}{dx} = p \cdot p(x) \quad \rightarrow \quad p(x) = A e^{ipx/\hbar}$$

(e)

$$\langle p|\psi \rangle = \int_{-\infty}^{\infty} dx \langle p|x \rangle \langle x|\psi \rangle = \int_{-\infty}^{\infty} dx p^*(x) \psi(x) = A \int_{-\infty}^{\infty} dx e^{-\frac{ipx}{\hbar}} \psi(x)$$

What if I choose the normalization $A = (2\pi\hbar)^{-\frac{1}{2}}$?

$$p(x) = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \quad \rightarrow \quad \langle p|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \psi(x) \exp\left(\frac{ipx}{\hbar}\right) = \tilde{\psi}(p) \quad \text{for } \eta = \frac{1}{\hbar}$$

Then $\langle p|\psi\rangle = \tilde{\psi}(p)$ is nothing but the Fourier transform of $\langle x|\psi\rangle = \psi(x)$. This implies:

$$\langle p|p'\rangle = \int dx \langle p|x\rangle \langle x|p'\rangle = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx e^{-i(p-p')x/\hbar} = \delta\left(\frac{p-p'}{\hbar}\right) \frac{1}{\hbar} = \delta(p-p')$$

So we have, in fact normalized $\langle x|p\rangle$. (Functions in a Hilbert space must be normalizable to unity, as for bound functions, or to a Dirac delta, as is the case here and for unbound wavefunctions.)

(f) The following is an informal way of evaluating this. (You can consider the $\langle x|$ on the left to denote the basis in which the operators and state are being written. It is *not* correct to view the bra as being pulled through the commutator however; we would then be operating a matrix on a scalar. The more formal version illustrating this is shown further below.)

$$\langle x|[x, P]|\psi\rangle = x \left(-i\hbar \frac{\partial}{\partial x}\right) \psi(x) + i\hbar \frac{\partial}{\partial x} (x\psi(x)) = i\hbar\psi(x) = i\hbar \langle x|\psi\rangle \quad \rightarrow \quad [x, P] = i\hbar$$

This is the usual commutator between a coordinate and its conjugate momentum. We therefore conclude that a given wavefunction written in a coordinate basis can be transformed to the momentum basis by the application of a Fourier transform. For the sake of completion, a more formal version of part (f) would read as follows, where we note that the terms $|x\rangle$ are eigenstates of \hat{x} , just as $|p\rangle$ denotes an eigenstate of \hat{p} above, and that $\langle x|D|x'\rangle$ differentiates terms containing x' .

$$\begin{aligned} \langle x|[\hat{x}, \hat{p}]|\psi\rangle &= \int \langle x|\hat{x}\hat{p} - \hat{p}\hat{x}|x'\rangle \langle x'|\psi\rangle dx' = \int \langle x|\hat{x}|x''\rangle \langle x''|\hat{p}|x'\rangle \langle x'|\psi\rangle dx' dx'' - \int \langle x|\hat{p}|x''\rangle \langle x''|\hat{x}|x'\rangle \langle x'|\psi\rangle dx' dx'' \\ &= -i\hbar \left[\int x'' \langle x|x''\rangle \langle x''|D|x'\rangle \langle x'|\psi\rangle dx' dx'' - \int \langle x|D|x''\rangle \langle x''|x'\rangle x' \langle x'|\psi\rangle dx' dx'' \right] \\ &= -i\hbar \left[\int x'' \delta(x-x'') [\partial_{x''} \delta(x''-x')] \psi(x') dx' dx'' - \int [\partial_x \delta(x-x'')] \delta(x''-x') x' \psi(x') dx' dx'' \right] \\ &= i\hbar \left[\int [\partial_x \delta(x-x')] x' \psi(x') dx' - \int x [\partial_x \delta(x-x')] \psi(x') dx' \right] = i\hbar \left[\frac{d}{dx} (x\psi(x)) - x \frac{d}{dx} \psi(x) \right] \end{aligned}$$

Note that this recovers the result above. The abstracted commutator (devoid of any particular basis or state), can be written $[x, p] = i\hbar\mathbb{1}$, or simply $[x, p] = i\hbar$. A fun fact for further context: this applies to any set of coordinates and momenta x and p related in classical terms by $p = \partial_x L$, where L is the Lagrangian for a system. The Heisenberg uncertainty principle can be derived from this commutator (this will be done in class), and thereby applies over any conjugate set of variables in the same way. Getting from one variable to the other by Fourier transform as shown above “closes” a theoretical loop of sorts; the uncertainty principle can also be derived from Fourier transforms independent of any reference to quantum mechanics. It is a direct consequence of the fact that we are working in mathematical system in which our variables must be related in the way derived above.

Note also that the integral transform definition of P is still consistent with all of this (just a nice check):

$$\begin{aligned} \langle p|P|\psi\rangle &= -i\hbar \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dx' \langle p|x\rangle \langle x|D|x'\rangle \langle x'|\psi\rangle = -\frac{i\hbar}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \int_{-\infty}^{\infty} dx' \psi(x') \delta(x-x') \\ &= -\frac{i\hbar}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \frac{d\psi}{dx} = -i\hbar \left(\frac{ip}{\hbar} \tilde{\psi}(p)\right) = p\tilde{\psi}(p) \\ \langle p|P|\psi\rangle &= \langle p|P^\dagger|\psi\rangle = p \langle p|\psi\rangle = p\tilde{\psi}(p) \end{aligned}$$

(I have used the identity for the Fourier Transform of the derivative of a function to simplify. I have also used the fact that P is hermitian, even though we have not proven this strictly above.)

A further note on the utility of this result: What this means is that if I expand a wavefunction in coordinate space (as you are accustomed to doing), you use $\hat{x} = x$ and $\hat{p} = -i\hbar\partial_x$. You could however expand in the momentum basis and use

$\hat{p} = p$ and $\hat{x} = i\hbar\partial_p$. In some cases the integrations might be easier one way than the other, so it is worth being aware of both options.

$$\langle x \rangle \rightarrow \int dx \psi^*(x) x \psi(x) \leftrightarrow \int dp \tilde{\psi}^*(p) \left(i\hbar \frac{\partial}{\partial p} \right) \tilde{\psi}(p) \quad \text{and} \quad \langle p \rangle \rightarrow \int dx \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x) \leftrightarrow \int dp \tilde{\psi}^*(p) p \tilde{\psi}(p)$$

3.4 Problem 13

Let $|a'\rangle$ and $|a''\rangle$ be eigenstates of a Hermitian operator A with eigenvalues a' and a'' respectively. ($a' \neq a''$). The Hamiltonian is given below, where b is some real number.

$$H = b|a'\rangle\langle a''| + b|a''\rangle\langle a'|$$

(a) $|a'\rangle$ and $|a''\rangle$ are not eigenstates of the Hamiltonian. Do you see why this is true? Determine the eigenstates and corresponding eigenvalues.

(b) Suppose the system is in a state $|a'\rangle$ at $t = 0$. Determine the state vector for $t > 0$.

(c) Determine the probability for finding the system in $|a''\rangle$ for $t > 0$ if the system is known to be in a state $|a'\rangle$ at $t = 0$.

Solution

(a) Begin by evaluating $H|a'\rangle$ and $H|a''\rangle$, noting that $\langle a'|a''\rangle = 0 = \langle a''|a'\rangle$.

$$H|a'\rangle = b(|a'\rangle\langle a''| + |a''\rangle\langle a'|)|a'\rangle = b|a''\rangle \quad H|a''\rangle = b(|a'\rangle\langle a''| + |a''\rangle\langle a'|)|a''\rangle = b|a'\rangle$$

It is then clear that H is swapping us between $|a'\rangle$ and $|a''\rangle$. We proceed by constructing the matrix form of H in order to find an eigenbasis:

$$H = \begin{pmatrix} \langle a'|H|a'\rangle & \langle a'|H|a''\rangle \\ \langle a''|H|a'\rangle & \langle a''|H|a''\rangle \end{pmatrix} = \begin{pmatrix} 0 & b \\ b & 0 \end{pmatrix} \rightarrow \begin{vmatrix} -\lambda & b \\ b & -\lambda \end{vmatrix} = 0 \rightarrow \lambda = \pm b$$

We see that the eigenvalues are $\pm b$, and notate the associated normalized eigenstates by $|b\rangle$ and $|-b\rangle$. Solve these the usual way to obtain:

$$|b\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |-b\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

(b) Recall that the time evolution operator is of the form $U = e^{-iHt/\hbar}$. When applied to an eigenstate of the Hamiltonian with energy E this results in a term $e^{-iEt/\hbar}$. We write the vector $|a'\rangle$ in terms of the eigenbasis.

$$|a'\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}|b\rangle + \frac{1}{\sqrt{2}}|-b\rangle$$

Then we may apply the evolution operator to obtain:

$$|a'\rangle_t = U|a'\rangle = \frac{1}{\sqrt{2}}e^{-ibt/\hbar}|b\rangle + \frac{1}{\sqrt{2}}e^{ibt/\hbar}|-b\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{-ibt/\hbar} + \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} e^{ibt/\hbar} = \begin{pmatrix} \cos\left(\frac{bt}{\hbar}\right) \\ -i \sin\left(\frac{bt}{\hbar}\right) \end{pmatrix}$$

(c) Then the probability of the system being in $|a''\rangle$ for $t > 0$ after starting in $|a'\rangle$ is given by:

$$P = |\langle a''|a'\rangle_t|^2 \rightarrow |a''\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow P = \sin^2\left(\frac{bt}{\hbar}\right)$$

4

4.1 Problem 14

Consider a particle subject to the potential $V(x) = -V_0\delta(x)$ where $V_0 > 0$.

(a) What are the boundary conditions? What are the units of V_0 ?

(b) Look for a bound state using the variational approach and a trial function $\phi(x) = Ae^{-\alpha|x|}$. Give the energy and normalized wave function of the bound state.

(c) Show that the trial wave function in part (b) is an exact solution to the Schrödinger equation for this system.

(d) Repeat part (b) with a different trial wavefunction shown below to determine the minimum expected energy $\langle E \rangle$. (L is a variational parameter).

$$\psi(x) = \begin{cases} 1 + x/L & x \in [-L, 0] \\ 1 - x/L & x \in (0, L] \end{cases}$$

Compare with the results you found in part (b).

Solution

(a) We note that $\delta(x)$ has units of m^{-1} ($[\delta(x)] = [x]^{-1}$). Then for V to have units of Joules, $[V_0] = Jm$. We require that the wavefunction be continuous across the boundary (consider what would happen to the probability current if this were not the case). We obtain a relation for the discontinuity in the derivative by integrating the Schrödinger equation over the delta function. We define a small region $x \in [-\epsilon, \epsilon]$, and are interested in the limit as $\epsilon \rightarrow 0$.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2} - V_0 \delta(x) \phi(x) - E \phi(x) = 0 \quad \rightarrow \quad \lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \left[\frac{\partial^2 \phi}{\partial x^2} + \frac{2m}{\hbar^2} (V_0 \delta(x) + E) \phi(x) \right] dx$$

This gives a discontinuity in the derivative according to:

$$\lim_{\epsilon \rightarrow 0} \phi'(\epsilon) - \phi'(-\epsilon) + \frac{2mV_0}{\hbar^2} \phi(0) = 0 \quad \rightarrow \quad \phi'_2(0) - \phi'_1(0) = -\frac{2mV_0\phi(0)}{\hbar^2}$$

(b)

$$\langle H \rangle = \frac{\frac{1}{2m} \int |p\phi|^2 dx - V_0 \phi(0)}{\int |\phi|^2 dx} = \frac{\frac{\hbar^2 \alpha^2}{2m} \int e^{-2\alpha|x|} dx - V_0}{\int e^{-2\alpha|x|} dx} = \frac{\frac{\hbar^2 \alpha^2}{2m} - V_0}{\frac{1}{\alpha}} = \frac{\hbar^2 \alpha^2}{2m} - V_0 \alpha$$

We then minimize $\langle H \rangle$ and plug the value of α back in to obtain a measure of the energy.

$$\frac{\partial \langle H \rangle}{\partial \alpha} = 0 = \frac{\hbar^2 \alpha}{m} - V_0 \quad \rightarrow \quad \alpha = \frac{mV_0}{\hbar^2} \quad \rightarrow \quad \langle H \rangle = \frac{\hbar^2}{2m} \left(\frac{mV_0}{\hbar^2} \right) - V_0 \frac{mV_0}{\hbar^2} = -\frac{mV_0^2}{2\hbar^2}$$

We then normalize ϕ by evaluating $1 = \int |\phi|^2 dx = \frac{A^2}{\alpha}$. This gives $A = \sqrt{\alpha}$.

$$\phi(x) = \sqrt{\frac{mV_0}{\hbar^2}} \exp \left[-\frac{mV_0}{\hbar^2} |x| \right]$$

(c) It will be useful to write $|x| = x\varepsilon(x)$ where ε is the alternating function (you may also know it as $\text{sgn}(x)$). Note that $\partial_x \varepsilon(x) = 2\delta(x)$. Plug the solution into the Schrödinger equation.

$$\begin{aligned} & \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V_0 \delta(x) \right] \exp \left[-\frac{mV_0}{\hbar^2} |x| \right] \stackrel{?}{=} -\frac{mV_0^2}{2\hbar^2} \exp \left[-\frac{mV_0}{\hbar^2} |x| \right] \\ & \left[-\frac{\hbar^2}{2m} \left(\frac{mV_0}{\hbar^2} \right)^2 - \frac{\hbar^2}{2m} \left(-\frac{mV_0}{\hbar^2} \right) 2\delta(x) - V_0 \delta(x) \right] \exp \left[-\frac{mV_0}{\hbar^2} |x| \right] \stackrel{?}{=} E \exp \left[-\frac{mV_0}{\hbar^2} |x| \right] \end{aligned}$$

The δ -functions on the LHS cancel, such that both sides are in fact equal, and we see that we have been using an exact solution.

(d) As usual we require the continuity of the wavefunction at all points, thus $\psi_1(0) = \psi_2(0)$, where region 1 is for negative x and region 2 is for positive x .

$$\psi(x) = \begin{cases} 1 + x/L & x \in [-L, 0] \quad \rightarrow \quad \psi_1 \\ 1 - x/L & x \in (0, L] \quad \rightarrow \quad \psi_2 \end{cases}$$

We obtain a relation for the discontinuity in the derivative by integrating the Schrödinger equation over the delta function as in part (a), to obtain the following.

$$\lim_{\epsilon \rightarrow 0} \psi'(\epsilon) - \psi'(-\epsilon) + \frac{2mV_0}{\hbar^2} \psi(0) = 0 \quad \rightarrow \quad \psi'_2(0) - \psi'_1(0) = -\frac{2mV_0\psi(0)}{\hbar^2}$$

$$\langle H \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\frac{\hbar^2}{m} \int_0^L \left| \frac{\partial \psi_2}{\partial x} \right|^2 dx - V_0 \psi(0)}{2 \int_0^L \left(1 - \frac{x}{L}\right)^2 dx} = \frac{\frac{\hbar^2}{mL} - V_0}{\frac{2L}{3}} = \frac{3}{2} \left(\frac{\hbar^2}{mL^2} - \frac{V_0}{L} \right)$$

$$\frac{d\langle H \rangle}{dL} = 0 = -3 \frac{\hbar^2}{mL^3} + \frac{3V_0}{2L^2} \quad \rightarrow \quad L = \frac{2\hbar^2}{mV_0}$$

Then plugging L back into $\langle H \rangle$ gives:

$$\langle H \rangle = -\frac{3mV_0}{8\hbar^2}$$

We have an energy slightly closer to zero than the actual value with this approximation, but we see that the variational method still gives us a relatively good result for this trial wavefunction. (By plotting the wavefunctions one may see that trial function from part (d) and the exact solution in parts (b) and (c) are qualitatively quite similar.)

4.2 Problem 15

Calculate the following Commutators:

- (a) $[x, p]$ (b) $[x^2, p]$ (c) $[x, p^2]$ (d) $[x^n, p]$ (e) $[x, p^n]$ (f) $[x_1x_2, p_1p_2]$ (g) $[x_1p_2, x_2p_1]$

Solution

- (a) $[x, p] = i\hbar$. See part (e) of previous problem.
 (b) $[x^2, p] = x[x, p] + [x, p]x = 2i\hbar x$.
 (c) $[x, p^2] = p[x, p] + [x, p]p = 2i\hbar p$.
 (d) $[x^n, p] = x[x^{n-1}, p] + [x, p]x^{n-1} = x^2[x^{n-2}, p] + x[x, p]x^{n-2} + i\hbar x^{n-1} = \dots = i\hbar n x^{n-1}$.
 (e) $[x, p^n] = ni\hbar p^{n-1}$ by same logic.
 (f) $[x_1x_2, p_1p_2] = i\hbar(p_1x_1 + x_2p_2)$.
 (g) $[x_1p_2, x_2p_1] = i\hbar(x_2p_2 - x_1p_1)$.

4.3 Problem 16

The 1D SHO can be expressed/solved in terms of the following operators:

$$H = \frac{p^2}{2M} + \frac{1}{2}M\omega^2 x^2 = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) \quad ; \quad a = \sqrt{\frac{M\omega}{2\hbar}} \left(x + \frac{ip}{M\omega} \right) \quad , \quad a^\dagger = \sqrt{\frac{M\omega}{2\hbar}} \left(x - \frac{ip}{M\omega} \right)$$

- (a) Calculate the commutator $[a, a^\dagger]$.
 (b) Given the operator $N = a^\dagger a$, where $N|n\rangle = n|n\rangle$, compute $E_n = \langle n | H | n \rangle$.
 (c) Compute $[a, H]|n\rangle$ and $[a^\dagger, H]|n\rangle$. Show that $H(a|n\rangle) = E_{n-1}(a|n\rangle)$ and $H(a^\dagger|n\rangle) = E_{n+1}(a^\dagger|n\rangle)$.
 (d) Determine $a|n\rangle$ and $a^\dagger|n\rangle$.
 (e) Write out the matrix elements $\langle n | x | m \rangle$, $\langle n | p | m \rangle$, $\langle n | x^2 | m \rangle$, and $\langle n | p^2 | m \rangle$. Write out enough elements in matrix form to get a sense of how this looks.
 (f) Sum matrices to obtain a matrix for H . Does your result make sense?
 (g) From part (e), compute $\Delta x \Delta p$ of the n^{th} state.

Solution

(a)

$$[a, a^\dagger] = \frac{M\omega}{2\hbar} \left[x + \frac{ip}{M\omega}, x - \frac{ip}{M\omega} \right] = \frac{M\omega}{2\hbar} \frac{i}{M\omega} (-[x, p] + [p, x]) = \frac{i}{2\hbar} (-2i\hbar) = 1$$

(b)

$$H = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right) = \hbar\omega N + \frac{\hbar\omega}{2} \rightarrow \langle H \rangle = E_n = \hbar\omega \left(n + \frac{1}{2} \right) \quad \text{for } n = 0, 1, 2, \dots$$

(c)

$$[a, H] = \hbar\omega[a, a^\dagger a] = \hbar\omega[a, a^\dagger]a = \hbar\omega a \rightarrow [a, H]|n\rangle = \hbar\omega a|n\rangle \rightarrow H(a|n\rangle) = (E_n - \hbar\omega)(a|n\rangle)$$

Similarly:

$$[a^\dagger, H]|n\rangle = -\hbar\omega a^\dagger|n\rangle \rightarrow H(a^\dagger|n\rangle) = (E_n + \hbar\omega)(a^\dagger|n\rangle)$$

Thus we see that a^\dagger raises us one energy level, and a lowers us one level.

(d) We may then say that $a|n\rangle = C_1|n-1\rangle$ and that $a^\dagger|n\rangle = C_2|n+1\rangle$. We apply the definitions and commutator results above to evaluate expectation values.

$$\langle n|a^\dagger a|n\rangle = |C_1|^2 = n \rightarrow a|n\rangle = \sqrt{n}|n-1\rangle$$

$$\langle n|aa^\dagger|n\rangle = |C_2|^2 = n+1 \rightarrow a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

(e) Solve the system of given relations defining a and a^\dagger to write x and p in terms of the ladder operators, and then apply these in calculating the matrix elements.

$$x = \sqrt{\frac{\hbar}{2M\omega}}(a + a^\dagger) \quad p = i\sqrt{\frac{M\omega\hbar}{2}}(a^\dagger - a)$$

$$\langle n|x|m\rangle = \sqrt{\frac{\hbar}{2M\omega}}(\sqrt{m}\delta_{n,m-1} + \sqrt{m+1}\delta_{n,m+1})$$

$$\langle n|p|m\rangle = -i\sqrt{\frac{M\omega\hbar}{2}}(\sqrt{m}\delta_{n,m-1} - \sqrt{m+1}\delta_{n,m+1})$$

$$\langle n|x^2|m\rangle = \frac{\hbar}{2M\omega}(\sqrt{m(m-1)}\delta_{n,m-2} + m\delta_{n,m} + (m+1)\delta_{n,m} + \sqrt{(m+1)(m+2)}\delta_{n,m+2})$$

$$\langle n|p^2|m\rangle = -\frac{M\omega\hbar}{2}(\sqrt{m(m-1)}\delta_{n,m-2} - m\delta_{n,m} - (m+1)\delta_{n,m} + \sqrt{(m+1)(m+2)}\delta_{n,m})$$

These may be equivalently represented by:

$$x = \sqrt{\frac{\hbar}{2M\omega}} \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \\ \vdots & & & & \ddots \end{pmatrix} \quad p = i\sqrt{\frac{M\omega\hbar}{2}} \begin{pmatrix} 0 & -1 & 0 & 0 & \dots \\ 1 & 0 & -\sqrt{2} & 0 & \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \\ 0 & 0 & \sqrt{3} & 0 & \\ \vdots & & & & \ddots \end{pmatrix}$$

$$x^2 = \frac{\hbar}{2M\omega} \begin{pmatrix} 1 & 0 & \sqrt{2} & \dots \\ 0 & 3 & 0 & \\ \sqrt{2} & 0 & 5 & \\ \vdots & & & \ddots \end{pmatrix} \quad p^2 = -\frac{M\omega\hbar}{2} \begin{pmatrix} -1 & 0 & \sqrt{2} & \dots \\ 0 & -3 & 0 & \\ \sqrt{2} & 0 & -5 & \\ \vdots & & & \ddots \end{pmatrix}$$

(f)

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2 = \hbar\omega \begin{pmatrix} \frac{1}{2} & 0 & 0 & \dots \\ 0 & \frac{3}{2} & 0 & \\ 0 & 0 & \frac{5}{2} & \\ \vdots & & & \ddots \end{pmatrix}$$

This is a thoroughly unsurprising result, which can be obtained directly from $H = \hbar\omega(a^\dagger a + \frac{1}{2})$ as well. We are in the energy eigenbasis, so H should be diagonal with the energy eigenvalues populating the diagonal. This is exactly what we find.

(g)

$$\langle n|x|n\rangle = 0 = \langle n|p|n\rangle \quad \langle n|x^2|n\rangle = \frac{\hbar}{2M\omega}(2n+1) \quad \langle n|p^2|n\rangle = \frac{M\omega\hbar}{2}(2n+1) \quad \rightarrow \quad \Delta x \Delta p = \frac{\hbar}{2}(2n+1) \geq \frac{\hbar}{2}$$

4.4 Problem 17

(a) Evaluate the following for some operator Ω .

$$\frac{d}{dt} \langle \Omega \rangle$$

(Hint: Consider using the time-dependent Schrödinger equation to rewrite terms containing $|\dot{\psi}\rangle$.)

(b) The result above is known as Ehrenfest's theorem. What classical equation does the result remind you of? What does the relationship suggest is a classical quantity analogous to the commutators used in quantum theory? Discuss.

(c) Prove the following relationship where X and P denote a coordinate and conjugate momentum (both expectation values are time dependent):

$$m \frac{d\langle X \rangle}{dt} = \langle P \rangle$$

Solution

(a)

$$\frac{d}{dt} \langle \Omega \rangle = \frac{d}{dt} \langle \psi | \Omega | \psi \rangle = \langle \dot{\psi} | \Omega | \psi \rangle + \left\langle \psi \left| \frac{\partial \Omega}{\partial t} \right| \psi \right\rangle + \langle \psi | \Omega | \dot{\psi} \rangle$$

The time-dependent Schrödinger equation can be written:

$$i\hbar \frac{d}{dt} |\psi\rangle = i\hbar |\dot{\psi}\rangle = H |\psi\rangle \quad \rightarrow \quad |\dot{\psi}\rangle = -\frac{i}{\hbar} H |\psi\rangle \quad , \quad \langle \dot{\psi} | = \frac{i}{\hbar} \langle \psi | H$$

Plugging these results into the first relationship for $d_t \langle \Omega \rangle$, we obtain:

$$\frac{d}{dt} \langle \Omega \rangle = \frac{i}{\hbar} \langle \psi | H \Omega | \psi \rangle + \left\langle \psi \left| \frac{\partial \Omega}{\partial t} \right| \psi \right\rangle - \frac{i}{\hbar} \langle \psi | \Omega H | \psi \rangle = \frac{i}{\hbar} \langle \psi | [H, \Omega] | \psi \rangle + \left\langle \psi \left| \frac{\partial \Omega}{\partial t} \right| \psi \right\rangle = \frac{1}{i\hbar} \langle [\Omega, H] \rangle + \langle \partial_t \Omega \rangle$$

If Ω has no explicit time dependence, this reduces to

$$\frac{d\langle \Omega \rangle}{dt} = \frac{1}{i\hbar} \langle [\Omega, H] \rangle$$

(b) This result looks an awful lot like the following result from classical mechanics, describing the time evolution of some phase-space parameter ω , where the curly braces denote Poisson brackets:

$$\frac{d\omega}{dt} = \{\omega, H\} + \frac{\partial \omega}{\partial t} \quad \text{If } \omega \neq \omega(t) \quad \rightarrow \quad \frac{d\omega}{dt} = \{\omega, H\}$$

It would then be reasonable to suppose that the commutator in the quantum mechanical equation behaves very much like the Poisson Bracket in classical mechanics. One can show that this is true and applies quite generally (although we do not have the time to do so here): for an equation with a Poisson bracket $\{a, b\}$ in a classical setting, substituting in a commutator $[A, B]/i\hbar$ will give a correct quantum-mechanical statement. For instance, in classical mechanics for a conjugate coordinate and momentum x and p , $\{x, p\} = 1$ becomes $[\hat{x}, \hat{p}]/i\hbar = 1 \rightarrow [\hat{x}, \hat{p}] = i\hbar$ in the quantum case, where \hat{x} and \hat{p} now denote operators.

(c)

$$\frac{d\langle X \rangle}{dt} = \frac{1}{i\hbar} \langle [X, H] \rangle = \frac{1}{i\hbar} \langle [X, P^2/2m + V(x)] \rangle = \frac{1}{2mi\hbar} \langle 2i\hbar P \rangle = \frac{\langle P \rangle}{m}$$

5

5.1 Problem 18

Consider a particle subject to the potential

$$V(x) = \begin{cases} -V_0\delta(x-a) & x > 0 \\ \infty & x \leq 0 \end{cases}$$

where $V_0 > 0$ and $a > 0$. Does a bound state exist for this system?

Solution

We note that $\psi = 0$ for all $x \leq 0$, and that the solutions to the Schrödinger equation are exponential for a bound state ($E < 0$). We define ψ_1 over $x \in [0, a]$ and ψ_2 over $x \in [a, \infty)$. Since we would like a function that decays as $x \rightarrow \infty$ and which is zero at $x = 0$ we propose the following:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V_0 \delta(x-a) \psi(x) = -|E| \psi(x) \quad \rightarrow \quad k^2 = \frac{2m|E|}{\hbar^2} \quad \rightarrow \quad \psi_1 = A \sinh(kx) \quad \text{and} \quad \psi_2 = B e^{-kx}$$

The boundary conditions are obtained the same way as in workshop problem 4.1, and are:

$$\begin{aligned} \psi_1(a) - \psi_2(a) &= 0 & \psi_1'(a) - \psi_2'(a) &= -\frac{2mV_0\psi(a)}{\hbar^2} \\ A \sinh(ka) - B e^{-ka} &= 0 & -k B e^{-ka} - A k \cosh(ka) &= -\frac{2mV_0 B e^{-ka}}{\hbar^2} \end{aligned}$$

This system can be expressed as:

$$\begin{pmatrix} \sinh(ka) & -e^{-ka} \\ k \cosh(ka) & e^{-ka} \left(k - \frac{2mV_0}{\hbar^2}\right) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = 0$$

For a solution to the system of equations to exist, we require that the determinant of the matrix be zero.

$$\begin{vmatrix} \sinh(ka) & -e^{-ka} \\ k \cosh(ka) & e^{-ka} \left(k - \frac{2mV_0}{\hbar^2}\right) \end{vmatrix} = \sinh(ka) e^{-ka} \left(k - \frac{2mV_0}{\hbar^2}\right) + k \cosh(ka) e^{-ka} = 0$$

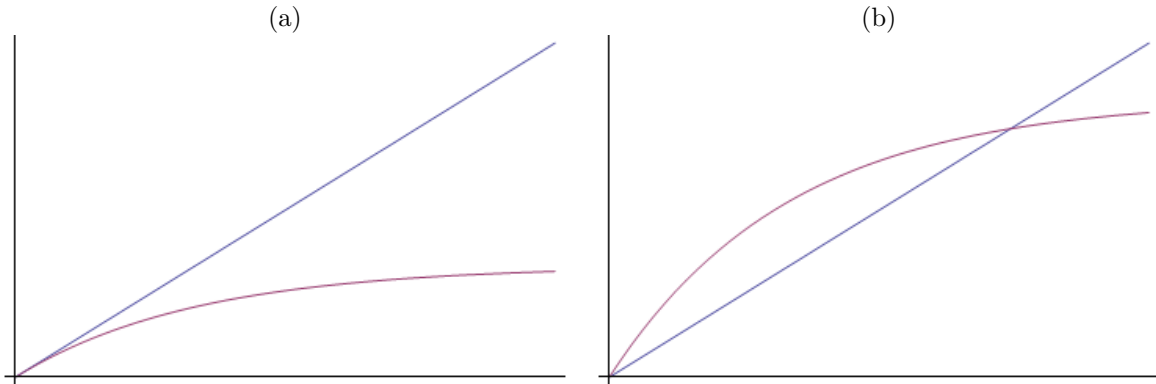
We reduce this equation down:

$$\left(k - \frac{2mV_0}{\hbar^2}\right) \sinh(ka) = -k \cosh(ka) \quad \rightarrow \quad \frac{2mV_0}{\hbar^2} = k(\coth(ka) + 1)$$

And arrive at:

$$\frac{mV_0}{k\hbar^2} = \frac{e^{2ka}}{e^{2ka} - 1} \quad \rightarrow \quad \eta \equiv 2ka \quad \rightarrow \quad \frac{\hbar^2 \eta}{2mV_0 a} = 1 - e^{-\eta}$$

We plot each side of the transcendental equation to see if we have a solution.



In case (a), where the LHS equation passes above the RHS we only have an intersection corresponding to the trivial solution $\eta \propto k \propto |E|^{1/2} = 0$. In case (b) however, we have a nontrivial solution for a bound state energy. We quantify this; for a bound state to exist we must have:

$$\left. \frac{d}{d\eta} (1 - e^{-\eta}) \right|_{\eta=0} = 1 > \frac{\hbar^2}{2mV_0 a} \quad \rightarrow \quad \text{Bound State when: } V_0 > \frac{\hbar^2}{2ma}$$

5.2 Problem 19

Two potentials are shown below, where $V_0 > 0$, $V_2 > V_1 > 0$, and $a > 0$.

$$V_1(x) = \left\{ \begin{array}{ll} 0 & x < 0 \\ V_1 & 0 < x < a \\ V_2 & x > a \end{array} \right\} \quad V_2(x) = \left\{ \begin{array}{ll} 0 & x < -a \\ -V_0 & -a < x < 0 \\ V_0 & 0 < x < a \\ 0 & x > a \end{array} \right\}$$

(a) Consider a particle incident from the left in system 1, with energy $E > V_2$. Set up, but *do not solve* a system of equations you can use to calculate the transmission and reflection coefficients for this system. Write expressions for the transmission and reflection coefficients in terms of wave amplitudes.

(b) What are the transmission and reflection coefficients in system 1 if the particle is incident with an energy $E < V_2$?

(c) Repeat part (a) in system 2 for a particle incident from the left with energy $E > V_0$.

(d) What if the particle in part (c) had an energy $0 < E < V_0$?

Solution

(a) Number the regions in system 1 as 1-3, from left to right. Then make the following assignments for wave functions, which are solutions to the Schrödinger equation in each region.

$$\begin{aligned} \psi_1(x) &= e^{ik_1x} + Be^{-ik_1x} & \psi_2(x) &= Ce^{ik_2x} + De^{-ik_2x} & \psi_3(x) &= Fe^{ik_3x} \\ k_1 &\equiv \sqrt{\frac{2mE}{\hbar^2}} & k_2 &\equiv \sqrt{\frac{2m(E - V_1)}{\hbar^2}} & k_3 &\equiv \sqrt{\frac{2m(E - V_2)}{\hbar^2}} \end{aligned}$$

We must have the wavefunction and its derivative continuous across each boundary. This results in the following equations:

$$\begin{aligned} \psi_1(0) = \psi_2(0) &\rightarrow 1 + B = C + D \\ \psi_1'(0) = \psi_2'(0) &\rightarrow ik_1(1 - B) = ik_2(C - D) \\ \psi_2(a) = \psi_3(a) &\rightarrow Ce^{ik_2a} + De^{-ik_2a} = Fe^{ik_3a} \\ \psi_2'(a) = \psi_3'(a) &\rightarrow ik_2(Ce^{ik_2a} - De^{-ik_2a}) = ik_3Fe^{ik_3a} \end{aligned}$$

This can be rewritten more nicely as:

$$\begin{pmatrix} -1 & 1 & 1 & 0 \\ k_1 & k_2 & -k_2 & 0 \\ 0 & e^{iak_2} & e^{-iak_2} & -e^{iak_3} \\ 0 & k_2e^{iak_2} & -k_2e^{-iak_2} & -k_3e^{iak_3} \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \end{pmatrix} = \begin{pmatrix} 1 \\ k_1 \\ 0 \\ 0 \end{pmatrix}$$

The reflection coefficient is $R = |B|^2$ and the transmission coefficient is $T = (k_3/k_1)|F|^2$. For those interested, one can solve for the coefficients and obtain:

$$\begin{aligned} B &= \frac{(k_1 - k_2)(k_2 + k_3) + e^{2iak_2}(k_1 + k_2)(k_2 - k_3)}{(k_1 + k_2)(k_2 + k_3) + e^{2iak_2}(k_1 - k_2)(k_2 - k_3)} \\ C &= \frac{2k_1(k_2 + k_3)}{(k_1 + k_2)(k_2 + k_3) + e^{2iak_2}(k_1 - k_2)(k_2 - k_3)} \\ D &= \frac{2k_1e^{2iak_2}(k_2 - k_3)}{(k_1 + k_2)(k_2 + k_3) + e^{2iak_2}(k_1 - k_2)(k_2 - k_3)} \\ F &= -\frac{4k_1k_2e^{ia(k_2 - k_3)}}{-(k_1 + k_2)(k_2 + k_3) + e^{2iak_2}(k_2 - k_1)(k_2 - k_3)} \end{aligned}$$

(b) Since the wave function must now decay in region 3, there is no chance of the particle being transmitted to infinity. Therefore $R = 1$ and $T = 0$.

(c) Number the regions in system 2 as 1-4, from left to right. We then follow the same process as in part (a):

$$\psi_1(x) = e^{ik_1x} + Be^{-ik_1x} \quad \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \quad \psi_3(x) = Fe^{ik_3x} + Ge^{-ik_3x} \quad \psi_4(x) = He^{ik_1x}$$

$$k_1 = k_4 = \sqrt{\frac{2mE}{\hbar^2}} \quad k_2 = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \quad k_3 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

The boundary conditions are applied at $x = 0, \pm a$, to obtain:

$$\begin{pmatrix} e^{iak_1} & -e^{-iak_2} & -e^{iak_2} & 0 & 0 & 0 \\ k_1 e^{iak_1} & k_2 e^{-iak_2} & -k_2 e^{iak_2} & 0 & 0 & 0 \\ 0 & 1 & 1 & -1 & -1 & 0 \\ 0 & k_2 & -k_2 & -k_3 & k_3 & 0 \\ 0 & 0 & 0 & e^{iak_3} & e^{-iak_3} & -e^{iak_1} \\ 0 & 0 & 0 & k_3 e^{iak_3} & -k_3 e^{-iak_3} & -k_1 e^{iak_1} \end{pmatrix} \begin{pmatrix} B \\ C \\ D \\ F \\ G \\ H \end{pmatrix} = \begin{pmatrix} -e^{-ik_1 a} \\ k_1 e^{-ik_1 a} \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

The reflection coefficient is given by $R = |B|^2$ and the transmission coefficient is given by $T = |H|^2$.

(d) This change in the energy of the incident particle only affects region 3. We may replace the ψ_3 in part (c) with

$$\psi_3(x) = F e^{-k_3 x} + G e^{k_3 x}$$

and then proceed in the same fashion. This does not imply that $T \rightarrow 0$ as in part (b) however, since region 3 does not extend to infinity. There is a nonzero chance that the particle will tunnel through the classically forbidden region and continue onto region 4.

5.3 Problem 20

Consider the 3-dimensional anisotropic oscillator described by the Hamiltonian:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2} m \omega^2 (x^2 + 4y^2 + 9z^2)$$

(a) Write down a general expression for the energy eigenvalues, and list the first eight energies. What is the degeneracy of each of these states?

(b) Write out the wavefunctions corresponding to the first three energies.

Solution

(a) Consider $\frac{1}{2} m \omega^2 (x^2 + 4y^2 + 9z^2) = \frac{m}{2} (\omega^2 x^2 + (2\omega)^2 y^2 + (3\omega)^2 z^2)$. Then:

$$E = \hbar \omega \left(n_x + 2n_y + 3n_z + \frac{1}{2} + 2\frac{1}{2} + 3\frac{1}{2} \right) = \hbar \omega (n_x + 2n_y + 3n_z + 3)$$

Energy	(n_x, n_y, n_z)	No. of combinations
$3\hbar\omega$	all 0	1
$4\hbar\omega$	(1,0,0)	1
$5\hbar\omega$	(2,0,0), (0,1,0)	2
$6\hbar\omega$	(3,0,0), (1,1,0), (0,0,1)	3
$7\hbar\omega$	(4,0,0), (0,2,0), (2,1,0), (1,0,1)	4
$8\hbar\omega$	(5,0,0), (3,1,0), (1,2,0), (2,0,1), (0,1,1)	5
$9\hbar\omega$	(6,0,0), (4,1,0), (2,2,0), (0,3,0), (1,1,1), (0,0,2), (3,0,1)	7
$10\hbar\omega$	(7,0,0), (5,1,0), (3,2,0), (1,3,0), (2,1,1), (1,0,2), (4,0,1), (0,2,1)	8

(b) We use the convention from Liboff (table 7.1), where $\xi_i^2 \equiv \frac{m\omega_i}{\hbar^2} x_i^2$, and $A_n = (2^n n! \sqrt{\pi})^{-\frac{1}{2}}$. For the case above, we may take $\xi_x^2 = m\omega x^2/\hbar^2$, $\xi_y^2 = 2m\omega y^2/\hbar^2$, and $\xi_z^2 = 3m\omega z^2/\hbar^2$. Then:

$$\begin{aligned} E_{000} = 3\hbar\omega &\quad \rightarrow \quad \psi(\xi_x, \xi_y, \xi_z) = A_0^3 e^{-(\xi_x^2 + \xi_y^2 + \xi_z^2)/2} \\ E_{100} = 4\hbar\omega &\quad \rightarrow \quad \psi(\xi_x, \xi_y, \xi_z) = \left(A_0^2 e^{-(\xi_y^2 + \xi_z^2)/2} \right) \cdot \left(2A_1 \xi_x e^{-\xi_x^2/2} \right) \\ E_{010} = 5\hbar\omega &\quad \rightarrow \quad \psi(\xi_x, \xi_y, \xi_z) = \left(A_0^2 e^{-(\xi_x^2 + \xi_z^2)/2} \right) \cdot \left(2A_1 \xi_y e^{-\xi_y^2/2} \right) \\ E_{200} = 5\hbar\omega &\quad \rightarrow \quad \psi(\xi_x, \xi_y, \xi_z) = \left(A_0^2 e^{-(\xi_y^2 + \xi_z^2)/2} \right) \cdot \left(A_2 (4\xi_x^2 - 2) e^{-\xi_x^2/2} \right) \end{aligned}$$

5.4 Problem 21

Consider the matrices

$$\sigma_x = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

- (a) Find a matrix σ_z such that $[\sigma_y, \sigma_z] = i\sigma_x$, and $[\sigma_z, \sigma_x] = i\sigma_y$, and $Tr(\sigma_z) = 0$.
 (b) Compute $[\sigma_x, \sigma_y]$. What does this say about σ_x , σ_y , and σ_z ?
 (c) Compute $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$. What are the eigenvalues of σ^2 ?
 (d) Determine the kets $|\pm \frac{1}{2}\rangle$, which are the eigen-kets of σ_z corresponding the eigenvalues $\pm \frac{1}{2}$. Define $\sigma_{\pm} = \sigma_x \pm i\sigma_y$, and compute $\sigma_{\pm}|\pm \frac{1}{2}\rangle$. What do you notice?

Solution

- (a) Set up a suitable system of equations, guess and check, or know the answer by some other means to obtain:

$$\sigma_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

(b) You will notice that for this choice of σ_z we have $[\sigma_x, \sigma_y] = i\sigma_z$, which means σ_x , σ_y , and σ_z are closed under commutation.

(c)

$$\sigma^2 = \frac{1}{4} \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right] = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}$$

The eigenvalue is $\frac{3}{4}$ with degeneracy 2.

(d) The eigenvectors of σ_z are given by (this is trivial since σ_z is diagonal):

$$|+1/2\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |-1/2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\sigma_+ = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \sigma_- = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{i}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

With these definitions, we can see the following:

$$\sigma_+ \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \quad , \quad \sigma_- \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad , \quad \sigma_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad , \quad \sigma_- \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

We conclude that σ_{\pm} are raising and lowering operators, moving us on a ladder with only two states (raising above $|\frac{1}{2}\rangle$ and lowering below $|\frac{-1}{2}\rangle$ both give zero.)

6

6.1 Problem 22

The following are theorems that have been useful throughout the course, and will continue to prove useful as the semester progresses. Prove (a)-(e), then discuss (f). Then try to make connections between these and problems 6.2-6.3.

- (a) A Hermitian operator has real eigenvalues.
- (b) Eigenvectors of a Hermitian operator with distinct eigenvalues are orthogonal.
- (c) The operator which transforms an orthonormal set of basis vectors into another is unitary.
- (d) If A is a Hermitian matrix, then there exists a unitary matrix U such that $U^\dagger A U$ is diagonal.
- (e) If Ω and Λ are two commuting Hermitian matrices/operators with non-degenerate eigenvalues, then the eigenstates of Ω are also eigenstates of the Λ .
- (f) Extend part (e) to account for the possibility of degeneracies. Discuss how one might prove that for any commuting and Hermitian Ω and Λ there exists some set of shared eigenstates. (This is provable, but this question is asking for an informal discussion rather than a formal proof, due to time constraints.)

Solution

(a) Let A be a Hermitian operator, such that $A = A^\dagger$. Let $|a\rangle$ be an eigenvector/eigenstate of A with eigenvalue a . Then:

$$A|a\rangle = a|a\rangle \rightarrow \langle a|A|a\rangle = a\langle a|a\rangle \quad \text{and} \quad \langle a|A^\dagger = \langle a|A = a^*\langle a| \rightarrow \langle a|A|a\rangle = a^*\langle a|a\rangle$$

By subtracting the results of each expression we obtain $(a - a^*)\langle a|a\rangle = 0$. Since the inner product of a vector with itself is positive semi-definite (i.e. $\langle a|a\rangle \geq 0$), for the relationship to hold for any $|a\rangle$ and a , we must have $a = a^*$, meaning that a is real.

(b) Let A be a hermitian operator and $|a_1\rangle$ and $|a_2\rangle$ be eigenstates of A with eigenvalues a_1 and a_2 , respectively. Since the eigenvalues are distinct, we require $a_1 \neq a_2$. Then we may do the following:

$$A|a_1\rangle = a_1|a_1\rangle \rightarrow \langle a_2|A|a_1\rangle = a_1\langle a_2|a_1\rangle \quad \text{and} \quad A|a_2\rangle = a_2|a_2\rangle \rightarrow \langle a_2|A = a_2\langle a_2| \rightarrow \langle a_2|A|a_1\rangle = a_2\langle a_2|a_1\rangle$$

We again take the difference of the results, to obtain the equation $(a_1 - a_2)\langle a_2|a_1\rangle = 0$. Since $a_1 \neq a_2$ by assumption, we must have $\langle a_2|a_1\rangle = 0$.

(c) We define a set of orthonormal basis vectors $|e_i\rangle$, and let U be the operator which takes it to another set of orthonormal basis vectors $|a_i\rangle$. Then:

$$|a_i\rangle = U|e_i\rangle \rightarrow \langle a_j| = \langle e_j|U^\dagger \rightarrow \langle a_j|a_i\rangle = \langle e_j|U^\dagger U|e_i\rangle$$

Since both sets of vectors are orthonormal we have $\langle a_j|a_i\rangle = \delta_{ij} = \langle e_j|e_i\rangle$. Then the above is true when $U^\dagger U = \mathbb{I}$, or U is unitary.

(d) Let $|e_i\rangle$ be the standard orthonormal basis, and $|a_i\rangle$ be an orthonormal eigenbasis of the operator A . U is the matrix that transforms the standard basis to the eigenbasis. Then:

$$\begin{aligned} |a_i\rangle = U|e_i\rangle \text{ and } A|a_i\rangle = a_i|a_i\rangle &\rightarrow \langle a_j|A|a_i\rangle = a_i\langle a_j|a_i\rangle = a_i\delta_{ij} \\ &= \langle e_j|U^\dagger A U|e_i\rangle = a_i\delta_{ij} \end{aligned}$$

This shows that $U^\dagger A U$ is diagonal, with the eigenvalues of A as the matrix elements down the diagonal. Then U diagonalizes A .

(e) Let Ω and Λ be commuting operators ($[\Omega, \Lambda] = 0$), and $|\omega_i\rangle$ represent the complete set of eigenstates of Ω corresponding to eigenvalues ω_i . We further assume that neither Ω nor Λ have degenerate eigenvalues. Since $[\Omega, \Lambda] = 0$, we may write $(\Omega\Lambda - \Lambda\Omega)|\omega_i\rangle = 0$. From here we do the following:

$$\Omega\Lambda|\omega_i\rangle = \Lambda\Omega|\omega_i\rangle = \omega_i(\Lambda|\omega_i\rangle)$$

Since $\Omega(\Lambda|\omega_i\rangle) = \omega_i(\Lambda|\omega_i\rangle)$ we see that $\Lambda|\omega_i\rangle$ is also an eigenvector of Ω with eigenvalue ω_i . This is only possible if $\Lambda|\omega_i\rangle = \lambda_i|\omega_i\rangle$. This means that all eigenstates of Ω are also eigenstates of Λ , and that the same matrix which diagonalizes Ω would diagonalize Λ .

(f) We now consider the possibility of degeneracy in the eigenvalues ω_i . Let $|\omega_i, j\rangle$ be an N_i -fold degenerate eigenstate of Ω , where $j = 1, 2, \dots, N_i$, such that $\Omega|\omega_i, j\rangle = \omega_i|\omega_i, j\rangle$. Note that for a non-degenerate state we simply have $N_i = 1$ for that particular i . For the sake of formality, we state that Ω is a linear operator over an N -dimensional vector space \mathbb{V} .

There are a few results and observations we need to motivate this discussion. (1) A linear operator on \mathbb{V} is diagonalizable iff \mathbb{V} can be written as the direct sum of the eigenspaces of the operator, (2) all Hermitian operators are diagonalizable, as shown above, and (3) an operator which is Hermitian on \mathbb{V} will also be Hermitian within each subspace \mathbb{W}_i . This means that each eigenspace of Ω \mathbb{W}_i (necessarily a subspace of \mathbb{V}) has dimensionality N_i such that $\sum_i N_i = N$, or that all of the states $|\omega_i, j\rangle$ are orthogonal and span \mathbb{V} . To summarize, we are saying that:

$$\langle \omega_i, k | \omega_i, j \rangle = \delta_{jk} \quad \forall i \quad \text{and} \quad \mathbb{W}_1 \oplus \mathbb{W}_2 \oplus \dots \oplus \mathbb{W}_{i_{max}} = \mathbb{V} \quad \text{or} \quad \mathbb{W}_i \cap \sum_{i \neq j} \mathbb{W}_j = \{0\} \quad \forall j$$

We have already shown that $\langle \omega_k, j | \omega_i, j \rangle = \delta_{ik} \quad \forall j$ in part (b). The result we are interested in follows reasonably well once we have digested the above. We proceed by noting something we used in workshop 1. Consider a linear combination of $|\omega_i, j\rangle$ for fixed i :

$$\Omega \left(\sum_j^N \alpha_j |\omega_i, j\rangle \right) = \sum_j^N \alpha_j \Omega |\omega_i, j\rangle = \sum_j^N \omega_i \alpha_j |\omega_i, j\rangle = \omega_i \left(\sum_j^N \alpha_j |\omega_i, j\rangle \right)$$

It is therefore obvious that a superposition of degenerate eigenstates of Ω is still an eigenstate of Ω . Then we can say the following as we did in part (e):

$$[\Omega, \Lambda] = 0 \quad \rightarrow \quad \Omega \left(\Lambda \sum_j^N \alpha_j |\omega_i, j\rangle \right) = \Lambda \Omega \left(\sum_j^N \alpha_j |\omega_i, j\rangle \right) = \omega_i \left(\Lambda \sum_j^N \alpha_j |\omega_i, j\rangle \right)$$

This reduces the question down somewhat. Can we find sets of coefficients α_j such that we construct a linear combination of $|\omega_i, j\rangle$ within each subspace \mathbb{W}_i which create N_i eigenvectors of Λ ? Part (d) tells us yes, because if Λ is Hermitian in \mathbb{V} it must also be Hermitian within each subspace \mathbb{W}_i . Therefore we conclude that we have the freedom to perform a change of basis that diagonalizes Λ in each subspace, which solves our problem.

Note that parts (e) and (f) show that given two commuting Hermitian operators, each eigenbasis of Ω is also an eigenbasis of Λ iff the eigenvalues of the operators are non-degenerate. If there are degeneracies however, we will be able to find a common set of eigenvectors, but not every eigenbasis of one operator will also be an eigenbasis of the other. Those wishing to see the same thought process explained differently may wish to read

http://ocw.mit.edu/courses/physics/8-04-quantum-physics-i-spring-2013/study-materials/MIT8_04S13_OnCommEigenbas.pdf

which was referenced in creating this solution.

This problem can also be understood by looking at the matrix representations of the operators Ω and Λ directly. Clearly Ω is diagonal in its own eigenbasis, and Λ , which commutes with Ω , must then be block diagonal in an eigenbasis of Ω .

$$\Omega = \begin{pmatrix} \omega_1 & 0 & 0 \\ 0 & \omega_1 & 0 \\ 0 & 0 & \omega_2 \end{pmatrix} \quad \rightarrow \quad \Lambda = \begin{pmatrix} \boxed{?} & \boxed{?} & 0 \\ \boxed{?} & \boxed{?} & 0 \\ 0 & 0 & \boxed{\lambda_2} \end{pmatrix}$$

Since ω_1 has multiplicity 2 in the example above, the corresponding eigenspace is not necessarily already diagonalized, but can be in order to obtain a common basis. Since ω_2 is non-degenerate, this portion of Λ is already diagonal and will already share an eigenvector. A further example of how this works can be found in problem 6.3.

One final point to ensure that the utility of this result is clear. In homework problem 4.2 you were given a 2D SHO, and states $|0, 0\rangle$ with $E = \hbar\omega$, $|1, 0\rangle$ and $|0, 1\rangle$ with $E = 2\hbar\omega$, where these are indexed according to $|n_x, n_y\rangle$. These are states written in the energy eigenbasis (eigenbasis of H), and you were given two operators A and B which you had shown were Hermitian and commuted with H . You were asked to find an eigenbasis common to H and A , and one common to H and B . You were lucky with A , because the eigenstates of H were already eigenstates of A . For B however, you found that $|0, 0\rangle$ was an eigenstate of B (which it had to be, since the energy eigenvalue $\hbar\omega$ was non-degenerate), but then for B , you had to take a linear combination of the two states in the $2\hbar\omega$ -subspace in order to diagonalize B .

6.2 Problem 23

Consider a Hamiltonian given by the 3×3 matrix

$$H = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 0 & 5 \\ 0 & 5 & 0 \end{pmatrix}$$

- (a) Determine the Energy Eigenvalues.
 (b) Does H form a CSCO?

Solution

(a)

$$\det \begin{pmatrix} 3-\lambda & 0 & 0 \\ 0 & -\lambda & 5 \\ 0 & 5 & -\lambda \end{pmatrix} = 0 \quad \rightarrow \quad \lambda = 3, 5, -5$$

(b) Since the eigenvalues are non-degenerate, H completely describes the system and is a CSCO.

6.3 Problem 24

Consider a system with Hamiltonian H and operator A given by:

$$H = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad A = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 2 & 0 \end{pmatrix}$$

- (a) Do H and A commute? If yes, give a basis of eigenvectors common to H and A .
 (b) Which among the set of operators H , A , $\{H, A\}$, and $\{H^2, A\}$ form a CSCO?

Solution

(a) We find that $[H, A] = 0$. H has eigenvalues $-2, 1$, and 1 and eigenvectors:

$$|-2\rangle_H = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |1\rangle_{Ha} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |1\rangle_{Hb} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

A has eigenvalues $-2, 2, 5$, with eigenvectors:

$$|-2\rangle_A = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \quad |2\rangle_A = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \quad |5\rangle_A = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

We look for a set of eigenvectors common to both operators. We do this in the same way as in workshop 1, noting that any linear combination of $|1\rangle_{Ha}$ and $|1\rangle_{Hb}$ will still be an eigenvector of H with eigenvalue 1.

$$|-2\rangle_A = \frac{1}{\sqrt{2}}|1\rangle_{Ha} - \frac{1}{\sqrt{2}}|1\rangle_{Hb} \quad |2\rangle_A = \frac{1}{\sqrt{2}}|1\rangle_{Ha} + \frac{1}{\sqrt{2}}|1\rangle_{Hb}$$

We therefore reindex our vectors according to $|\lambda_H, \lambda_A\rangle$, and propose the following for the shared set:

$$|1, -2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \quad |1, 2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \quad |-2, 5\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

(b) H cannot be a CSCO on its own because it is degenerate. A is however a CSCO since its eigenvalues are non-degenerate, and since $[H, A] = 0 = [H^2, A]$ these are also complete sets of commuting operators.

6.4 Problem 25

Consider a particle subject to the Hamiltonian below, where ϵ is a constant.

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega^2x^2 - \epsilon x + V(y) \quad V(y) = \begin{cases} 0 & y \in [-L/2, L/2] \\ \infty & \text{else} \end{cases}$$

Determine the energy spectrum, wavefunctions, and comment on parity and possibility of degenerate states.

Hint: Consider an SHO with a linear transformation in x , namely $x \rightarrow x - x_0$.

Solution

Consider an SHO with $x \rightarrow x - x_0$

$$H_x = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2(x - x_0)^2 = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2(x^2 - 2xx_0 + x_0^2)$$

We match this up with the given Hamiltonian, and conclude that $\epsilon = m\omega^2 x_0$. Then:

$$H = \frac{p_x^2 + p_y^2}{2m} + \frac{1}{2}m\omega^2 \left(x - \frac{\epsilon}{m\omega^2}\right)^2 - \frac{1}{2}m\omega^2 \left(\frac{\epsilon}{m\omega^2}\right)^2 + V(y)$$

Since $\epsilon^2/2m\omega^2$ is a constant, this simply shifts the whole spectrum, but does not otherwise affect the problem. We can then write the spectrum, where $n_x = 0, 1, 2, \dots$ and $n_y = 1, 2, 3, \dots$

$$E = \hbar\omega \left(n_x + \frac{1}{2}\right) + \frac{n_y^2 \pi^2 \hbar^2}{2mL^2} - \frac{\epsilon^2}{2m\omega^2}$$

We can then also write the wavefunctions, where ξ follows the conventions in Liboff, and A_n is the SHO normalization from Liboff table 7.1. \mathcal{H} denotes a Hermite polynomial.

$$\text{Let } \xi_x^2 = \frac{m\omega}{\hbar} \left(x - \frac{\epsilon}{m\omega^2}\right)^2 \quad \rightarrow \quad \psi(x, y) = \sqrt{\frac{2}{L}} A_{n_x} e^{\xi_x^2/2} \mathcal{H}_{n_x}(\xi_x) \begin{cases} \cos\left(\frac{n_y \pi y}{L}\right) & n_y \text{ odd} \\ \sin\left(\frac{n_y \pi y}{L}\right) & n_y \text{ even} \end{cases}$$

The parity is determined by $(-1)^{n_x}(-1)^{n_y+1} = (-1)^{n_x+n_y+1}$.

For an arbitrary choice of m , ω and ϵ , the spectra in x and y will not necessarily line up and create degeneracies. They could however be tuned in such a way that particular states in each dimension end up combining to create degeneracies.

6.5 Problem 26

In cartesian coordinates, the parity operator transforms $x \rightarrow -x$, $y \rightarrow -y$, and $z \rightarrow -z$.

- (a) What does a parity transformation do in polar and spherical coordinates?
- (b) Find an H in spherical coordinates where $[H, \pi] = 0$.

Solution

(a) Parity works differently in an even number and odd number of dimensions. For polar coordinates, we let $\varphi \rightarrow -\varphi$, which mirrors the functions across the x -axis. (A mirroring through the origin in an even-numbered coordinate system would be equivalent to a single rotation, which is not useful).

For spherical coordinates we may mirror through the origin. This could naively be achieved by letting $r \rightarrow -r$, but r cannot be negative. We can however achieve the same result by letting $\theta \rightarrow \pi - \theta$ and $\varphi \rightarrow \pi + \varphi$.

- (b) Consider the following:

$$H = \frac{1}{2m} \left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\varphi^2}{r^2 \sin^2 \theta} \right) + V(r)$$

Since $\dot{\mathbf{r}}^2 = (-\dot{\mathbf{r}})^2$ nothing happens to the kinetic energy under parity transformation. We leave $V(r)$ only as a function of r however, because r is the only coordinate that is unaffected under parity transformation.

7

7.1 Problem 27

Consider an SHO where $\langle H \rangle = n\hbar\omega$ and $n \geq 2$, in the state

$$|\psi\rangle = A|n\rangle + B|n-2\rangle$$

- (a) Determine A and B .
- (b) Determine ΔH .
- (c) Show $\Delta x \Delta p \geq \hbar/2$ for all time t . (Hint: use parity arguments.)

Solution

- (a) We use the fact that $|A|^2 + |B|^2 = 1$.

$$\langle H \rangle = |A|^2 \hbar\omega \left(n + \frac{1}{2} \right) + |B|^2 \hbar\omega \left(n - 2 + \frac{1}{2} \right) = \hbar\omega \left(n + \frac{1}{2} - 2|B|^2 \right) = \hbar\omega n$$

We then solve to obtain $|B|^2 = \frac{1}{4}$ and $|A|^2 = \frac{3}{4}$. Therefore:

$$|\psi\rangle = \frac{\sqrt{3}}{2}|n\rangle + \frac{1}{2}|n-2\rangle$$

- (b)

$$\langle H^2 \rangle = \frac{3}{4} \left[\hbar\omega \left(n + \frac{1}{2} \right) \right]^2 + \frac{1}{4} \left[\hbar\omega \left(n - \frac{3}{2} \right) \right]^2 = (\hbar\omega)^2 \left[\frac{3}{4} \left(n^2 + n + \frac{1}{4} \right) + \frac{1}{4} \left(n^2 - 3n + \frac{9}{4} \right) \right] = (\hbar\omega)^2 \left[n^2 + \frac{3}{4} \right]$$

We already know $\langle H \rangle^2$ from the problem statement, so

$$\Delta H = \left(\langle H^2 \rangle - \langle H \rangle^2 \right)^{\frac{1}{2}} = \frac{\sqrt{3}}{2} \hbar\omega$$

(c) Notice that $|\psi\rangle$ has either odd or even parity. In a coordinate basis, it is evident that \hat{x} and \hat{p} both have odd parity (x has odd parity, and taking the derivative of an odd or even function results in one of the opposite parity). Let $|\Psi\rangle = U|\psi\rangle$ be the time dependent version of $|\psi\rangle$ where U is the time evolution operator. Then by parity arguments, the following is evident because the overall expressions in these integrands are odd upon expansion over a coordinate.

$$\langle x \rangle_t = \langle \Psi | x | \Psi \rangle = 0 \quad \langle p \rangle_t = \langle \Psi | p | \Psi \rangle = 0$$

Next we consider $\langle x^2 \rangle_t$. Note that the commutator $[a, a^\dagger] = 1$ implies $aa^\dagger + a^\dagger a = 2aa^\dagger - 1$.

$$\begin{aligned} \langle x^2 \rangle_t &= \frac{\hbar}{2m\omega} \langle \Psi | a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a | \Psi \rangle = \frac{\hbar}{2m\omega} \langle \Psi | [a^2 + a^{\dagger 2} + 2aa^\dagger - 1] \left(\frac{\sqrt{3}}{2} e^{-iE_n t/\hbar} |n\rangle + \frac{1}{2} e^{-iE_{n-2} t/\hbar} |n-2\rangle \right) \\ &= \frac{\hbar}{2m\omega} \langle \Psi | \left[\frac{\sqrt{3}}{2} e^{-i\omega(n+1/2)t} \left(\sqrt{n(n-1)} |n-2\rangle + (2n+1) |n\rangle \right) + \frac{1}{2} e^{-i\omega(n-3/2)t} \left(\sqrt{n(n-1)} |n\rangle + (2n-3) |n-2\rangle \right) \right] \\ &= \frac{\hbar}{2m\omega} \left[\frac{\sqrt{3}}{2} e^{-i\omega(n+1/2)t} \left(\frac{\sqrt{n(n-1)}}{2} e^{i\omega(n-3/2)t} + (2n+1) \frac{\sqrt{3}}{2} e^{i\omega(n+1/2)t} \right) + \dots \right. \\ &\quad \left. \dots + \frac{1}{2} e^{-i\omega(n-3/2)t} \left(\sqrt{n(n-1)} \frac{\sqrt{3}}{2} e^{i\omega(n+1/2)t} + \frac{2n-3}{2} e^{i\omega(n-3/2)t} \right) \right] \\ &= \frac{\hbar}{2m\omega} \left[\frac{\sqrt{3}}{4} \sqrt{n(n-1)} (e^{2i\omega t} + e^{-2i\omega t}) + \frac{3}{4}(2n+1) + \frac{1}{4}(2n-3) \right] = \frac{\hbar}{2m\omega} \left[\frac{\sqrt{3n(n-1)}}{2} \cos(2\omega t) + 2n \right] = \Delta x^2 \end{aligned}$$

We perform a similar calculation to obtain $\langle p^2 \rangle_t$. We shorten it greatly by noticing some similarities with the above.

$$x^2 = \frac{\hbar}{2m\omega} (a^2 + a^{\dagger 2} + a^\dagger a + aa^\dagger) = \frac{\hbar}{2m\omega} (a^2 + a^{\dagger 2} + 2aa^\dagger - 1) \quad \rightarrow \quad p^2 = \frac{m\omega\hbar}{2} (2a^\dagger a - 1 - a^2 - a^{\dagger 2})$$

We see that we can simply change the sign on the last two terms and the calculation is otherwise identical. Therefore:

$$\Delta p^2 = \frac{m\omega\hbar}{2} \left[\frac{-\sqrt{3n(n-1)}}{2} \cos(2\omega t) + 2n \right]$$

We may now verify against the uncertainty principle (recall that $n \geq 2$):

$$\Delta x \Delta p = \frac{\hbar}{2} \left[4n^2 - \frac{3n(n-1)}{4} \cos^2(2\omega t) \right]^{\frac{1}{2}} \geq \frac{\hbar}{2} \sqrt{4n^2 - \frac{3n(n-1)}{4}} > \frac{\hbar}{2}$$

7.2 Problem 28

Consider a particle subject to the potential

$$V(x) = \begin{cases} -V & |x| < a \\ 0 & \text{else} \end{cases}$$

with $V > 0$. Look for an even-parity state with vanishingly small (or zero) energy.

- Determine the wavefunctions in each region.
- Apply boundary conditions to find a condition on V and a . What values of V are possible?
- Show that the result from part (b) agrees with the result derived in class for bound states of even parity in the finite well, namely:

$$\xi^2 + \eta^2 = \frac{2mVa^2}{\hbar^2} \quad , \quad \eta = \xi \tan \xi \quad (\text{Recall } \xi = ka, \eta = \kappa a)$$

Solution

(a) Let region 1 be for $x < -a$, region 2 for $-a < x < a$, and region 3 for $x > a$. We note that the solutions will be eigenfunctions of the parity operator, since the potential is symmetric.

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_{1,3}}{\partial x^2} = 0 \quad \rightarrow \quad \psi_1(x) = Ax + B \quad \xrightarrow{EV \rightarrow EN} \quad \psi_3(x) = -Ax + B$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_2}{\partial x^2} - V\psi_2(x) = 0 \quad \rightarrow \quad \psi_2(x) = C \cos(kx) + D \sin(kx) \quad \text{for } k = \frac{\sqrt{2mV}}{\hbar}$$

We note that except for $A = B = 0$ this state will not be normalizable, but since it is on the border of not being bound, we accept this. We must however still consider that this is still a well, and that having a divergent probability density at $x \rightarrow \pm\infty$, which dominates over finding the particle near the box does not appear physical. We require that $A = 0$ on these grounds. (Having a constant is also consistent with an approach where we take the limit as $k \rightarrow 0$ from the solutions of the bound case.) We apply the usual continuity conditions to these simplified wave-functions.

$$\psi_1 = \psi_3 = B \quad , \quad \psi_2 = C \cos(kx) \quad \rightarrow \quad B = C \cos(ka) \quad , \quad 0 = kC \sin(ka) \quad \rightarrow \quad \begin{pmatrix} 1 & -\cos(ka) \\ 0 & k \sin(ka) \end{pmatrix} \begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

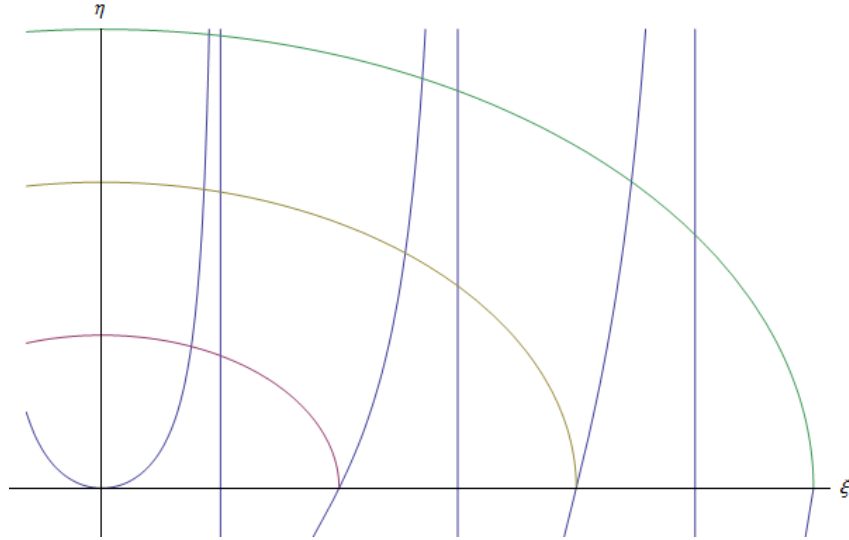
Having $\sin(ka) = 0$ implies:

$$ka = n\pi \quad \rightarrow \quad V = \frac{1}{2m} \left(\frac{n\pi\hbar}{a} \right)^2 \quad \text{for } n = 1, 2, 3, \dots$$

We now compare with the known result for the even-parity bound states of the finite square well. For $E = 0$:

$$\xi^2 = k^2 a^2 = \frac{2mVa^2}{\hbar^2} \quad \eta^2 = \kappa^2 a^2 = 0$$

See the following page for the plot of this result. We see that for $\eta = 0$, we find the solution exactly along the ξ -axis, which fall precisely on the roots of $\tan(\xi)$, which is where $ka = n\pi$. Therefore the result we have obtained above agrees with the previous work we have done on this potential in class.



7.3 Problem 29

Consider a particle subject to the potential

$$V(x) = V_1[\delta(x + b) + \delta(x - b)] + \begin{cases} -V_0 & |x| < a \\ 0 & \text{else} \end{cases}$$

with $b \geq a > 0$, and $V_1, V_0 > 0$. Look for a state with vanishingly small or zero energy.

(a) Determine the wavefunctions in each region.

(b) Apply boundary conditions to derive

$$\cot \zeta = \zeta \left(\frac{b}{a} - 1 - \frac{\hbar^2}{2maV_1} \right) \quad \text{for } \zeta \equiv \frac{a}{\hbar} \sqrt{2mV_0}$$

(c) Comment on the solutions of V_0 for the following cases (look a graphical solutions)

i) $\frac{b}{a} > 1 + \frac{\hbar^2}{2maV_1}$, ii) $\frac{b}{a} < 1 + \frac{\hbar^2}{2maV_1}$, iii) $\frac{b}{a} \gg 1$

Solution

(a) We number the regions in the problem from left to right in increasing order. We note that in the finite square well, only the even state solutions will have the possibility of appearing for any choice of V and a , and that the delta functions added here make it more difficult to create bound states. (Look at the roots in the graphical solution from class; the $E = 0$ condition once again sets us on the ξ axis, but the odd solution with cotangent instead of tangent does not have a root until $\xi = \pi/2$, meaning that the well can be “too shallow” for an odd bound state, even without the delta functions). We will once again work only with the even solutions in solving this problem, since they offer a more general look at the system. Following the same reasoning applied in problem 7.2, we write the following as the wavefunctions in each region:

$$\psi_1(x) = A \quad \psi_2(x) = Bx + C \quad \psi_3(x) = D \cos(kx) \quad \psi_4(x) = -Bx + C \quad \psi_5(x) = A \quad k = \frac{\sqrt{2mV}}{\hbar}$$

(b) We set up the usual boundary conditions for the coefficients. Note that since we have established certain symmetries in the problem that we only need “one side” of the problem, so to speak.

$$\psi_3(a) = \psi_4(a) \quad \rightarrow \quad D \cos(ka) = -Ba + C$$

$$\psi_3'(a) = \psi_4'(a) \quad \rightarrow \quad -Dk \sin(ka) = -B$$

$$\psi_4(b) = \psi_5(b) \quad \rightarrow \quad -Bb + C = A$$

$$\int_{b-\epsilon}^{b+\epsilon} dx \left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V_1\delta(x-b)\psi(x) \right) = 0 \quad \rightarrow \quad 0 + B = \frac{2mV_1A}{\hbar^2}$$

These can be summarized in the following homogeneous system of equations:

$$\begin{pmatrix} \frac{2mV_1}{\hbar^2} & -1 & 0 & 0 \\ 0 & 1 & 0 & -k \sin(ka) \\ 1 & b & -1 & 0 \\ 0 & a & -1 & \cos(ka) \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0$$

As usual, when confronted with this type of homogeneous solution and a question where we do not care to solve for A , B , C , or D , we note that the determinant must be zero for a solution to exist, and examine the conditions under which this is true. This requires:

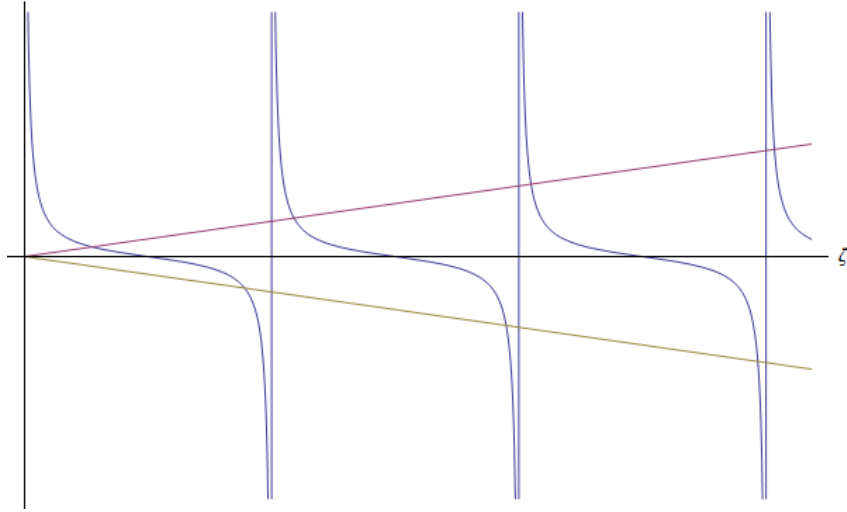
$$\frac{2mV_1}{\hbar^2} [(b-a)k \sin(ka) - \cos(ka)] - k \sin(ka) = 0 \quad \rightarrow \quad \frac{2mV_1}{\hbar^2} [(a-b)k + \cot(ka)] + k = 0$$

$$V_1 = \frac{\hbar^2}{2m} \frac{-k}{\cot(ka) + k(a-b)} \quad \rightarrow \quad \cot(ka) + ka \left(1 - \frac{b}{a}\right) + \frac{\hbar^2 ka}{2maV_1} = \cot(ka) + ka \left(1 - \frac{b}{a} + \frac{\hbar^2}{2maV_1}\right) = 0$$

Which gives us the desired result:

$$\cot(ka) = ka \left(\frac{b}{a} - 1 - \frac{\hbar^2}{2maV_1}\right) \quad \rightarrow \quad \cot \zeta = \zeta \left(\frac{b}{a} - 1 - \frac{\hbar^2}{2maV_1}\right)$$

(c) We may look at cases i) and ii) together:



The upper linear function is for $\frac{b}{a} > 1 + \frac{\hbar^2}{2maV_1}$, and the lower linear function is for $\frac{b}{a} < 1 + \frac{\hbar^2}{2maV_1}$. We see that the solutions for case i) are shifted to the right relative to those for case ii). This makes sense because it means that a deeper well can bind a particle despite the delta functions being closer to the well. For case iii) we observe that:

$$\frac{b}{a} \gg 1 \quad \rightarrow \quad \sin(ka) = 0 \quad \rightarrow \quad ka = n\pi \quad \text{for } n = 1, 2, 3, \dots$$

which is the same as in previous problem, which meets any expectations we might have had. (This is equivalent to saying that for very large slopes in the lines on the graphical solution, we will get intersections very near the asymptotes of $\cot \zeta$.)

8 Review for Midterm

Important Formulas and Results

Five systems / general types of problems you want to be familiar with: (1) Infinite Square Well, (2) Simple Harmonic Oscillator, (3) Delta-Function Potential, (4) Unbound State Barrier Problems (Transmission and Reflection), (5) Finite Square Well.

Important Concepts to Apply in these problems: (1) Calculating and Interpreting Expectation Values, (2) Time Evolution (including time-dependent expectation values), (3) Heisenberg Uncertainty Principle, (4) Generalizations to higher dimensions and degeneracies that may arise, (5) Superpositions of States, Probability, and Probability Amplitudes, (6) Operator Algebras (including matrix manipulation, use/role of Hermitian operators, ladder operators, Commutators, CSCOs, etc.), (7) Appropriate use of graphical solution techniques.

These topics are summarized on the equation sheet that has also been posted. You should know how to use every result on that sheet and qualitatively be able to explain where it comes from. If you are able to actually derive everything on that sheet, then you are in *very* good shape!

Suggestion: Study the homework first and foremost, followed by the workshop problems. Problems labeled “practice problems and other” below are those I find particularly representative of the kinds of topics that might be covered.

Workshop Problems Organized by Type

Math Practice / Notation 1.1, 1.2, 1.3, 2.1, 2.2, 2.3, 3.1, 3.3, 3.4, 6.5

Theoretical Foundations 1.3, 2.4, 3.1, 3.3, 4.4, 6.1, 6.2, 6.3

Practice Problems and Other 1.4, 2.5, 3.2, 3.4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3, 5.4, 6.4, 7.1, 7.2, 7.3

8.1 Short Exercises

1. Plot any of the following functions that you cannot sketch without a reference. Notice their roots, behavior at 0 and $\pm\infty$, parity, and any other salient features.

$\sinh(x)$, $\cosh(x)$, $\tanh(x)$, $e^{-|x|}$, $\Theta(x)$ (Heaviside), $\text{sgn}(x)$, The first 4 states of the SHO.

Understand the derivatives of Θ and sgn in terms of their plots.

2. Define bound and unbound states.
3. Define a CSCO.
4. Write the time evolution operator. Why is it generally necessary to know some state in terms of energy eigenstates to use it?
5. What is the action of the parity operator on a function? Which functions are eigenfunctions of \mathbb{P} and with what eigenvalues? Construct operators which project out the even or odd part of any function.

Solution

1. Make the plots yourself! Mathematica has Hermite polynomials built in if you need it, and the derivatives of interest are proportional to dirac delta functions. The scaling factor on the delta functions is proportional to the size of the discontinuity in the functions.
2. Bound states are those for which the particle is confined to some region of space. Confinement leads to quantized energies, each of which corresponds to a bound state(s). A bound state is normalizable if $E < V$ at $x = \pm\infty$, which means that the particle has no amplitude to tunnel to $\pm\infty$. An unbound state is one for which $V < E$ at $x = \infty$ or $x = -\infty$, where the particle is away from any kind of local minimum / unconfined (which is what you are working with in a barrier/scattering problem). An unbound state cannot exist in a potential which tends towards positive infinity at both edges (in this case all states are bound).
3. CSCO means complete set of commuting operators or complete set of commuting observables. It is a set of operators which are Hermitian, commute with each other, and thereby have shared eigenstates. The set is “complete” if the eigenvalues of all the operators in the set are able to completely distinguish between all of the states. (An operator with degenerate eigenvalues cannot be a CSCO alone – it needs another operator(s) with the same eigenstates but different eigenvalues, such that the set of eigenvalues totally characterizes the state.)

Examples: 2D SHO: H_x and H_y form a CSCO, as do H and either H_x and H_y . None of these alone are able to distinguish between states however.

4. $U = \exp[-iHt/\hbar]$. In order to substitute a number for H , the operator must act on a state corresponding to a single energy, namely an energy eigenstate.
5. $\mathbb{P}f(x) = f(-x)$ in one dimension. Eigenfunctions are either even ($f(x) = f(-x)$; eigenvalue 1), or odd ($f(x) = -f(-x)$; eigenvalue -1). See Liboff, problem 6.18 for the projection problem (p. 180). If you are uncomfortable with the parity operator you are equally encouraged to do problem 6.16, and review workshop problem 6.5 for further details and higher-dimensional cases.

8.2 Problem 30

A particle in one dimension has a first excited state eigenfunction associated with energy eigenvalue E_1 given by

$$\psi_1(x) = x\psi_0(x),$$

where ψ_0 is the ground state wavefunction with energy eigenvalue E_0 . The potential vanishes at $x = 0$.

- (a) Apply the Schrödinger equation to ψ_0 and ψ_1 , and solve for the wavefunction $\psi_0(x)$.
- (b) Determine the potential $V(x)$ in which the particle moves, and a numerical answer for the ratio $\frac{E_1}{E_0}$. What type of system do you infer the above describes?

Solution

Problem from Prof. Das' book.

(a)

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad \rightarrow \quad H\psi_0 = E_0\psi_0 \quad , \quad H\psi_1 = E_1\psi_1 = xE_1\psi_0$$

We expand these out, and reduce the equation containing E_1 :

$$\frac{d^2\psi_0}{dx^2} - \frac{2m}{\hbar^2}(V(x) - E_0)\psi_0 = 0 \tag{8.1}$$

$$\frac{d^2\psi_1}{dx^2} - \frac{2m}{\hbar^2}(V(x) - E_1)\psi_1 = 0 \quad \rightarrow \quad x \frac{d^2\psi_0}{dx^2} + 2 \frac{d\psi_0}{dx} - \frac{2mx}{\hbar^2}(V(x) - E_1)\psi_0 = 0 \tag{8.2}$$

We multiply through (8.1) by x , and then subtract this modified form of (8.1) from (8.2).

$$x \frac{d^2\psi_0}{dx^2} - \frac{2mx}{\hbar^2}(V(x) - E_0)\psi_0 = 0 \quad \rightarrow \quad 2 \frac{d\psi_0}{dx} - \frac{2mx}{\hbar^2}(E_0 - E_1)\psi_0 = 0$$

This is a first order, separable ODE for ψ_0 , which we can proceed to solve.

$$\frac{\partial\psi_0}{\partial x} = \frac{m}{\hbar^2}(E_0 - E_1)x\psi_0 \quad \rightarrow \quad \ln \psi_0 = \frac{m}{\hbar^2}(E_0 - E_1) \frac{x^2}{2} + C \quad \rightarrow \quad \psi_0 = A \exp \left[-\frac{m}{2\hbar^2} x^2 (E_0 - E_1) \right]$$

(b) Next, obtain the equation below by differentiating (8.2), which is of the same form as the original ground state equation (8.1) once the result for the single derivative above is plugged in.

$$\frac{d^2\psi_0}{dx^2} - \frac{m}{\hbar^2}(E_0 - E_1) \left(\psi_0 + x \frac{d\psi_0}{dx} \right) = 0 \quad \rightarrow \quad \frac{d^2\psi_0}{dx^2} - \frac{m}{\hbar^2}(E_0 - E_1)\psi_0 - \frac{m^2}{\hbar^4} x^2 (E_0 - E_1)^2 \psi_0 = 0$$

We infer that

$$V(x) - E_0 = \frac{1}{2} \left(E_0 - E_1 + \frac{m}{\hbar^2} (E_0 - E_1)^2 x^2 \right) \quad \rightarrow \quad V(x) = \frac{3}{2} E_0 - \frac{1}{2} E_1 + \frac{m}{2\hbar^2} (E_0 - E_1)^2 x^2$$

We then apply the boundary condition that $V(0) = 0$, and obtain:

$$\frac{3}{2} E_0 = \frac{1}{2} E_1 \quad \rightarrow \quad \frac{E_1}{E_0} = 3 \quad \rightarrow \quad V(x) \frac{m}{2\hbar^2} (E_0 - 3E_0)^2 x^2 = \frac{2mE_0^2}{\hbar^2} x^2 = \frac{1}{2} m\omega^2 x^2 \quad \text{for suitable } \omega$$

We have a quadratic potential, which is a form of the SHO, and have found that $E_1/E_0 = \frac{3}{2}\hbar\omega/\frac{1}{2}\hbar\omega = 3$. This is self-consistent, and consistent with all previous results derived in this class.

8.3 Problem 31

Consider a particle subject to the following potential, with $V_0, V_1 > 0$.

$$V(x) = V_0\delta(x) - V_1[\delta(x - a) + \delta(x + a)]$$

Comment on the existence of:

- (a) an odd parity bound state.
- (b) an even parity bound state.
- (c) a bound state for $a = 0$. Of which parity?
- (d) a bound state for $a \rightarrow \infty$. Parity?

This is a qualitative question, but your arguments should be founded on an understanding of how to solve the system mathematically, and an intuition built up from the homework regarding how you expect the solutions to go.

Solution

In order to gain extra practice, you may wish to demonstrate each of the following points with more mathematical rigor, especially if you do not find the following arguments convincing at first glance.

(a) Note that any continuous odd function $f(x)$ must satisfy $f(0) = 0$. Therefore an odd solution would not “feel” the repulsive delta function at $x = 0$, and only sees the two attractive ones at $x = \pm a$. We know that for even one attractive delta we have a bound state, and we will for two as well.

(b) An even parity state will feel both the attractive and repulsive potentials, and so the overall ability of the potential to bind will depend on the relative strengths of V_1 and V_0 . Solving the $E = 0$ case would be the simplest way to determine the conditions under which a bound state might be possible.

(c) Here the delta functions are all on top of each other. As long as $2V_1 > V_0$ this will be an overall attractive delta and single even-parity bound state will exist.

(d) Sending $a \rightarrow \infty$ essentially makes the effects of the attractive parts of the potential negligible, leaving only the repulsive portion at $x = 0$. No bound state can exist under these conditions.

8.4 Problem 32

A canonical coherent state is an eigenstate of the 1D SHO annihilation operator, which you examined in HW problem 4.1. Let $|\alpha\rangle$ be a canonical coherent state with eigenvalue α such that $a|\alpha\rangle = \alpha|\alpha\rangle$. Part (a) was completed on your homework in a slightly different way, and you then proceeded to determine that the distribution of energies to create such a state follows a Poisson distribution, and the typical uncertainties for such a distribution. We now examine the dynamics of this system.

(a) Redo this if you want the practice, or move forward using the homework results. Write $|\alpha\rangle$ as a linear combination $\sum_n C_n|n\rangle$ of states $|n\rangle$ of the 1D SHO. Find a recursion relation to determine the coefficients C_n in terms of C_0 , then determine C_0 by normalizing the state. Compare with results from the homework.

(b) Let $|\psi_\alpha\rangle$ be the time-dependent form of the state $|\alpha\rangle$, obtained by using the time evolution operator. Write and simplify $|\psi_\alpha\rangle$ using the results from the previous parts.

(c) Calculate the time-dependent expectation values $\langle x \rangle_t = \langle \psi_\alpha | x | \psi_\alpha \rangle$ and $\langle p \rangle_t = \langle \psi_\alpha | p | \psi_\alpha \rangle$. (Do not do the whole calculation twice. Once you obtain one, you should be able to obtain the other with relatively little work.)

(d) Find the wavefunction $\langle x | \alpha \rangle$.

(e) What do you notice about the results from parts (c) and (d) / How does the behavior of this system compare with that of a classical SHO? How does this system move? How is the Heisenberg uncertainty principle satisfied (a qualitative answer based on a plot is sufficient)?

Solution

(a) We begin by expanding $|\alpha\rangle$ in terms of the energy eigenstates of the SHO.

$$|\alpha\rangle = \sum_n |n\rangle \langle n | \alpha \rangle = \sum_n C_n |n\rangle \quad \rightarrow \quad \text{Determine Coefficients } C_n = \langle n | \alpha \rangle$$

We use the property that $a|\alpha\rangle = \alpha|\alpha\rangle$ to proceed.

$$\begin{aligned} a|\alpha\rangle &= \sum_n C_n a|n\rangle = \sum_{n=1}^{\infty} C_n \sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} C_{n+1} \sqrt{n+1}|n\rangle \\ &= \alpha|\alpha\rangle = \alpha \sum_n C_n |n\rangle \end{aligned}$$

We obtain the recursion relation $\alpha C_n = \sqrt{n+1}C_{n+1}$. If we begin with C_0 and apply this repeatedly, we see that $C_n = \frac{\alpha^n}{\sqrt{n!}}C_0$. Therefore:

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle$$

We determine C_0 by normalization.

$$\begin{aligned} \langle\alpha|\alpha\rangle &= 1 = \left(\sum_m \langle m| \frac{(\alpha^*)^m}{\sqrt{m!}} C_0^* \right) \left(\sum_n \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle \right) = \sum_{n,m} |C_0|^2 \frac{(\alpha^*)^m \alpha^n}{\sqrt{m!n!}} \delta_{nm} = |C_0|^2 \sum_n \frac{|\alpha|^{2n}}{n!} \\ \rightarrow |C_0|^2 &= \left(\sum_n \frac{|\alpha|^{2n}}{n!} \right)^{-1} = e^{-|\alpha|^2} \end{aligned}$$

(b) The evolution operator is $U = e^{-iHt/\hbar}$. We want to calculate $|\psi_\alpha\rangle = U|\alpha\rangle$.

$$|\psi_\alpha\rangle = e^{-iHt/\hbar} \sum_n \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle = C_0 \sum_n \frac{\alpha^n}{\sqrt{n!}} e^{-iE_n t/\hbar} |n\rangle = C_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t(n+1/2)} |n\rangle$$

(c) We calculate $\langle x \rangle_t$ first.

$$\langle\psi_\alpha|x|\psi_\alpha\rangle = |C_0|^2 \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m \alpha^n}{\sqrt{n!m!}} e^{i\omega t(m-n)} \langle m|x|n\rangle$$

The term $\langle m|x|n\rangle$ is of interest.

$$x = \sqrt{\frac{\hbar}{2M\omega}}(a + a^\dagger) \rightarrow \langle m|x|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}(\langle m|a|n\rangle + \langle m|a^\dagger|n\rangle) = \sqrt{\frac{\hbar}{2M\omega}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})$$

We plug this result into the first expression above and simplify:

$$\begin{aligned} \langle x \rangle_t &= |C_0|^2 \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m \alpha^n}{\sqrt{n!m!}} e^{i\omega t(m-n)} \sqrt{\frac{\hbar}{2M\omega}} (\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \left(\sum_{n=1}^{\infty} \frac{(\alpha^*)^{n-1} \alpha^n}{\sqrt{n!(n-1)!}} e^{i\omega t((n-1)-n)} \sqrt{n} + \sum_{n=0}^{\infty} \frac{(\alpha^*)^{n+1} \alpha^n}{\sqrt{n!(n+1)!}} e^{i\omega t((n+1)-n)} \sqrt{n+1} \right) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \left(\sum_{n=1}^{\infty} \frac{\alpha|\alpha|^{2(n-1)}}{(n-1)!} e^{-i\omega t} + \sum_{n=0}^{\infty} \frac{\alpha^*|\alpha|^{2n}}{n!} e^{i\omega t} \right) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) = \sqrt{\frac{\hbar}{2M\omega}} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) \end{aligned}$$

We then note that $\langle p \rangle_t = M\partial_t \langle x \rangle_t$, such that we may write the following:

$$\langle p \rangle_t = i\sqrt{\frac{\hbar M\omega}{2}} (\alpha^* e^{i\omega t} - \alpha e^{-i\omega t})$$

(d) We write the operator a in a coordinate representation, and then solve the resulting differential equation from the requirement that $\langle x|a|\alpha\rangle = \alpha\langle x|\alpha\rangle$. I'll start writing the mass lower case again since there is no longer an index m to confuse it with.

$$a = \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega} \frac{\partial}{\partial x} \right) \rightarrow \sqrt{\frac{m\omega}{2\hbar}} \left(x + \frac{\hbar}{m\omega} \frac{\partial}{\partial x} \right) \alpha(x) = \alpha \cdot \alpha(x) \rightarrow \left[x\sqrt{\frac{m\omega}{2\hbar}} - \alpha + \sqrt{\frac{\hbar}{2m\omega}} \frac{d}{dx} \right] \alpha(x) = 0$$

$$\frac{d\alpha}{dx} = \sqrt{\frac{2m\omega}{\hbar}} \left(\alpha - x\sqrt{\frac{m\omega}{2\hbar}} \right) \alpha(x) = \left(\sqrt{\frac{2m\omega}{\hbar}}\alpha - \frac{m\omega}{\hbar}x \right) \alpha(x)$$

We propose a slightly modified Gaussian of the form $f(x) = e^{-bx^2+cx}$ since $\partial_x f(x) = (-2bx+c)f(x)$, which is of the same form as the above.

$$b = \frac{m\omega}{2\hbar} \quad , \quad c = \alpha\sqrt{\frac{2m\omega}{\hbar}} \quad \rightarrow \quad \langle x|\alpha\rangle = \alpha(x) = A \exp \left[-\frac{m\omega}{2\hbar}x^2 + x\alpha\sqrt{\frac{2m\omega}{\hbar}} \right]$$

This is a shifted Gaussian. We can make this more apparent and easier to work with by completing the square in the exponential:

$$\begin{aligned} \langle x|\alpha\rangle &= A \exp \left[-\frac{m\omega}{2\hbar}x^2 + x\alpha\sqrt{\frac{2\hbar}{m\omega}} \right] \quad \rightarrow \quad -\frac{m\omega}{2\hbar} \left(x^2 - x\alpha\frac{2\hbar}{m\omega}\sqrt{\frac{2m\omega}{\hbar}} \right) \quad \rightarrow \quad x^2 - 2\alpha\sqrt{\frac{2\hbar}{m\omega}}x \\ x^2 - 2\alpha\sqrt{\frac{2\hbar}{m\omega}}x &= x^2 - 2\alpha\sqrt{\frac{2\hbar}{m\omega}}x + \frac{2\alpha^2\hbar}{m\omega} - \frac{2\alpha^2\hbar}{m\omega} = \left(x - \alpha\sqrt{\frac{2\hbar}{m\omega}} \right)^2 - \frac{2\alpha^2\hbar}{m\omega} \end{aligned}$$

We absorb the extra constant into the normalization to obtain a function of the form:

$$\langle x|\alpha\rangle = B \exp \left[-\frac{m\omega}{2\hbar} \left(x - \alpha\sqrt{\frac{2\hbar}{m\omega}} \right)^2 \right]$$

(e) We may rearrange the result in part (c) into real and imaginary parts to write it purely in terms of sinusoidal functions. In analogy with a classical system, the “spring” begins at its equilibrium position for a purely imaginary α , and begins at the end of its range of motion for a purely real α . We can thereby see that the real and imaginary parts of α determine the initial conditions of the system at $t = 0$, and that the expectation values of position and momentum then oscillate as in a classical oscillator. This is however still a quantum system, and we can qualitatively see how the Heisenberg uncertainty principle is satisfied here; instead of two known values of position and momentum oscillating in time (which we could represent with oscillating Dirac delta functions), we have two distributions (Gaussian) whose centroids are oscillating as shown above. The width of these distributions tells us about the uncertainty in the position and momentum of the particle at any given time.

Specifically, for the case where α is real:

$$\langle x \rangle_t = \sqrt{\frac{\hbar}{2m\omega}} \alpha (e^{-i\omega t} + e^{i\omega t}) = \alpha \sqrt{\frac{2\hbar}{m\omega}} \cos(\omega t)$$

At $t = 0$ the expectation value of position is at its extreme (the “spring” is at its “most stretched”), which corresponds exactly to the shift observed in the peak of the Gaussian at $t = 0$ found in part (d). You can satisfy yourself that this will still work out as described above for complex α . We can infer all of the above with reasonable confidence without finding the fully time dependent $\langle x|\psi_\alpha\rangle$. All of this can be verified analytically with the time dependence along for the ride, or you can evaluate the partial sums in terms of the SHO eigenstates with mathematica to confirm. (Use the Poisson uncertainties in H derived on the homework to choose where to truncate a sum for a given α !)

9

9.1 Problem 33

Consider the first two energy levels of the 2D SHO.

- (a) Write out the unnormalized eigenfunctions in polar coordinates.
 (b) Write out the eigenfunctions of L_z . What are the possible values of m for each level?

Solution

- (a) We use notation such that $\psi_{n_x, n_y}(r, \varphi) = \langle r, \varphi | n_x, n_y \rangle$.

$$\psi_{00} \propto e^{-\alpha r^2} \quad \psi_{10} \propto r \cos \varphi e^{-\alpha r^2} \quad \psi_{01} \propto r \sin \varphi e^{-\alpha r^2}$$

- (b) Recall the following about the angular momentum operator L_z in a coordinate basis:

$$L_z \rightarrow -i\hbar \frac{\partial}{\partial \varphi} \quad \text{Eigenfunctions: } e^{im\varphi} \quad \text{with eigenvalues } m$$

We can write the following:

$$\begin{aligned} \psi_{00} \propto e^{-\alpha r^2} &\rightarrow m = 0 \\ \psi_{10} + i\psi_{01} \propto r e^{-\alpha r^2} e^{i\varphi} &\rightarrow m = 1 \\ \psi_{10} - i\psi_{01} \propto r e^{-\alpha r^2} e^{-i\varphi} &\rightarrow m = -1 \end{aligned}$$

Notice that the states with $m = \pm 1$ have the same energy. You may wish to re-examine homework problems 3.3 and 4.2 in order to put these observations in their proper context. The following suggests that the states we listed as $\langle r, \varphi | n_x, n_y \rangle$ might be better expressed with a different set of eigenvalues appropriate for a polar representation rather than a spherical one. Consider instead $\langle r, \varphi | n_r, m \rangle$. This suggests a second CSCO composed of radial and angular operators.

9.2 Problem 34

In Einstein notation $\mathbf{A} \cdot \mathbf{B} = A_i B_i$, where the sum over i is implicit. (You may find it convenient to denote a derivative in a particular coordinate by ∂_i , where i can be x, y , or z .) The cross product in Einstein notation is written using the Levi-Cevita tensor. In particular if we have $\mathbf{C} = \mathbf{A} \times \mathbf{B}$, then that can be written $C_i = \epsilon_{ijk} A_j B_k$, where the index i is fixed since it appears on both sides of the equation, and there is an implicit sum over j and k . Recall that the Levi-Cevita tensor is given by

$$\epsilon_{ijk} = \begin{cases} +1 & ijk \text{ are cyclically permuted} \\ -1 & ijk \text{ are anti-cyclically permuted} \\ 0 & i = j \text{ or } i = k \text{ or } j = k \end{cases}$$

- (a) Write out $\nabla \cdot \mathbf{C}$ in Einstein notation.
 (b) Prove the following vector identity using Einstein notation:

$$\nabla \cdot (\mathbf{A} \times \mathbf{B}) = (\nabla \times \mathbf{A}) \cdot \mathbf{B} - \mathbf{A} \cdot (\nabla \times \mathbf{B})$$

(c) Expand $\nabla \times [\phi(\mathbf{r} \times \mathbf{A})]$ in Einstein notation, and then rewrite your result in vector notation. You may find the identity $\epsilon_{ijk} \epsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}$ useful.

- (d) Using $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, show that $[L_i, r_j] = i\hbar \epsilon_{ijk} r_k$ and $[L_i, p_j] = i\hbar \epsilon_{ijk} p_k$.

Solution

- (a) In general, the divergence of some vector quantity can be notated:

$$\nabla \cdot \mathbf{C} = \frac{\partial C_i}{\partial x_i} = \partial_i C_i$$

For $\mathbf{C} = \mathbf{A} \times \mathbf{B}$ in particular, we may write:

$$\nabla \cdot (\mathbf{A} \times \mathbf{B}) = \partial_i \epsilon_{ijk} A_j B_k = \epsilon_{ijk} \partial_i A_j B_k = \epsilon_{ijk} (A_j \partial_i B_k + B_k \partial_i A_j) \dots$$

(b) which is continued below:

$$\begin{aligned}\nabla \cdot (\mathbf{A} \times \mathbf{B}) &= \partial_i \epsilon_{ijk} A_j B_k = \epsilon_{ijk} \partial_i A_j B_k = \epsilon_{ijk} (B_k \partial_i A_j + A_j \partial_i B_k) = \epsilon_{kij} B_k \partial_i A_j - \epsilon_{jik} A_j \partial_i B_k \\ &= (\nabla \times \mathbf{A}) \cdot \mathbf{B} - \mathbf{A} \cdot (\nabla \times \mathbf{B})\end{aligned}$$

(c)

$$\begin{aligned}\{\nabla \times [\phi(\mathbf{r} \times \mathbf{A})]\}_i &= \epsilon_{ijk} \partial_j [\phi(\mathbf{r} \times \mathbf{A})]_k = \epsilon_{ijk} \partial_j [\epsilon_{klm} \phi r_l A_m] = \epsilon_{ijk} \epsilon_{klm} [\phi r_l \partial_j A_m + \phi A_m \partial_j r_l + r_l A_m \partial_j \phi] \\ &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) [\phi r_l \partial_j A_m + \phi A_m \delta_{jl} + r_l A_m \partial_j \phi] \\ &= \phi r_i \partial_j A_j - \phi r_j \partial_j A_i + \phi A_j \delta_{ij} - \phi A_i \delta_{jj} + r_i A_j \partial_j \phi - r_j A_i \partial_j \phi\end{aligned}$$

We note that since there is an implicit sum over j , δ_{jj} is effectively the trace of a 3×3 identity matrix (since we are in three dimensions), and consequently $\delta_{jj} = 3$. We convert the following expansion back into vector notation:

$$\nabla \times [\phi(\mathbf{r} \times \mathbf{A})] = \phi[\mathbf{r}(\nabla \cdot \mathbf{A}) - (\mathbf{r} \cdot \nabla)\mathbf{A} - 2\mathbf{A}] + \mathbf{r}(\mathbf{A} \cdot \nabla\phi) - \mathbf{A}(\mathbf{r} \cdot \nabla\phi)$$

(d) Note that $L_i = \epsilon_{ijk} r_j p_k$. Then we may do the following:

$$\begin{aligned}[L_i, r_n] &= \epsilon_{ijk} [r_j p_k, r_n] = -i\hbar \epsilon_{ijk} r_j \delta_{kn} = i\hbar \epsilon_{inj} r_j \\ [L_i, p_n] &= \epsilon_{ijk} [r_j p_k, p_n] = i\hbar \epsilon_{ink} p_k\end{aligned}$$

9.3 Problem 35

Review some of the relationships between angular momentum operators discussed in class in parts (a)-(c).

(a) Using $[L_i, L_j] = i\hbar \epsilon_{ijk} L_k$, compute $[L^2, L_i]$ where $L^2 = L_x^2 + L_y^2 + L_z^2$. What does this imply?

(b) Using $L_z |l, m\rangle = m\hbar |l, m\rangle$, evaluate $[L_{\pm}, L_z] |l, m\rangle$ where $L_{\pm} = L_x \pm iL_y$. What happens when L_{\pm} acts on a state?

(c) Using $L^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle$, show $L_{\pm} |l, m\rangle = \hbar \sqrt{l(l+1) - m(m \pm 1)} |l, m \pm 1\rangle$.

(d) Construct the matrix of L_x for $l = 1$. What are the possible values of L_x ? Write out the eigenfunctions of L_x in the L_z basis.

(e) Write out the functions $\langle \varphi, \theta | 1, -1 \rangle$, $\langle \varphi, \theta | 1, 0 \rangle$, and $\langle \varphi, \theta | 1, 1 \rangle$, where the kets are of the form $|l, m\rangle$.

Solution

(a)

$$[L^2, L_i] = [L_j^2, L_i] = i\hbar \epsilon_{jik} L_j L_k + i\hbar \epsilon_{jik} L_k L_j \quad \text{but} \quad \epsilon_{ijk} L_j L_k = -\epsilon_{ijk} L_k L_j \quad \rightarrow \quad [L^2, L_i] = 0$$

We conclude that L^2 and L_i share some eigenbasis. Note that since the L_i for different i do not commute, that the eigenbasis will have to be shared between L^2 and only one of the three L_i . We continue by defining eigenkets $|l, m\rangle$, which are simultaneous eigenkets of both L^2 and L_z .

(b) $[L_{\pm}, L_z] = \mp \hbar L_{\pm}$ using the above. But then it follows that:

$$\mp \hbar L_{\pm} |l, m\rangle = (L_{\pm} L_z - L_z L_{\pm}) |l, m\rangle \quad \rightarrow \quad L_z (L_{\pm} |l, m\rangle) = \hbar(m \pm 1) (L_{\pm} |l, m\rangle)$$

We conclude that L_{\pm} are ladder operators, which move us between different projections on a given state. In other words, $L_{\pm} |l, m\rangle = C_{\pm} |l, m \pm 1\rangle$.

(c) Notice that since $L_i = L_i^{\dagger} \forall i$ we may say that $L_+ = L_-^{\dagger}$ and vice versa. We now find the proportionality constants C_{\pm} defined in the line above.

$$\langle l, m | L_- L_+ |l, m\rangle = |C_+|^2 = \langle l, m | (L_x - iL_y)(L_x + iL_y) |l, m\rangle = \langle l, m | L^2 - L_z^2 - \hbar L_z |l, m\rangle$$

where we have used $(L_x - iL_y)(L_x + iL_y) = L_x^2 + L_y^2 + iL_x L_y - iL_y L_x = L^2 - L_z^2 + i[L_x, L_y]$. Then:

$$|C_+|^2 = \hbar^2 [l(l+1) - m^2 - m] = \hbar^2 [l(l+1) - m(m+1)]$$

We repeat this with L_+ and L_- reversed in order to determine $|C_-|^2$:

$$\langle l, m | L_+ L_- |l, m\rangle = |C_-|^2 = \hbar^2 [l(l+1) - m(m-1)]$$

These results can then be summarized by:

$$L_{\pm}|l, m\rangle = \hbar\sqrt{l(l+1) - m(m \pm 1)}|l, m \pm 1\rangle = \hbar\sqrt{(l \mp m)(l \pm m + 1)}|l, m \pm 1\rangle$$

(d) Notice that the definitions of L_{\pm} can be added or subtracted to obtain:

$$L_x = \frac{1}{2}(L_- + L_+) \quad L_y = \frac{i}{2}(L_- - L_+)$$

We can construct matrices for L_+ and L_- with $l = 1$ according to the following:

$$\begin{pmatrix} \langle 11|L_+|11\rangle & \langle 11|L_+|10\rangle & \langle 11|L_+|1-1\rangle \\ \langle 10|L_+|11\rangle & \langle 10|L_+|10\rangle & \langle 10|L_+|1-1\rangle \\ \langle 1-1|L_+|11\rangle & \langle 1-1|L_+|10\rangle & \langle 1-1|L_+|1-1\rangle \end{pmatrix}$$

This allows us to determine:

$$L_+ = \hbar\sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad L_- = \hbar\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \quad \rightarrow \quad L_x = \frac{L_+ + L_-}{2} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

We then find the eigenvalues and eigenvectors in the usual way. We find that the eigenvalues are $0, \pm\hbar$, and that the corresponding eigenvectors are:

$$0 \rightarrow \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad \hbar \rightarrow \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \quad -\hbar \rightarrow \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

(e) Functions $\langle \varphi, \theta | l, m \rangle$ (the coordinate representations of the angular momentum eigenstates) are given by the spherical harmonics $Y_l^m(\varphi, \theta)$. Many can be found in Liboff, table 9.1, including the following:

$$Y_1^1 = -\frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta e^{i\varphi} \quad Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos\theta \quad Y_1^{-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \sin\theta e^{-i\varphi}$$

Note that this implies that the eigenvectors found in part (d) can also be written (See Liboff 9.100):

$$\frac{1}{\sqrt{2}}(Y_1^1 - Y_1^{-1}) \quad \frac{1}{2}(Y_1^1 + \sqrt{2}Y_1^0 + Y_1^{-1}) \quad \frac{1}{2}(Y_1^1 - \sqrt{2}Y_1^0 + Y_1^{-1})$$

9.4 Problem 36

A system of two spin-1/2 particles is in the state

$$|\psi\rangle = \frac{1}{\sqrt{5}}|++\rangle + \frac{2}{\sqrt{5}}|+-\rangle.$$

What are the possible values of J^2 and J_z ? With what probabilities?

Solution

First we need the CG coefficients for this system. These have been worked out in class, and we list them again below. (Work these out by starting at the top or bottom of the ladder, raising and lowering, and using orthonormality considerations if you do not remember how to find these.) We are considering the system $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$.

$$|11\rangle = |++\rangle \quad |10\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \quad |00\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \quad |1-1\rangle = |--\rangle$$

We need to make this change of basis because the states in the coupled basis above are the eigenstates of J^2 and J_z . The possible values of J^2 are $2\hbar^2$ ($j = 1$) and $0\hbar^2$ ($j = 0$). The possible values of J_z are \hbar and $0\hbar$.

$$|\psi\rangle = \frac{1}{\sqrt{5}}|++\rangle + \frac{2}{\sqrt{5}}|+-\rangle = \frac{1}{\sqrt{5}}|11\rangle + \frac{2}{\sqrt{5}}\frac{1}{\sqrt{2}}(|10\rangle + |00\rangle) = \sqrt{\frac{1}{5}}|11\rangle + \sqrt{\frac{2}{5}}|10\rangle + \sqrt{\frac{2}{5}}|00\rangle$$

We can read off the probabilities from the state in this form:

$$J^2 = \begin{cases} 2\hbar^2 \\ 0 \end{cases} \quad \text{with probabilities} \quad \begin{matrix} 3/5 \\ 2/5 \end{matrix} \quad J_z = \begin{cases} \hbar \\ 0 \end{cases} \quad \text{with probabilities} \quad \begin{matrix} 1/5 \\ 4/5 \end{matrix}$$

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10.1 Problem 37

In workshop problem 9.4 you were asked to determine the possible values of J^2 and J_z , and their corresponding probabilities, given the state below for a system of two spin- $\frac{1}{2}$ particles.

$$|\psi\rangle = \frac{1}{\sqrt{5}}|++\rangle + \frac{2}{\sqrt{5}}|+-\rangle.$$

Repeat the calculation for two spin-1 particles, letting $+$ and $-$ denote projections of $m = \pm 1$ instead of $m = \pm \frac{1}{2}$. You should begin by finding the appropriate Clebsch-Gordan coefficients.

Solution

We begin by finding the CG coefficients. The uncoupled representation will be notated with $|\pm, \pm\rangle$ as above, while the coupled with $|J, m_J\rangle$. The uncoupled states will be notated with $+$ ($m = +1$), \cdot ($m = 0$), and $-$ ($m = -1$). We start at the top of the ladder and lower:

$$\begin{aligned} |22\rangle &= |++\rangle \quad \rightarrow \quad J_-|22\rangle = (j_{1-} + j_{2-})|++\rangle \\ \sqrt{2 \cdot 3 - 2 \cdot 1}|21\rangle &= \sqrt{1 \cdot 2 - 1 \cdot 0}|\cdot+\rangle + \sqrt{1 \cdot 2 - 1 \cdot 0}|+\cdot\rangle \quad \rightarrow \quad |21\rangle = \sqrt{\frac{1}{2}}|\cdot+\rangle + \sqrt{\frac{1}{2}}|+\cdot\rangle \end{aligned}$$

We repeat this continuing down the ladder with each subsequent result to obtain the rest of the $|2, m_2\rangle$ states. I'll omit the algebra below.

$$\begin{aligned} J_-|21\rangle &= (j_{1-} + j_{2-}) \left(\sqrt{\frac{1}{2}}|\cdot+\rangle + \sqrt{\frac{1}{2}}|+\cdot\rangle \right) \quad \rightarrow \quad |20\rangle = \sqrt{\frac{1}{6}}|+-\rangle + \sqrt{\frac{2}{3}}|\cdot\cdot\rangle + \sqrt{\frac{1}{6}}|-+\rangle \\ &\rightarrow \quad |2-1\rangle = \sqrt{\frac{1}{2}}|\cdot-\rangle + \sqrt{\frac{1}{2}}|-\cdot\rangle \quad \rightarrow \quad |2-2\rangle = |--\rangle \end{aligned}$$

We determine $|11\rangle$ by considering orthonormality conditions. Specifically, $|11\rangle$ shares uncoupled states with $|21\rangle$, and we make an orthogonal $|11\rangle$:

$$|11\rangle = \sqrt{\frac{1}{2}}|\cdot+\rangle - \sqrt{\frac{1}{2}}|+\cdot\rangle$$

We apply the same lowering process as before to obtain the next two states down the ladder with $J = 1$:

$$\rightarrow \quad |10\rangle = \sqrt{\frac{1}{2}}|+-\rangle - \sqrt{\frac{1}{2}}|-+\rangle \quad \rightarrow \quad |1-1\rangle = \sqrt{\frac{1}{2}}|\cdot-\rangle - \sqrt{\frac{1}{2}}|-\cdot\rangle$$

Finally, we note that our last state $|00\rangle$ must be orthogonal to both $|20\rangle$ and $|10\rangle$, which it will share uncoupled states with. The following satisfies this requirement:

$$|00\rangle = \sqrt{\frac{1}{3}}|+-\rangle + \sqrt{\frac{1}{3}}|\cdot\cdot\rangle + \sqrt{\frac{1}{3}}|-+\rangle$$

Recall that the CG coefficients are of the form $\langle m_{j_1}, m_{j_2} | J, m_J \rangle$, and that since they are real, $\langle m_{j_1}, m_{j_2} | J, m_J \rangle = \langle J, m_J | m_{j_1}, m_{j_2} \rangle$. We can expand them either way. We have two states of interest due to $|\psi\rangle$, namely $|++\rangle$ and $|+-\rangle$, which we would like to rewrite in the coupled basis. Clearly $|++\rangle = |22\rangle$. We consider $|+-\rangle$. There are three coupled states which could contribute to it:

$$|+-\rangle = \sum_{J, m_J} |Jm_J\rangle \langle Jm_J | +- \rangle \quad \rightarrow \quad |+-\rangle = |20\rangle \langle 20 | +- \rangle + |10\rangle \langle 10 | +- \rangle + |00\rangle \langle 00 | +- \rangle$$

We are simply expanding the ket in the coupled basis over the uncoupled basis (both are complete orthonormal sets).

$$|\psi\rangle = \sqrt{\frac{1}{5}}|22\rangle + \sqrt{\frac{2}{5}} \left(\sqrt{\frac{1}{6}}|20\rangle + \sqrt{\frac{1}{2}}|10\rangle + \sqrt{\frac{1}{3}}|00\rangle \right) = \sqrt{\frac{1}{5}}|22\rangle + \sqrt{\frac{2}{15}}|20\rangle + \sqrt{\frac{2}{5}}|10\rangle + \sqrt{\frac{4}{15}}|00\rangle$$

With the state rewritten in this way, we can now simply read off the answers.

$$J^2 = \left\{ \begin{array}{l} 6\hbar^2 \\ 2\hbar^2 \\ 0 \end{array} \right. \quad \text{with probabilities} \quad \left\{ \begin{array}{l} 1/3 \\ 2/5 \\ 4/15 \end{array} \right\} \quad J_z = \left\{ \begin{array}{l} 2\hbar \\ 0 \end{array} \right. \quad \text{with probabilities} \quad \left\{ \begin{array}{l} 1/5 \\ 4/5 \end{array} \right\}$$

10.2 Problem 38

The Runge-Lenz vector is given by:

$$\mathbf{K} = \frac{1}{2me^2} (\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}) + \frac{\mathbf{r}}{r}$$

(a) Show that this is equivalent to

$$\mathbf{K} = \frac{1}{me^2} (\mathbf{L} \times \mathbf{p} - i\hbar\mathbf{p}) + \frac{\mathbf{r}}{r}$$

(b) To compute $[H, \mathbf{K}]$ you will find it necessary to compute $[p_i, 1/r]$. Compute this commutator.

(c) Does the result from part (a) hold if motion is constrained to the xy plane (i.e. in two dimensions)? Why?

Solution

(a) We expand one of the cross products being careful about order of operations.

$$\begin{aligned} \{\mathbf{p} \times \mathbf{L}\}_i &= \epsilon_{ijk} p_j L_k = \epsilon_{ijk} ([p_j, L_k] + L_k p_j) = \epsilon_{ijk} \epsilon_{jkm} i\hbar p_m - (\mathbf{L} \times \mathbf{p})_i \\ &= (\delta_{kk} - 1) \delta_{im} i\hbar p_m - (\mathbf{L} \times \mathbf{p})_i = 2i\hbar p_i - (\mathbf{L} \times \mathbf{p})_i \end{aligned}$$

Then we may rearrange the $\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L}$ term in \mathbf{K} to read:

$$\mathbf{L} \times \mathbf{p} - \mathbf{p} \times \mathbf{L} = 2\mathbf{L} \times \mathbf{p} - 2i\hbar\mathbf{p} \quad \rightarrow \quad \mathbf{K} = \frac{1}{me^2} (\mathbf{L} \times \mathbf{p} - i\hbar\mathbf{p}) + \frac{\mathbf{r}}{r}$$

(b) We will calculate the commutator with the aid of a trial function to make it extra-clear:

$$[p_i, 1/r]\psi = p_i \frac{1}{r} \psi - \frac{1}{r} p_i \psi = -i\hbar \left(\psi \frac{\partial}{\partial r_i} r^{-1} + \frac{1}{r} \frac{\partial \psi}{\partial r_i} - \frac{1}{r} \frac{\partial \psi}{\partial r_i} \right) = -i\hbar \left(-\frac{1}{r^2} \frac{\partial r}{\partial r_i} \right) \psi = \frac{i\hbar r_i}{r^3} \psi$$

This can be summarized:

$$\left[p_i, \frac{1}{r} \right] = \frac{i\hbar r_i}{r^3} \quad \leftrightarrow \quad \left[\mathbf{p}, \frac{1}{r} \right] = \frac{i\hbar \mathbf{r}}{r^3}$$

(c) The result from part (a) does not hold in two dimensions, where $L = L_z$ and \mathbf{p} and \mathbf{r} only have two components. The clearest mathematical reason for this is that δ_{kk} evaluates to 2 in 2-dimensions rather than 3, which changes the result somewhat. You are free to evaluate this out the long way with suitable simplifications however if you wish. The change in evaluating the delta results in:

$$\mathbf{K} = \frac{1}{2me^2} (2\mathbf{L} \times \mathbf{p} - i\hbar\mathbf{p}) + \frac{\mathbf{r}}{r}$$

for two-dimensions instead of the result derived above for 3. (In general you would clearly like to use the 3D result. This part of the problem is here simply to draw your attention to the fact that there is a difference, and that you can spot it if you are being careful about your use of Einstein notation.)

10.3 Problem 39

Consider the system of three particles each with $S^2 = 2\hbar^2$. The Hamiltonian is shown below, where λ is a constant.

$$H = \lambda \sum_{i \neq j} \mathbf{S}_i \cdot \mathbf{S}_j$$

(a) Write out all the states of the system in the coupled representation. What are the possible values of S_{total}^2 and the degeneracies of each?

(b) Write H in a form which is diagonal (i.e. change of basis). Determine the eigenvalues of H and the degeneracies of each. Compute the average eigenvalue. Why should we expect this result? (Hint: compute the trace of H .)

(c) Compute the average eigenvalue for a general sum on i and j (i can equal j). Does the result make sense?

Solution

(a) We have a system of 3 spin-1 particles. The coupling of the Hilbert spaces can be denoted by:

$$1 \otimes 1 \otimes 1 = (2 \oplus 1 \oplus 0) \otimes 1 = 3 \oplus 2 \oplus 1 \oplus 2 \oplus 1 \oplus 0 \oplus 1$$

The first expansion above denotes the coupling possibilities for the first two particles. There are $3^3 = 27$ states, and we distinguish states with $|S_{Total}, S_1 + S_2, S_z\rangle$. We list them out clarify the above:

State	Range of m	No. of States
$ 3, 2, m\rangle$	$-3 \rightarrow 3$	7
$ 2, 2, m\rangle$	$-2 \rightarrow 2$	5
$ 1, 2, m\rangle$	$-1 \rightarrow 1$	3
$ 2, 1, m\rangle$	$-2 \rightarrow 2$	5
$ 1, 1, m\rangle$	$-1 \rightarrow 1$	3
$ 0, 1, m\rangle$	0	1
$ 1, 0, m\rangle$	$-1 \rightarrow 1$	3
Total		27

This implies that $S^2 = (12, 6, 2, 6, 2, 0, 2)\hbar^2$ are (7, 5, 3, 5, 3, 1, 3)-fold degenerate.

(b) We first write out H explicitly.

$$H = \lambda(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_1 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_2 + \mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_1)$$

We then note that

$$S_T^2 = (S_1 + S_2 + S_3)^2 = S_1^2 + S_2^2 + S_3^2 + 2\mathbf{S}_1 \cdot \mathbf{S}_2 + 2\mathbf{S}_2 \cdot \mathbf{S}_3 + 2\mathbf{S}_1 \cdot \mathbf{S}_3$$

Since \mathbf{S}_i and \mathbf{S}_j correspond to different particles, $[\mathbf{S}_i, \mathbf{S}_j] = 0$ for $i \neq j$. (They exist in different Hilbert spaces.) Then H can be rewritten as follows:

$$H = \lambda(S_T^2 - S_1^2 - S_2^2 - S_3^2) = \lambda(S_T^2 - 6\hbar^2) = \lambda(6, 0, -4, 0, -4, -6, -4)\hbar^2 \quad \text{are } (7, 5, 3, 5, 3, 1, 3)\text{-fold denegerate.}$$

This indicates that average eigenvalue is 0, since we may evaluate the trace of the Hamiltonian in the basis in which it is diagonal in order to obtain:

$$Tr(H) = \hbar^2 \lambda(6 \cdot 7 + 5 \cdot 0 - 4 \cdot 3 + 5 \cdot 0 - 4 \cdot 3 - 6 - 4 \cdot 3) = 0$$

Since the trace is invariant under unitary transformation, we may take the trace in the energy eigenbasis and expect it to be the same regardless of the basis in which we might be expressing the matrix. We expect the overall trace of the Hamiltonian to be zero because the trace of any angular momentum is zero (we are summing over all possible projections $m = -s \rightarrow s$, so then $Tr(S_{ik}) = 0$). A remark on the notation here: I am using the first subscript to denote which spin this is (i.e. i and j below are 1,2, or 3), and the second subscript to denote the coordinate of that particular spin (i.e. k below is $x, y, \text{ or } z$). So any single case would read like S_{1x} . The trace in this scheme can be separated by the first index (different Hilbert spaces), but not the coordinate.

$$Tr(H) = \lambda \sum_{i \neq j} Tr(S_{ik} S_{jk}) = \lambda \sum_{i \neq j} Tr(S_{ik}) Tr(S_{jk}) = 0$$

(We may separate the traces in the last step because each term corresponds to a different particle.) Since the original Hamiltonian must have trace zero, it would a problem if the average eigenvalue evaluated with this trace method (i.e. eigenvalue weighted by degeneracy) did not give zero. This is a good check of the solution.

(c) Let H_0 be the original Hamiltonian.

$$H = \lambda(S_1^2 + S_2^2 + S_3^2) + H_0 \quad \rightarrow \quad Tr(H) = \lambda Tr(S_1^2 + S_2^2 + S_3^2) + Tr(H_0) = \lambda Tr(6\hbar^2) + 0 = 27(6\lambda\hbar^2)$$

The average is then $6\lambda\hbar^2$.

10.4 Problem 40

(a) Find the eigenvalues of the spin operator \mathbf{S} of an electron in the direction \hat{n} which lies in the xz plane. (You should be able to say what you expect for this before doing the problem. Do you find what you should?)

(b) Given a particular projection measured at some angle w.r.t. z , comment on how you would obtain the probability of obtaining a particular measurement along z itself. (I am not asking you to do the math in workshop. It is good practice to actually compute the probabilities if you wish do so later however.)

Solution

(a) Consider $\mathbf{S} \cdot \hat{\mathbf{n}} = S_x \sin \theta + S_z \cos \theta$. We use the Pauli matrices for S_x and S_z .

$$\mathbf{S} \cdot \hat{\mathbf{n}} = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}$$

We determine that the eigenvalues of this matrix are $\pm \frac{\hbar}{2}$ in the usual way. (If we remove the factor $\frac{\hbar}{2}$ in front, the eigenvalues of the matrix itself are ± 1 , which we use below to simplify calculation of the eigenvectors). This is what we would expect, because in principle what we called the z axis could have been anywhere. If the possibilities for the measurement were to change based on the direction of an arbitrarily defined set of coordinates, we would have a problem.

(b) Recall from workshop problem 5.4 that the eigenvectors of S_z are the most convenient eigenvectors, since we generally work in the S_z basis where it is a diagonal matrix. It is therefore simple to decompose any eigenvector into eigenvectors of z , and then read off the probabilities. To solve the problem, we would find the eigenvectors associated with the eigenvalues found in part (a), and take the mod-square of the appropriate components.

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11.1 Problem 41

Consider a particle with charge q and mass m in an excited state of the two-dimensional harmonic oscillator. A photon is emitted when the particle de-excites. The spontaneous emission rate (up to first order) is given by the following expression:

$$R = \frac{4\omega^3 q^2}{3\hbar c^3} |\langle \psi_f | \mathbf{r} | \psi_i \rangle|^2$$

ψ_i and ψ_f are the initial and final states, respectively, and ω is the frequency of the emitted photon.

- Calculate the transition rate from the first excited state to the ground state.
- Calculate the lifetime of the first excited state and the power radiated.

Solution

(a)

$$R = \frac{4\omega^3 q^2}{3\hbar c^3} |\langle \psi_f | \mathbf{r} | \psi_i \rangle|^2 \rightarrow \langle \psi_f | \mathbf{r} | \psi_i \rangle = \langle 00 | \mathbf{r} | 10 \rangle = \left\langle 00 \left| \sqrt{\frac{\hbar}{2m\omega'}} \begin{pmatrix} a_x + a_x^\dagger \\ a_y + a_y^\dagger \end{pmatrix} \right| 10 \right\rangle = \sqrt{\frac{\hbar}{2m\omega'}} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Notice that we happen to have put the excitation in x above, and that of the four ladder operators shown, only the term with a_x is giving us an answer. We could equally well have put the excitation in y however, and obtained the same result except for the vector, which will become irrelevant when we evaluate the mod-square anyway.

$$\text{Since } \frac{E_1 - E_0}{\hbar} = \omega \rightarrow \omega = \omega'$$

We evaluate the above to obtain:

$$R = \frac{2\omega^2 q^2}{3mc^3}$$

(b) The lifetime of a state is just the inverse of the transition rate, i.e.:

$$\tau = \frac{1}{R} = \frac{3mc^3}{2\omega^2 q^2}$$

Furthermore, the power emitted is given by the energy emitted times the rate of emission. The energy emitted in this transition is $E = \hbar\omega$. Therefore:

$$P = \frac{2\hbar\omega^3 q^2}{3mc^3}$$

11.2 Problem 42

The rotation operator U , which rotates an operator about the \hat{n} axis through an angle φ is given by $\exp(-i\mathbf{J} \cdot \hat{n}\varphi/\hbar)$ where \mathbf{J} is the angular momentum vector.

(a) For the case of spin-1/2, show

$$\exp\left(-\frac{i}{2}(\sigma \cdot \hat{n})\varphi\right) = \cos\left(\frac{\varphi}{2}\right) - i(\sigma \cdot \hat{n}) \sin\left(\frac{\varphi}{2}\right)$$

(b) Determine a U that rotates S_x into $-S_y$ and show that it works via the operation US_xU^\dagger for spin-1/2.

Solution

(a) We note that $(\sigma \cdot \hat{n})^2 = \mathbb{I}$ (identity matrix). Expand the exponential in series form about φ_0 :

$$\begin{aligned} \exp\left(-\frac{i}{2}(\sigma \cdot \hat{n})\varphi\right) &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{2}(\sigma \cdot \hat{n})\varphi\right)^n = \sum_{n=0, \text{EVEN}}^{\infty} \frac{(\sigma \cdot \hat{n})^n}{n!} \left(-\frac{i\varphi}{2}\right)^n + \sum_{n=1, \text{ODD}}^{\infty} \frac{(\sigma \cdot \hat{n})^n}{n!} \left(-\frac{i\varphi}{2}\right)^n \\ &= \sum_{n=0, \text{EVEN}}^{\infty} \frac{1}{n!} \left(-\frac{i\varphi}{2}\right)^n + (\sigma \cdot \hat{n}) \sum_{n=1, \text{ODD}}^{\infty} \frac{1}{n!} \left(-\frac{i\varphi}{2}\right)^n = \cos\left(\frac{\varphi}{2}\right) - i(\sigma \cdot \hat{n}) \sin\left(\frac{\varphi}{2}\right) \end{aligned}$$

(b) We apply the above and ascertain that it in fact does what it is supposed to do. If we rotate by $\frac{\pi}{2}$ about the z axis that should move us from x to y . Thus we get from S_x to $-S_y$ by trying the proposed scheme for $\hat{n} = -\hat{z}$ and $\frac{\pi}{2} = \varphi$.

$$\begin{aligned} US_xU^\dagger &= \frac{\hbar}{2} \left[\cos\left(\frac{\pi}{4}\right) + i\sigma_z \sin\left(\frac{\pi}{4}\right) \right] \sigma_x \left[\cos\left(\frac{\pi}{4}\right) - i\sigma_z \sin\left(\frac{\pi}{4}\right) \right] \\ &= \frac{\hbar}{2(2)} \left[\begin{pmatrix} 1+i & 0 \\ 0 & 1-i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1-i & 0 \\ 0 & 1+i \end{pmatrix} \right] \\ &= -\frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -S_y \end{aligned}$$

11.3 Problem 43

Use rotation operators and the properties of trace to prove the following:

- (a) $Tr(S_i S_j) = 0$ for $i \neq j$ where i and j are spatial directions.
- (b) $Tr(S_i^2) = Tr(S_j^2)$ (no sum, i and j are fixed). Combine this result with that of part (a) to find $Tr(S_i S_j)$.
- (c) $Tr(S_i S_j S_k) = 0$ for any two indices alike.
- (d) $Tr(S_i S_j S_k) = -Tr(S_j S_i S_k)$ for no two indices alike. Combine this result with that of part (c) to find $Tr(S_i S_j S_k)$.

Solution

- (a) Let U rotate about j sending $i \rightarrow -i$.

$$Tr(S_i S_j) = Tr(US_i U^\dagger U S_j U^\dagger) \rightarrow Tr(-S_i S_j) = -Tr(S_i S_j) \therefore Tr(S_i S_j) = 0 \text{ for } i \neq j$$

- (b) Let U rotate about j sending $i \rightarrow j$.

$$Tr(S_i S_i) = Tr(US_i U^\dagger U S_i U^\dagger) \rightarrow Tr(S_i^2) = Tr(S_j^2)$$

We conclude that $Tr(S_i S_j) = a\delta_{ij}$ for some number a . We find a as follows:

$$Tr(S_i^2) = \frac{Tr(S^2)}{3} = \frac{\hbar^2 s(s+1)(2s+1)}{3} \rightarrow Tr(S_i S_j) = \frac{\hbar^2 s(s+1)(2s+1)}{3} \delta_{ij}$$

- (c) Let us first consider $Tr(S_i S_i S_k)$, with a U which rotates about i sending $k \rightarrow -k$.

$$Tr(S_i S_i S_k) = Tr(US_i U^\dagger U S_i U^\dagger U S_k U^\dagger) \rightarrow Tr(S_i S_i S_k) = -Tr(S_i S_i S_k) = 0$$

Then let us consider $Tr(S_i S_i S_i)$ and a U which rotates about $j \neq i$ sending $i \rightarrow -i$.

$$Tr(S_i S_i S_i) = Tr(US_i U^\dagger U S_i U^\dagger U S_i U^\dagger) \rightarrow Tr(S_i S_i S_i) = -Tr(S_i S_i S_i) = 0$$

- (d) Let U rotate about k sending $i \rightarrow j$ and $j \rightarrow -i$.

$$Tr(S_i S_j S_k) = Tr(US_i U^\dagger U S_j U^\dagger U S_k U^\dagger) \rightarrow Tr(S_i S_j S_k) = -Tr(S_j S_i S_k)$$

We may therefore conclude that $Tr(S_i S_j S_k) = b\epsilon_{ijk}$ for some number b . We find b as follows:

$$\begin{aligned} Tr\{([S_i, S_j] + S_j S_i) S_k\} &= Tr(i\hbar\epsilon_{ijl} S_l S_k + S_j S_i S_k) = i\hbar\epsilon_{ijl} Tr(S_l S_k) + Tr(S_j S_i S_k) \\ &\rightarrow 2Tr(S_i S_j S_k) = \frac{i\hbar^3 s(s+1)(2s+1)}{3} \epsilon_{ijk} \rightarrow Tr(S_i S_j S_k) = \frac{i\hbar^3}{6} s(s+1)(2s+1) \epsilon_{ijk} \end{aligned}$$

11.4 Problem 44

(a) Determine the degeneracy of a general bound state of the hydrogen atom with principal quantum number n . Include spin of an electron in the derivation. Use the summation

$$\sum_{i=0}^m i = \frac{m(m+1)}{2}$$

(b) Explain qualitatively the effects one might take into consideration to break this degeneracy, and give the order of magnitudes of these splittings relative to the energies themselves. (I am asking you to summarize things which have been covered in greater detail in class.)

Solution

(a) Per level n and orbital ℓ there is a degeneracy $2\ell + 1$. We sum over the possible orbitals for a given n :

$$\sum_{\ell=0}^{n-1} 2\ell + 1 = 2 \sum_{\ell=0}^{n-1} \ell + n = (n-1)n + n = n^2 - n + n = n^2$$

This does not account for the spin of the electron yet. Since the spin is either up or down, the degeneracy including spin is $2n^2$.

(b) For further details concerning a derivation of these points, see your class notes and/or Liboff p. 589.

The so called “fine structure” correction for Hydrogen breaks the degeneracy. This correction includes spin-orbit coupling (interactions between the spin of an electron and its orbital angular momentum), and approximate relativistic effects. These each change the energy levels by approximately one part in 10^5 relative to the usual spectrum where the energy only depends on n .

There are also “hyperfine” corrections one can undertake to the spectrum, which are corrections several orders of magnitude smaller than those in the fine structure. These hyperfine corrections account for interactions due to the electric and magnetic fields of the atomic nucleus.

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12.1 Problem 45

This problem concerns the derivation and applications of the quantum-mechanical Virial theorem.

(a) Show that for any time-independent operator \hat{a} the relationship $\partial_t \langle \hat{a} \rangle = 0$ holds, where the expectation value is taken between eigenstates of the Hamiltonian.

(b) Consider the Hamiltonian:

$$H = \frac{p^2}{2m} + kx^n = T + V$$

Show that for the above system $2 \langle T \rangle = n \langle V \rangle$. (Hint: Choose $\hat{a} = xp$. This is the Virial Theorem.)

(c) We extend the above into three dimensions. First, show the following. (What choice for the operator A makes sense in analogy with the 1D choice for \hat{a} above?)

$$[H, A] = i\hbar \left(\mathbf{r} \cdot \nabla \mathbf{V} - \frac{p^2}{m} \right)$$

(d) Then compute $\langle \psi | [H, A] | \psi \rangle$ to show that $\langle \mathbf{r} \cdot \nabla \mathbf{V} \rangle = 2 \langle T \rangle$, which is a statement of the Virial theorem in 3 dimensions.

(e) Use the Virial theorem to show $\langle V \rangle = -2 \langle T \rangle$ for the Coulombic potential.

(f) Use the Virial theorem to show $\langle V \rangle = \langle T \rangle$ for the SHO.

Solution

Note that we are sloppy about notating \hat{a} with its hat below. a and \hat{a} denote the same operator here.

(a) We have $H|\psi\rangle = E|\psi\rangle$ and notate $\langle a \rangle = \langle \psi | a | \psi \rangle$. We invoke Heisenberg's equation of motion, (see workshop problem 4.4)

$$\frac{da}{dt} = \frac{1}{i\hbar} [a, H] \quad \rightarrow \quad \frac{d\langle a \rangle}{dt} = \frac{1}{i\hbar} \langle \psi | [a, H] | \psi \rangle = \frac{1}{i\hbar} (\langle aH \rangle - \langle Ha \rangle)$$

and note that since H is Hermitian $\langle \psi | H = \langle \psi | H^\dagger = E \langle \psi |$. This implies:

$$\frac{d\langle a \rangle}{dt} = \frac{1}{i\hbar} (E \langle a \rangle - E \langle a \rangle) = 0 \quad \rightarrow \quad \therefore \quad \langle \dot{a} \rangle = 0 = \langle [a, H] \rangle$$

(b) Let $a = xp$; we have established from part (a) that $\langle [xp, H] \rangle = 0$. We consider the commutator in this expression:

$$[xp, H] = x[p, H] + [x, H]p = x[p, V] + [x, T]p = x[p, kx^n] + \frac{1}{2m}[x, p^2]p = kx(-ni\hbar x^{n-1}) + \frac{1}{2m}(2i\hbar p)p = i\hbar(2T - nV)$$

Therefore, using the result from part (a):

$$\langle [xp, H] \rangle = i\hbar \langle 2T - nV \rangle = i\hbar(2 \langle T \rangle - n \langle V \rangle) = 0 \quad \rightarrow \quad 2 \langle T \rangle = n \langle V \rangle$$

(c) Consider the general Hamiltonian $H = T + V$ where $T = p^2/2m$ and V is only spatially dependent.

Let $A = \mathbf{r} \cdot \mathbf{p} = x_i p_i$.

$$\begin{aligned} \left[\frac{p_j^2}{2m} + V, x_i p_i \right] &= \frac{1}{2m} [p_j^2, x_i] + x_i [V, p_i] = \frac{p_j}{m} [p_j, x_i] p_i + x_i \left(i\hbar \frac{\partial V}{\partial x_i} \right) = -\frac{i\hbar}{m} p_j p_i \delta_{ij} + i\hbar x_i \frac{\partial V}{\partial x_i} \\ &= i\hbar \left(x_i \frac{\partial V}{\partial x_i} - \frac{p_i^2}{m} \right) = i\hbar \left(\mathbf{r} \cdot \nabla \mathbf{V} - \frac{p^2}{m} \right) \end{aligned}$$

(d) Once again we have $[H, A] = 0$, so...

$$i\hbar \left\langle \mathbf{r} \cdot \nabla \mathbf{V} - \frac{p^2}{m} \right\rangle = 0 \quad \rightarrow \quad \langle \mathbf{r} \cdot \nabla \mathbf{V} \rangle = \left\langle \frac{p^2}{m} \right\rangle = 2 \langle T \rangle$$

(e)

$$\left\langle \mathbf{r} \cdot \left(\frac{d}{dr} \frac{-1}{r} \right) \hat{r} \right\rangle = \left\langle \mathbf{r} \cdot \hat{r} \left(\frac{1}{r^2} \right) \right\rangle = \left\langle \frac{1}{r} \right\rangle = -\langle V \rangle \quad \rightarrow \quad \langle V \rangle = -2 \langle T \rangle$$

(f) In one dimension, simply let $n = 2$ in part (b), and the result $2 \langle T \rangle = 2 \langle V \rangle$ is obtained trivially. In three dimensions, the result is the same:

$$\mathbf{r} \cdot \nabla \mathbf{V} = x_i \frac{\partial x_i^2}{\partial x_i} = 2x_i^2 = 2V \quad \rightarrow \quad \langle V \rangle = \langle T \rangle$$

12.2 Problem 46

(a) Prove the Hellmann-Feynman Theorem (λ is a variational parameter):

$$\frac{dE}{d\lambda} = \langle \psi(\lambda) | \partial_\lambda H | \psi(\lambda) \rangle$$

(b) Using part (a) and E for the Hydrogen atom, show the Virial theorem. (Hint: pick the right variational parameter.)

(c) Using part (a) and E for the SHO, show the Virial theorem.

Solution

(a) $|\psi\rangle$ is an eigenstate of H , ie $H|\psi(\lambda)\rangle = E|\psi(\lambda)\rangle$.

$$\begin{aligned} \frac{dE}{d\lambda} &= \frac{d}{d\lambda} \langle H \rangle = \frac{d}{d\lambda} \langle \psi(\lambda) | H | \psi(\lambda) \rangle = \left\langle \frac{\partial \psi}{\partial \lambda} | H | \psi(\lambda) \right\rangle + \left\langle \psi(\lambda) \left| \frac{\partial H}{\partial \lambda} \right| \psi(\lambda) \right\rangle + \left\langle \psi(\lambda) | H \left| \frac{\partial \psi}{\partial \lambda} \right\rangle \right. \\ &= E \left(\left\langle \frac{\partial \psi}{\partial \lambda} | \psi \right\rangle + \left\langle \psi \left| \frac{\partial \psi}{\partial \lambda} \right\rangle \right) + \langle \partial_\lambda H \rangle = E \frac{d}{d\lambda} \langle \psi | \psi \rangle + \langle \partial_\lambda H \rangle = \langle \partial_\lambda H \rangle \end{aligned}$$

(b) For the H-atom, we may use e^2 as our variational parameter:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \quad \& \quad E = -\frac{me^4}{2\hbar^2 n^2} \quad \rightarrow \quad \frac{dE}{de^2} = -\frac{me^2}{\hbar^2 n^2} = \left\langle -\frac{1}{r} \right\rangle$$

It then follows that

$$\langle V \rangle = 2 \langle E \rangle = 2(\langle V \rangle + \langle T \rangle) \quad \rightarrow \quad \langle V \rangle = -2 \langle T \rangle$$

(c) For the SHO, we will choose m as our variational parameter:

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad \& \quad E = \hbar\omega \left(n + \frac{1}{2} \right) \quad \rightarrow \quad \frac{dE}{dm} = 0 = \left\langle \frac{1}{m} \left(-\frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \right) \right\rangle = \frac{1}{m}(-\langle V \rangle + \langle T \rangle)$$

which then shows that $\langle V \rangle = \langle T \rangle$.

12.3 Problem 47

The magnetic moment of an electron moving in a loop is $\mu = q(\mathbf{r} \times \mathbf{v})/2$. In the presence of a magnetic field \mathbf{B} the interaction energy is $V = -\mu \cdot \mathbf{B}$.

(a) Determine $|\mu|$. (Hint: write μ in terms of orbital angular momentum.)

(b) Determine the energy levels of the $2p$ state of the Hydrogen atom in the presence of $\mathbf{B} = B\hat{z}$.

Solution

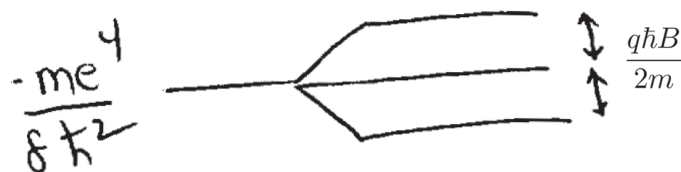
(a)

$$\mu = \frac{q(\mathbf{r} \times \mathbf{v})}{2} = \frac{q}{2m}(\mathbf{r} \times \mathbf{p}) = \frac{q\mathbf{L}}{2m} \quad \rightarrow \quad |\mu| = \frac{|q|\hbar}{2m} \sqrt{\ell(\ell+1)}$$

(b)

$$H = \frac{p^2}{2m} - \frac{e^2}{r} - \mu \cdot \mathbf{B} = H_0 - \frac{qB}{2m} L_z \quad \rightarrow \quad \text{Since } [H_0, L_z] = 0 \quad \rightarrow \quad E = -\frac{me^4}{2\hbar^2(2)^2} - \frac{q\hbar B}{2m} \begin{Bmatrix} -1 \\ 0 \\ 1 \end{Bmatrix}$$

This can be summarized by the diagram:



12.4 Problem 48

Consider an electron with Hamiltonian $H = \lambda S_z$. At $t = 0$, the electron is in a spin-up state along the y -axis. Determine the probability that at $t > 0$ the spin will be reversed.

Solution

Note that we notate the probabilities according to $p(x|I)$, which reads the probability of x given I . We are interested in seeing if a state $|+_y\rangle$ can evolve into a state $|-_y\rangle$ over time. This is expressed as follows, where we assume that the states are normalized:

$$p(-_y|+_y) = |\langle -_y | \exp[-iHt/\hbar] |+_y\rangle|^2$$

We can write out the states $|+_y\rangle$ and $|-_y\rangle$ in vector form. They are the eigenvectors of the operator S_y for spin one-half.

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \rightarrow \quad |+_y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad |-_y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ 1 \end{pmatrix}$$

Then the probability above can be calculated explicitly:

$$p(-_y|+_y) = \frac{1}{4} \left| (-i, 1) \left[\cos\left(\frac{\lambda t}{2}\right) \mathbb{I} - i\sigma_z \sin\left(\frac{\lambda t}{2}\right) \right] \begin{pmatrix} 1 \\ i \end{pmatrix} \right|^2 = \frac{1}{4} \left| (-i, 1) \begin{pmatrix} e^{-i\lambda t/2} \\ ie^{i\lambda t/2} \end{pmatrix} \right|^2 = \sin^2\left(\frac{\lambda t}{2}\right)$$

Note that we have made use of the identity derived in problem 11.2 in the context of a rotation operator. We may use it here since the same arguments allowing us to remove a dot product from the Taylor expansion in that problem apply here. ($\sigma_z^2 = \mathbb{I}$, which allows the spin operator to be removed from the summations).

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13.1 Problem 49

Consider an infinite square well extending from $x = 0$ to $x = L$. Calculate the energy of the n^{th} excited state using first order perturbation theory for the following two perturbations ($\lambda \ll 1$).

(a) $H_1 = \lambda V_0 \sin(\pi x/L)$.

(b) $H_1 = \lambda V_0 \delta(x - L/2)$.

Note that you can compare the solution of part (b) to the solution of HW problem 6.3 after workshop if you wish. What behaviors of the system does the first order approximation capture?

Solution

Problem and solution from Zettili, Quantum Mechanics Concepts and Applications (2nd Ed.). Recall that the usual energy and wavefunction are given by:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \quad \psi_n(x) = \langle x|n \rangle = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

We are in a non-degenerate system, so the energy correction is calculated as follows:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + E_n^{(1)} \quad \rightarrow \quad E_n^{(1)} = \langle n|H_1|n \rangle = \frac{2}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) H_1(x) dx$$

(a) We will derive a useful relation before proceeding with the actual calculation, namely:

$$\begin{aligned} \int \cos(nx) \sin(mx) dx &= \frac{1}{4i} \int (e^{inx} + e^{-inx})(e^{imx} - e^{-imx}) = \frac{1}{4i} \int (e^{i(m+n)x} - e^{-i(m+n)x} + e^{i(m-n)x} - e^{-i(m-n)x}) dx \\ &= \frac{1}{2} \int [\sin((m+n)x) + \sin((m-n)x)] dx = -\frac{1}{2} \left[\frac{\cos((m+n)x)}{m+n} + \frac{\cos((m-n)x)}{m-n} \right] \end{aligned}$$

Then we calculate $E_n^{(1)}$.

$$\begin{aligned} E_n^{(1)} &= \frac{2\lambda V_0}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) dx = \frac{\lambda V_0}{L} \int_0^L \left(1 - \cos\left(\frac{2n\pi x}{L}\right)\right) \sin\left(\frac{\pi x}{L}\right) dx \\ &= \frac{\lambda V_0}{\pi} \left[-\cos\left(\frac{\pi x}{L}\right) + \frac{\cos[(1-2n)\pi x/L]}{2(1-2n)} + \frac{\cos[(1+2n)\pi x/L]}{2(1+2n)} \right]_0^L = \frac{2\lambda V_0}{\pi} \frac{4n^2}{4n^2 - 1} \end{aligned}$$

Then the corrected energy spectrum up to first order is:

$$E_n = n^2 \left(\frac{\hbar^2 \pi^2}{2mL^2} + \frac{8\lambda V_0}{\pi(4n^2 - 1)} \right)$$

(b)

$$E_n^{(1)} = \frac{2\lambda V_0}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \delta(x - L/2) dx = \frac{2\lambda V_0}{L} \sin^2\left(\frac{n\pi}{2}\right)$$

As in the homework problem in which you solved this problem exactly, the odd-parity states (even n) are unaffected, whereas the first order perturbation is giving us an upward shift in the energy levels of even parity (odd n).

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} + \begin{cases} 0 & n \text{ even} \\ 2\lambda V_0/L & n \text{ odd} \end{cases}$$

13.2 Problem 50

Consider the 2D SHO, with Hamiltonian H_0 .

(a) Determine the energies of the three lowest states.

(b) Now apply the perturbation $H_1 = \delta m\omega^2 xy$ where $\delta \ll 1$. Determine the energy eigenvalues to first order in δ for the three lowest states.

(c) Solve $H = H_0 + H_1$ exactly. (Hint: Rewrite H in terms of a 45 degree counter-clockwise rotation of the coordinates and conjugate momenta.) Expand to first order in δ and compare with your result in part (b).

Solution

(a) $E = \hbar\omega, 2\hbar\omega, 2\hbar\omega$ as per results derived many times throughout the course.

(b) We calculate the ground state submatrix (1 element), and the first excited state submatrix (2×2 , in accordance with the degeneracies of the associated eigenvalues). Liboff section 13.2 should be consulted for further details on why this approach arises.

$$\langle 00 | xy | 00 \rangle = \frac{\hbar}{2m\omega} \langle 00 | (a_x + a_x^\dagger)(a_y + a_y^\dagger) | 00 \rangle = 0$$

We see that this perturbation leaves the ground state unchanged. Next for the first excited states:

$$\begin{pmatrix} \langle 10 | H_1 | 10 \rangle & \langle 01 | H_1 | 10 \rangle \\ \langle 10 | H_1 | 01 \rangle & \langle 01 | H_1 | 01 \rangle \end{pmatrix} = \delta m\omega^2 \frac{\hbar}{2m\omega} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\delta\hbar\omega}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where each inner product is reduced via the same procedure that was applied to the ground state. We are interested in the eigenvalues of this matrix, which will give us the corrections to the energies. We notate the eigenvalues of the H_1 submatrix as λ :

$$\lambda = \pm \frac{\delta\hbar\omega}{2} \quad \rightarrow \quad E_{00} = \hbar\omega \quad E_{01 \text{ or } 10} = 2\hbar\omega \pm \frac{\delta\hbar\omega}{2}$$

(c) The rotation referred to in the hint can be expressed mathematically as follows, where the lower case variables are the old ones, and the capital variables are the new:

$$P_{X,Y} = (p_x \pm p_y)/\sqrt{2} \quad X, Y = (x \pm y)/\sqrt{2}$$

You should satisfy yourself that upon making this change, the Hamiltonian shown below is equivalent to the original one:

$$H = \frac{P_X^2 + P_Y^2}{2m} + \frac{1}{2}m\omega^2(1 + \delta)X^2 + \frac{1}{2}m\omega^2(1 - \delta)Y^2$$

Since the variables are separated out now however, we can easily write an explicit form of the spectrum for this system:

$$E = \hbar\omega\sqrt{1 + \delta}(n_1 + 1/2) + \hbar\omega\sqrt{1 - \delta}(n_2 + 1/2)$$

We expand this to $O(\delta)$ and see that this approximation of the exact result matched precisely the one given by perturbation theory.

13.3 Problem 51

Spin and isospin are similar. By convention, $|p\rangle = |1/2, 1/2\rangle$ and $|n\rangle = |1/2, -1/2\rangle$ where $|p\rangle$ and $|n\rangle$ are the isospin states of a proton and neutron, respectively.

(a) Find the various states that can be constructed out of a two-nucleon system.

(b) Now consider the particles $|P\rangle = |1/2, 1/2\rangle$ and $|N\rangle = |1/2, -1/2\rangle$, where $|P\rangle$ and $|N\rangle$ are distinct from $|p\rangle$ and $|n\rangle$ by their masses. Assuming scattering only occurs in $I = 1$ states, compute the ratio of cross sections for the reactions

$$P + p \rightarrow P + p$$

$$P + n \rightarrow P + n$$

$$P + n \rightarrow N + p$$

(c) Repeat part (b) for scattering in $I = 0$ states.

Solution

(a) Have pp , pn , nn , and np . These can be notated in the fashion we are accustomed to for two spin- $\frac{1}{2}$ particles.

$$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0 \quad \rightarrow \quad |11\rangle = |++\rangle \quad |1-1\rangle = |--\rangle \quad |10\rangle = \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \quad |00\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$$

We make the following correspondences:

$$\begin{aligned} |pp\rangle &\rightarrow |++\rangle = |11\rangle & |pn\rangle &\rightarrow |+-\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |00\rangle) \\ |np\rangle &\rightarrow |-+\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |00\rangle) & |nn\rangle &\rightarrow |--\rangle = |1-1\rangle \end{aligned}$$

(b) Scattering cross-sections are proportional to the probability that a given interaction might occur. We may calculate the ratios between them without much trouble, even though the calculation of the absolute values of the cross sections is considerably more complicated, we may find the ratios with relative ease using the relationships determined above. For instance, $|Pp\rangle$ is always in an $I = 1$ state. $|Pn\rangle$ only has a probability of $\frac{1}{2}$ to be in an $I = 1$ state though, and an $I = 1$ event will result in $|Pn\rangle$ half the time and $|Np\rangle$ half the time. Therefore:

$$\sigma_{Pp \rightarrow Pp} : \sigma_{Pn \rightarrow Pn} : \sigma_{Pn \rightarrow Np} = 1 : \frac{1}{4} : \frac{1}{4} \quad \rightarrow \quad 4 : 1 : 1$$

(c) We apply the same logic, noting that for $I = 0$ nothing has changed except that no Pp events can occur in $I = 0$. Then the ratio of the cross-sections is:

$$0 : 1 : 1$$

13.4 Problem 52

Consider the spin-orbit coupling Hamiltonian (this is the term in fine structure)

$$H = \lambda(\mathbf{L} \cdot \mathbf{S})$$

Determine the energy levels for a spin one particle with general l . Show that the sum is zero.

Solution

Use $\mathbf{J} = \mathbf{L} + \mathbf{S}$ to write

$$H = \frac{\lambda}{2}(J^2 - L^2 - S^2)$$

Let's start with the case $\ell = 0$. We may write:

$$0 \otimes 1 = 1 = j \quad \rightarrow \quad j = s = 1 \quad \rightarrow \quad E = \frac{\lambda}{2}(J^2 - S^2) = 0$$

Now let's consider some $\ell > 0$, where $\ell \otimes 1 = \ell + 1 \oplus \ell \oplus \ell - 1$. This gives us three possibilities for j . We begin by considering $j = \ell + 1$.

$$E = \frac{\lambda}{2}((\ell + 1)(\ell + 2) - \ell(\ell + 1) - 2)\hbar^2 = \lambda\ell\hbar^2$$

For $j = \ell$ we have:

$$E = \frac{\lambda}{2}(-2)\hbar^2 = -\lambda\hbar^2$$

For $j = \ell - 1$ we have:

$$E = \frac{\lambda}{2}((\ell - 1)(\ell) - \ell(\ell + 1) - 2)\hbar^2 = \frac{\lambda}{2}(-2\ell - 2)\hbar^2 = -\lambda(\ell + 1)\hbar^2$$

We check that this is reasonable by summing these up (taking the trace of H , effectively), noting that the degeneracy for a given j is given by $2j + 1$:

$$(\lambda\ell\hbar^2)(2(\ell + 1) + 1) + (-\lambda\hbar^2)(2\ell + 1) + (-\lambda(\ell + 1)\hbar^2)(2(\ell - 1) + 1) = 0$$

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14.1 Problem 53

A particle is initially in the state $|\psi_i\rangle$ (for $t < 0$). At time $t = 0$ a small perturbation H_1 is applied to the system. The first-order transition probability is given by

$$P_{i \rightarrow f} = \frac{1}{\hbar^2} \left| \int_0^t e^{i\omega_{fi}t'} \langle \psi_f | H_1 | \psi_i \rangle dt' \right|^2$$

where $\omega_{fi} = \frac{1}{\hbar}(E_f - E_i)$.

(a) Consider a 1D SHO in the ground state subject to a perturbation $Ax^3e^{-t/\tau}$. Determine the possible final states and the probabilities of each as $t \rightarrow \infty$.

(b) Why doesn't the sum of the probabilities add up to one?

Solution

(a) We'll begin by determining the states the SHO could transition to from the ground state. This means we are interested in the expression $\langle n | x^3 | 0 \rangle$.

$$\begin{aligned} \langle n | x^3 | 0 \rangle &= \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} \langle n | (a^\dagger)^2 + a^\dagger a + a a^\dagger + a^2 (a^\dagger + a) | 0 \rangle = \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} \langle n | (a^\dagger)^3 + a^\dagger a a^\dagger + a (a^\dagger)^2 | 0 \rangle \\ &= \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} (\sqrt{6}\delta_{n3} + \delta_{n1} + 2\delta_{n1}) = \left(\frac{\hbar}{2m\omega} \right)^{\frac{3}{2}} (\sqrt{6}\delta_{n3} + 3\delta_{n1}) \end{aligned}$$

We conclude that the possible states are $n = 1$ and $n = 3$. We'll look at transitions from $0 \rightarrow 1$ first (noting that $\omega_{fi} = \omega$ in this case).

$$\begin{aligned} P_{0 \rightarrow 1} &= 9 \left(\frac{\hbar}{2m\omega} \right)^3 \frac{A^2}{\hbar^2} \left| \int_0^\infty e^{-t/\tau} e^{i\omega t} dt \right|^2 = \frac{9A^2\hbar}{8(m\omega)^3} \left| \frac{e^{-t(1/\tau - i\omega)}}{\frac{1}{\tau} - i\omega} \right|_0^\infty \Big|^2 = \frac{9A^2\hbar}{8(m\omega)^3} \left| \frac{-1}{\frac{1}{\tau} - i\omega} \right|^2 \\ &= \frac{9A^2\hbar}{8(m\omega)^3} \left(\frac{1}{\tau^2} + \omega^2 \right)^{-1} \end{aligned}$$

To calculate the transition probability for the $0 \rightarrow 3$ transition, we note that $\omega_{fi} = 3\omega$ for this case, and that apart from this and the coefficient out front nothing changes about the calculation. Thus:

$$P_{0 \rightarrow 3} = \frac{3A^2\hbar}{4(m\omega)^3} \left(\frac{1}{\tau^2} + 9\omega^2 \right)^{-1}$$

(b) It is relatively apparent that $P_{0 \rightarrow 1} + P_{0 \rightarrow 3} \neq 1$. This is alright however, because we are only considering the first order correction. Since this scheme is necessarily approximate, it is not surprising that we may have missed some aspects of the system which would rectify this situation.

14.2 Problem 54

Consider a perturbation due to linear Stark effect $H_1 = e(\mathbf{r} \cdot \mathbf{E})$.

(a) Can a first-order perturbation due to a linear Stark effect exist between the degenerate states $|n_1, n_2\rangle$ and $|n_2, n_1\rangle$ of the two dimensional infinite well? Assume the well is centered at the origin.

(b) Can a first order perturbation due to a linear Stark effect exist between degenerate states of the 3D SHO? The energy spectrum is $E = \hbar\omega(2n_r + \ell + 3/2)$, where ℓ determines the parity of the associated wave function. (The parity of the state $|n_r, \ell\rangle$ when written in the coordinate basis is $(-1)^\ell$.)

Solution

(a) Let $\mathbf{E} = E\hat{x}$. Then the question is whether or not the statement $\langle n_1 n_2 | x | n_2 n_1 \rangle$ is correct or not. Recall that the parity of the the eigenstates of the well goes as $(-1)^{n+1}$ in each spatial dimension. Consider the following:

$$\langle n_1 | x | n_2 \rangle \langle n_2 | n_1 \rangle \rightarrow ((-1)^{n_1+1}(-1)(-1)^{n_2+1}) ((-1)^{n_2+1}(-1)^{n_1+1}) = (-1)^{n_1+n_2+3}(-1)^{n_1+n_2+2} = -1$$

We conclude that for any combination of n_1 and n_2 the overall parity of the expression of interest is odd, and the matrix element must therefore always be zero. Therefore there is no first-order perturbation due to the linear Stark effect in the 2D infinite well.

(b) Let's pick $\mathbf{E} = E\hat{z}$ this time. We try the same sort of argument as in part (a). Consider:

$$\langle n'_r \ell' | z | n_r \ell \rangle \rightarrow (-1)^{\ell'}(-1)(-1)^\ell = (-1)^{\ell'+\ell+1}$$

Therefore we require that $\ell + \ell'$ be an odd number in order for a matrix element to be nonzero. But we have also specified that we are looking at degenerate states, which means that

$$2n'_r + \ell' = 2n_r + \ell \rightarrow 2(n'_r - n_r) = \ell - \ell'$$

Since the LHS of this last expression has a two in it, this implies that for degenerate states $\ell - \ell'$ can never be odd. Therefore such a first-order perturbation is not possible.

14.3 Problem 55

A Hydrogen atom, in the ground state, is placed between the plates of a parallel plate capacitor. A time-dependent, but spatially uniform electric field is applied as follows:

$$\mathbf{E} = \begin{cases} 0 & t < 0 \\ E_0 e^{-t/\tau} \hat{z} & t > 0 \end{cases}$$

To first-order, can the atom excite to the $2s$ state? How about the $2p$ states?

Solution

Recall that the parity of a state Y_ℓ^m is given by $(-1)^\ell$. The initial state for the system is the ground state $|100\rangle$, and the matrix elements of interest are of the form $\langle n' \ell' m' | z | n \ell m \rangle$. We are considering the possibility of transitions to the $2s$ state $\langle 200 |$ and $2p$ states $\langle 21m' |$. For the $2s$ state we observe that:

$$\langle 200 | z | 100 \rangle \rightarrow (-1)^0(-1)(-1)^0 = -1 \rightarrow \langle 200 | z | 100 \rangle = 0$$

For the $2p$ state we see that:

$$\langle 21m | z | 100 \rangle \rightarrow (-1)^1(-1)(-1)^0 = 1 \rightarrow \text{Possible so far}$$

Let's now consider which values of m would be possible, noting that $[L_z, z] = 0$.

$$\langle n' \ell' m' | [L_z, z] | n \ell m \rangle = 0 = \langle n' \ell' m' | L_z z - z L_z | n \ell m \rangle = (m - m') \langle n' \ell' m' | z | n \ell m \rangle$$

This last expression must equal zero one way or another, so if $(m - m') \neq 0$ then $\langle n' \ell' m' | z | n \ell m \rangle$ must be zero. Therefore the only possible transition is to the state $|210\rangle$.

14.4 Problem 56

Consider a Hydrogen atom subjected to the perturbation $H_1 = Axy$ (quadrupole Stark effect). Construct the first-order $n = 3$ submatrix. Do not evaluate any integrals; identify which elements must be zero and then identify non-zero elements with constants of your choosing.

Solution

First-order perturbation theory requires us to consider the matrix elements of the perturbing Hamiltonian calculated within all combinations of degenerate eigenstates of the unperturbed Hamiltonian. Let's begin by considering the perturbing Hamiltonian $H_1 = Axy = A(r \cos \theta \cos \varphi)(r \cos \theta \sin \varphi)$. The parity of H_1 is even, and the eigenfunctions of the unperturbed Hydrogen atom have parity that goes as $(-1)^\ell$. Therefore any matrix elements for which $\ell - \ell'$ is odd will include an integral in θ and φ that is overall odd, and will therefore go to zero. Matrix elements marked with a black zero in the grid below have been discarded because of this consideration.

Furthermore the φ dependence of H_1 can be rearranged as follows:

$$\cos \varphi \sin \varphi = \frac{1}{4i}(e^{i\varphi} + e^{-i\varphi})(e^{i\varphi} - e^{-i\varphi}) = \frac{1}{4i}(e^{2i\varphi} - e^{-2i\varphi})$$

We note that the integral below for integer p and q obeys:

$$\int_0^{2\pi} e^{-ip\varphi} e^{iq\varphi} d\varphi = 2\pi\delta_{pq}$$

In calculating the matrix elements $\langle 3\ell'm' | H_1 | 3\ell m \rangle$ the spherical harmonics from each wavefunction will contribute $e^{i(m-m')\varphi}$ to the integral. Combined with the φ dependence of H_1 , we conclude that only matrix elements with $\Delta m = \pm 2$ will survive integration with respect to φ . Elements discarded for this reason, which were not already discarded due to parity considerations, are marked below with a red zero.

The remaining matrix elements are marked with constants. We obtain a total of 6 matrix elements which need to be calculated, when we consider that the matrix must be Hermitian and mirror elements across accordingly.

nlm	300	31-1	310	311	32-2	32-1	320	321	322
300	0	0	0	0	a	0	0	0	b
31-1	0	0	0	c	0	0	0	0	0
310	0	0	0	0	0	0	0	0	0
311	0	c^*	0	0	0	0	0	0	0
32-2	a^*	0	0	0	0	0	d	0	0
32-1	0	0	0	0	0	0	0	e	0
320	0	0	0	0	d^*	0	0	0	f
321	0	0	0	0	0	e^*	0	0	0
322	b^*	0	0	0	0	0	f^*	0	0

In matrix form this reads:

$$H_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & a & 0 & 0 & 0 & b \\ 0 & 0 & 0 & c & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a^* & 0 & 0 & 0 & 0 & 0 & d & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e & 0 \\ 0 & 0 & 0 & 0 & d^* & 0 & 0 & 0 & f \\ 0 & 0 & 0 & 0 & 0 & e^* & 0 & 0 & 0 \\ b^* & 0 & 0 & 0 & 0 & 0 & f^* & 0 & 0 \end{pmatrix}$$

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15.1 Problem 57

Consider the momentum eigenstates $\psi(x) = e^{\pm ikx}$ in one dimension of length L .

(a) What condition on k makes $\psi(x) = \psi(x + L)$?

(b) In the continuum, the number of states is determined by the expression below, where $\rho(E)$ is the density of states.

$$\int \rho(E)dE = \frac{L}{2\pi} \int dk$$

Determine $\rho(E)$ for a free particle.

(c) Determine $d\rho(E)$ for a free particle in three dimensions (in terms of the differential solid angle in k -space).

Solution

(a)

$$e^{ikx} = e^{ik(x+L)} \rightarrow kL = 2\pi n \quad \text{for } n \in \mathbb{Z}$$

(b) Note that this is all performed in the continuum, which means that we are looking at the (non-quantized) unbound states of a free particle. The density of states tells us how many states we can expect to find within a certain interval of energies.

$$\begin{aligned} \int \rho(E)dE &= \frac{L}{2\pi} \int dk \rightarrow E = \frac{\hbar^2 k^2}{2m} \rightarrow dE = \frac{\hbar^2}{m} k dk \\ \int \rho(E)dE &= \frac{L}{2\pi} \int \frac{m}{\hbar^2 k} dE \rightarrow \rho(E) = \frac{Lm}{2\pi\hbar\sqrt{2mE}} \end{aligned}$$

(c) We begin by generalizing the expression given above for one dimension into three. Note that $d\Omega_k$ is the differential solid angle in k -space.

$$\int \rho(E)dE = \frac{L}{2\pi} \int dk \rightarrow \int \rho(E)dE = \frac{L^3}{(2\pi)^3} \int k^2 dk d\Omega_k$$

The expression we found above relating dk and dE holds, so we do the following:

$$\int \rho(E)dE = \frac{L^3}{(2\pi)^3} \int k^2 dk d\Omega_k = \frac{V}{(2\pi)^3} \int \frac{km}{\hbar^2} dE d\Omega_k \rightarrow d\rho(E) = \frac{mV\sqrt{2mE}}{(2\pi)^3\hbar^3} d\Omega_k$$

Note that we have repeatedly used $k = \sqrt{2mE}/\hbar$ above, and that the differential volume $k^2 dk d\Omega_k$ in k -space is directly analogous to $d^3x = r^2 dr d\Omega$ for regular spatial integrals.

Effectively what we are saying with this problem is that we are considering a very large box for $V = L^3$, where very large means that the difference in energies between states has become so small that we can model the behavior with integrals rather than discrete sums. This is in general how we treat the continuum. (You may recall that similar approaches are used regularly in statistical mechanics.)

15.2 Problem 58

Consider the perturbation shown below, where Ω is a time-independent operator (we are looking at the transition probability for a Harmonic Perturbation).

$$V(t) = \Omega e^{i\omega t} + \Omega^\dagger e^{-i\omega t}$$

(a) Compute the first-order transition probability (in terms of the undetermined spatial component). Disregard the cross-terms because they will not play a role in the next part.

(b) Take the limit of the transition rate (probability per unit time) for $t \rightarrow \infty$. Use the identity

$$\lim_{a \rightarrow \infty} \frac{\sin^2(ax)}{\pi a x^2} = \delta(x)$$

(c) From part (b) what physical effect does $e^{\pm i\omega t}$ have on the transition rate?

(d) How does this result change when transitions are to the continuum?

Solution

(a) This is effectively a statement to set up the problem using the first-order transition probability used in problem 1 of workshop 14:

$$P_{i \rightarrow f} = \frac{1}{\hbar^2} \left| \int_0^t \langle \psi_f | \Omega | \psi_i \rangle e^{i\omega t'} e^{i\omega_{fi} t'} dt' \right|^2 + \frac{1}{\hbar^2} \left| \int_0^t \langle \psi_f | \Omega^\dagger | \psi_i \rangle e^{-i\omega t'} e^{i\omega_{fi} t'} dt' \right|^2$$

We are already neglecting the cross terms by taking the mod-square of each individual term.

(b) The transition rate R is given by $R = P_{i \rightarrow f}/t$. We are interested in $\lim_{t \rightarrow \infty} R$. We'll reduce the expression above and then take the limit.

$$\begin{aligned} R &= \lim_{t \rightarrow \infty} \frac{1}{\hbar^2 t} \left(\left| \langle \psi_f | \Omega | \psi_i \rangle \frac{1 - e^{i(\omega + \omega_{fi})t}}{i(\omega + \omega_{fi})} \right|^2 + \left| \langle \psi_f | \Omega^\dagger | \psi_i \rangle \frac{1 - e^{i(-\omega + \omega_{fi})t}}{i(\omega_{fi} - \omega)} \right|^2 \right) \\ &= \lim_{t \rightarrow \infty} \frac{1}{\hbar^2} \left[|\langle \Omega \rangle_{fi}|^2 \left| \frac{e^{i(\omega_{fi} + \omega)t} - 1}{\omega_{fi} + \omega} \right|^2 + |\langle \Omega^\dagger \rangle_{fi}|^2 \left| \frac{e^{i(\omega_{fi} - \omega)t} - 1}{\omega_{fi} - \omega} \right|^2 \right] \\ &= \lim_{t \rightarrow \infty} \frac{4}{\hbar^2} \left[|\langle \Omega \rangle_{fi}|^2 \frac{\sin^2[(\omega_{fi} + \omega)t/2]}{(\omega_{fi} + \omega)^2} + |\langle \Omega^\dagger \rangle_{fi}|^2 \frac{\sin^2[(\omega_{fi} - \omega)t/2]}{(\omega_{fi} - \omega)^2} \right] \\ &= \frac{2\pi}{\hbar} [|\langle \psi_f | \Omega | \psi_i \rangle|^2 \delta(E_f - E_i + \hbar\omega) + |\langle \psi_f | \Omega^\dagger | \psi_i \rangle|^2 \delta(E_f - E_i - \hbar\omega)] \end{aligned}$$

(c) Let's stop and interpret this result for a moment, because the two terms have two different meanings. In the first, we see that the initial energy is necessarily higher than the final energy. In that case, we are looking at a system initially in an excited state, which de-excites and emits a photon of energy $\hbar\omega$ under the effect of the perturbation at hand. This process is referred to as stimulated emission. The second term goes the opposite way: the perturbation causes the absorption of a photon of energy $\hbar\omega$ leading to an excitation. So the terms $e^{\pm i\omega t}$ correspond to the absorption or emission of a photon of energy $\hbar\omega$.

(d) In the continuum (unbound states) we must modify our expressions a bit. In particular, we want to consider the number of final states which exist between the energies E_f and $E_f + dE_f$; we use the density of states ρ , which we explored in problem 1, which is defined such that $E_f + dE_f = \rho(E_f)dE_f$. We integrate our final result over the possible states in the continuum case, instead of just leaving the delta functions in place for the quantized states above:

$$R = \int \frac{P_{if}(t)}{t} \rho(E_f) dE_f$$

Integrating the delta functions will then use their sifting property over the density of states. We consider the absorbing and emitting cases below, notated as R_a and R_e , respectively.

$$R_a = \frac{2\pi}{\hbar} |\langle \psi_f | \Omega^\dagger | \psi_i \rangle|^2 \int \delta(E_f - E_i - \hbar\omega) \rho(E_f) dE_f = \frac{2\pi}{\hbar} |\langle \psi_f | \Omega^\dagger | \psi_i \rangle|^2 \rho(E_f) \Big|_{E_f = E_i + \hbar\omega}$$

$$R_e = \frac{2\pi}{\hbar} |\langle \psi_f | \Omega | \psi_i \rangle|^2 \int \delta(E_f - E_i + \hbar\omega) \rho(E_f) dE_f = \frac{2\pi}{\hbar} |\langle \psi_f | \Omega | \psi_i \rangle|^2 \rho(E_f) \Big|_{E_f = E_i - \hbar\omega}$$

These first order results treating transitions to or from the continuum to first order are often referred to as Fermi's Golden Rule. Those wishing for further practice with this should repeat the derivation we have performed above to obtain

$$R = \frac{2\pi}{\hbar} |\langle \psi_f | H_1 | \psi_i \rangle|^2 \rho(E_i)$$

in the case where the perturbation H_1 is constant in time. (This derivation is similar to, and slightly easier than the one done above, and I highly recommend it as practice.)

15.3 Problem 59

Comment on the calculation of the integral

$$\int z e^{i\mathbf{k} \cdot \mathbf{r}} e^{-r/a_0} d^3x$$

Solution

Suppose we are interested in using the result of problem 2 to calculate a transition probability for the ionization of a Hydrogen atom due to Stark effect. This corresponds to an excitation of a particular quantized state of the H-atom to the continuum. We could reasonably model the continuum state (ψ_f) with a plane-wave (as motivated in problem 1), and would then use a Hydrogen wavefunction as the other state (ψ_i). This would give us a radial integral of the form shown above.

Now let's consider the following regarding the actual evaluation of such an integral:

$$\int z e^{i\mathbf{k}\cdot\mathbf{r}} e^{-r/a_0} d^3x = -i \frac{\partial}{\partial k_z} \int e^{i\mathbf{k}\cdot\mathbf{r}} e^{-r/a_0} d^3x$$

The integral left over after re-writing with the parametric differentiation is invariant under a change of direction of \mathbf{k} . We'll choose \mathbf{k} along z then, so that when we re-write $\mathbf{k} \cdot \mathbf{r} = kr \cos \theta$ the angle θ will be the polar angle in spherical coordinates. We call the integral below $f(k)$.

$$-i \frac{\partial}{\partial k_z} \int e^{ikr \cos \theta} e^{-r/a_0} r^2 \sin \theta dr d\theta d\varphi = -i \frac{\partial}{\partial k_z} f(k) = -i f'(k) \frac{\partial k}{\partial k_z} = -i f'(k) \cos \theta_k$$

Consider how this can reduce the amount of work involved in this sort of calculation.

15.4 Problem 60

A Hydrogen atom is subjected to $V = Axyz$.

- Show that the $n = 1$ and $n = 2$ levels are unaffected up to first-order in A .
- Construct the $n = 3$ first-order correction submatrix of H . Identify non-zero elements with constants of your choosing.
- Make the matrix block-diagonal. When doing so, you must conserve the property $H = H^\dagger$.
- Determine the eigenvalues in terms of your constants.
- Explain why all of the non-zero matrix elements can be expressed in terms of a single radial integral.

Solution

(a) Note that H_1 is overall odd in this problem, and that xy creates a selection rule $\Delta m = \pm 2$. The only way to get $\Delta m = \pm 2$ for the $n = 0$ and $n = 1$ submatrices are for the matrix elements with $m' = -1$ and $m = +1$ or vice versa. But these are both $\ell = 1$ states, so these matrix elements are zero due to parity. Therefore there are no non-zero matrix elements within the $\ell = 0$ and $\ell = 1$ regions of any submatrix. (And for $n = 0$ and $n = 1$ this is all there is.)

(b) We apply the same approach and labeling as in problem 14.4.

$n\ell m$	300	31-1	310	311	32-2	32-1	320	321	322
300	0	0	0	0	0	0	0	0	0
31-1	0	0	0	0	0	0	0	c	0
310	0	0	0	0	a	0	0	0	b
311	0	0	0	0	0	d	0	0	0
32-2	0	0	a^*	0	0	0	0	0	0
32-1	0	0	0	d^*	0	0	0	0	0
320	0	0	0	0	0	0	0	0	0
321	0	c^*	0	0	0	0	0	0	0
322	0	0	b^*	0	0	0	0	0	0

(c) Let's number the columns of the matrix above 1-9. Then consider manipulating the columns so that they now go in the order (3,5,9,2,8,4,6,1,7) according to that numbering. Change the order of the rows in the same way in order to preserve $H = H^\dagger$. (Notice that the order in which we happened to write each state down the sides was arbitrary to begin with so this should be no problem. Also, exchanging two rows or columns only affects the determinant of a matrix up to

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Problem 61

Consider the following Hamiltonian, where $B \ll A$:

$$H = AJ_z + BJ_y$$

- Determine the eigenvalues of H up to $O(B^2)$.
- Determine the eigenvalues of H exactly.
- Expand the result from part (b) to $O(B^2)$ and show that it agrees with part (a).

Solution

(a) We take $H_0 = AJ_z$ and $H_1 = BJ_y$. The eigenstates of H_0 are of the form $|jm\rangle$. We begin with the first order corrections:

$$E^{(1)} = \langle jm | BJ_y | jm \rangle = \frac{B}{2i} \langle jm | J_+ - J_- | jm \rangle = 0$$

There are no first order corrections, so we proceed to second order. The general formula is shown below.

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle n^{(0)} | H_1 | m^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

We have $E_n^{(0)} = An\hbar$ for the purposes of that notation, and wish to evaluate:

$$\begin{aligned} E_m^{(2)} &= \frac{B^2}{4} \sum_{m \neq m'} \frac{|\langle jm | J_+ - J_- | j'm' \rangle|^2}{Am\hbar - Am'\hbar} = \frac{B^2\hbar}{4A} \left[\frac{|\sqrt{j(j+1) - m(m-1)}|^2}{m - (m-1)} + \frac{|\sqrt{j(j+1) - m(m+1)}|^2}{m - (m+1)} \right] \\ &= \frac{B^2\hbar}{4A} [j(j+1) - m(m-1) - [j(j+1) - m(m+1)]] = \frac{B^2\hbar}{4A} (2m) = \frac{B^2\hbar}{2A} m \end{aligned}$$

So the energy up to $O(B^2)$ is given by:

$$E = Am\hbar + \frac{B^2\hbar}{2A} m$$

(b) Now let's solve it exactly. Note that any Hamiltonian of the form $H = C\mathbf{J} \cdot \hat{\mathbf{n}}$ will have eigenvalues $Cm\hbar$ when the projections are measured along the $\hat{\mathbf{n}}$ axis. Consider:

$$H = AJ_z + BJ_y = C\mathbf{J} \cdot \hat{\mathbf{n}} = C(J_x, J_y, J_z) \cdot (0, B, A) \frac{1}{\sqrt{A^2 + B^2}} \rightarrow C = \sqrt{A^2 + B^2} \rightarrow E = \sqrt{A^2 + B^2} m\hbar$$

(c) Now we have eigenvalues, and can expand assuming $B \ll A$ to check against part (a).

$$E = \sqrt{A^2 + B^2} m\hbar = m\hbar A \sqrt{1 + \frac{B^2}{A^2}} \approx Am\hbar \left(1 + \frac{B^2}{2A^2} \right) = Am\hbar + \frac{B^2\hbar}{2A} m$$

We see that is in perfect agreement with the perturbative result to the same order.

Problem 62

Consider the Hamiltonian

$$H = A\mathbf{J}^2 + BJ_z^2$$

- Determine the eigenvalues and eigenvectors of H .
- Consider a perturbation $H_1 = Cxz$. Justify why the first-order perturbations vanish.

Solution

(a) The eigenvalues are easily determined in the coupled basis, and the basis states in the coupled basis are eigenstates of H . Consider:

$$H|jm\rangle = (AJ^2 + BJ_z^2)|jm\rangle = \hbar^2(Aj(j+1) + Bm^2)|jm\rangle$$

That takes care of both the eigenvalues and eigenvectors.

(b) Notice that H breaks up the degeneracy between the $|jm\rangle$ states that the eigenvalues J^2 and J_z alone would leave. Except for possible specific integer relationships between A and B , which we will neglect in this treatment, the only degeneracy is between $\pm m$ for a given j . In this case, we would in general need to evaluate matrix elements of the form where $m' = \pm m$.

$$\langle jm' | xz | jm \rangle$$

Note that xz is even, and implies a selection rule of $\Delta m = \pm 1$. (See workshop problems 14.4 and 15.4 if you do not immediately see why.) But when j and m are the same on both sides, the selection rule $\Delta m = \pm 1$ would not be satisfied, and this expectation value is always zero. Likewise, when $m \neq 0$ and $m' = -m$, the difference $m' - m$ is at least two, also violating the selection rule.

The part we are ignoring: There are almost certainly special cases choices of A and B for which states with a different j and m could create the same energy. This is more difficult to deal with, and we will not consider this case.

Problem 63

Consider an H -atom with an angular wavefunction

$$AY_2^0 + BY_2^1$$

where $|A|^2 + |B|^2 = 1$.

- (a) Determine the expectation of \mathbf{L}^2 and L_z .
- (b) Determine the expectation of L_x .
- (c) Determine the minimum value of energy that can be measured.

Solution

Let $|\psi\rangle = A|20\rangle + B|21\rangle$ where the states are labeled according to $|\ell m\rangle$

- (a) In order to calculate $\langle L^2 \rangle$ we consider the following:

$$\langle L^2 \rangle = (A^* \langle 20| + B^* \langle 21|) L^2 (A|20\rangle + B|21\rangle) = (A^* \langle 20| + B^* \langle 21|) 6\hbar^2 (A|20\rangle + B|21\rangle) = 6\hbar^2 (|A|^2 + |B|^2) = 6\hbar^2$$

For L_z :

$$\langle L_z \rangle = \langle \psi | L_z (A|20\rangle + B|21\rangle) = \langle \psi | (\hbar B |21\rangle) = \hbar |B|^2$$

- (b) Recall that $L_x = \frac{1}{2}(L_+ + L_-)$.

$$L_x |\psi\rangle = \frac{1}{2} (L_+ + L_-) (A|20\rangle + B|21\rangle) = \frac{\hbar\sqrt{6}}{2} [A(|2-1\rangle + |21\rangle) + B|20\rangle] + B|22\rangle$$

$$\langle L_x \rangle = \frac{\hbar\sqrt{6}}{2} (B^* A + A^* B)$$

(c) We have $\ell = 2$, and ℓ ranges up to $n - 1$. So $n = 3$ is the smallest principle quantum number of a Hydrogen state for which the above could be the angular wavefunction.

Problem 64

Consider four spin- $\frac{1}{2}$ particles.

- (a) How many states does the system have?
- (b) Determine the possible values of \mathbf{S}^2 and S_z .
- (c) Determine a CSCO.

Solution

(a) Each particle has 2 states, and there are 4 particles. The number of states is given by $2^4 = 16$.

(b)

$$\frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} \otimes \frac{1}{2} = (1 \oplus 0) \otimes \frac{1}{2} \otimes \frac{1}{2} = \left(\frac{3}{2} \oplus \frac{1}{2} \oplus \frac{1}{2} \right) \otimes \frac{1}{2} = (2 \oplus 1) \oplus (1 \oplus 0) \oplus (1 \oplus 0)$$

The possible values of $S^2 \rightarrow \hbar^2 S(S+1)$ are thus $6\hbar^2$, $2\hbar^2$, and 0. We check that above expansion is consistent with part (a), using the fact that there are $2S+1$ projections for each S . We see that $5+3+3+1+3+1=16$, which agrees with the above. The possible values of S_z are $\pm 2\hbar$, $\pm 1\hbar$, and 0.

(c) The simplest CSCO is $\{S_1^2, S_2^2, S_3^2, S_4^2, S_{1z}, S_{2z}, S_{3z}, S_{4z}\}$, although many others are possible.

Problem 65

Consider a system of $j_i = \frac{1}{2}$ with Hamiltonian

$$H = A(\mathbf{J}_1 \cdot \mathbf{J}_2)(\mathbf{J}_3 \cdot \mathbf{J}_4)$$

(a) Determine the eigenvalues of H and the degeneracies of each.

(b) Show that the sum of the above is zero and explain why.

(c) Determine a CSCO.

Solution

(a) Let $\mathbf{J}_{12} = \mathbf{J}_1 + \mathbf{J}_2$ and $\mathbf{J}_{34} = \mathbf{J}_3 + \mathbf{J}_4$.

$$H = \frac{A}{4}(J_{12}^2 - J_1^2 - J_2^2)(J_{34}^2 - J_3^2 - J_4^2) \rightarrow \frac{A}{4} \left(J_{12}^2 - \frac{3\hbar^2}{2} \right) \left(J_{34}^2 - \frac{3\hbar^2}{2} \right)$$

Clearly, J_{12} and J_{34} commute with each other, and each can take on values of 0 or 1 (since each contains two spins). Each value occurs in 1 and 3 states respectively in each of the two-spin subspaces. Thus we have the following combinations to consider in putting in numbers for J_{12} and J_{34} :

$$J_{12} = J_{34} = 1 \quad (9 \text{ states}) \quad J_{12} = 1, J_{34} = 0 \text{ or } J_{12} = 0, J_{34} = 1 \quad (3 \text{ states each}) \quad J_{12} = J_{34} = 0 \quad (1 \text{ state})$$

Then we have the following eigenvalues:

$$\begin{aligned} E &= \frac{A}{4} \left(2\hbar^2 - \frac{3\hbar^2}{2} \right) \left(2\hbar^2 - \frac{3\hbar^2}{2} \right) = \frac{A\hbar^4}{16} \rightarrow 9 \times \\ E &= \frac{A}{4} \left(0 - \frac{3\hbar^2}{2} \right) \left(2\hbar^2 - \frac{3\hbar^2}{2} \right) = -\frac{3A\hbar^4}{16} \rightarrow 6 \times \\ E &= \frac{A}{4} \left(0 - \frac{3\hbar^2}{2} \right) \left(0 - \frac{3\hbar^2}{2} \right) = \frac{9A\hbar^4}{16} \rightarrow 1 \times \end{aligned}$$

(b) The weighted sum of the eigenvalues is:

$$\frac{A\hbar^4}{16} (1 \cdot 9 - 3 \cdot 6 + 9 \cdot 1) = 0$$

This is expected because it is equivalent to taking the Trace of H and we have:

$$Tr(H) = A Tr[(J_{1i} J_{2i})(J_{3k} J_{4k})] = A Tr(J_{1i}) Tr(J_{2i}) Tr(J_{3k}) Tr(J_{4k}) = 0$$

(The second subscript indicates a particular spatial coordinate of each angular momentum operator. The operation of splitting up the trace is allowed for different angular momenta which are in separate subspaces, but not different spatial directions corresponding to the same operator.)

(c) Once again $\{J_1^2, J_2^2, J_3^2, J_4^2, J_{1z}, J_{2z}, J_{3z}, J_{4z}\}$ works, but it is more interesting to consider a CSCO containing the Hamiltonian. Note that since the Hamiltonian contains only dot products, it is a scalar and must therefore be rotationally invariant. Consider $\{H, J_1^2, J_2^2, J_3^2, J_4^2, J^2, J_{12z}, J_{34z}\}$.

Problem 66

Consider three spin one-half particles with the Hamiltonian

$$H = A(\mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_2)$$

- (a) Determine the eigenvalues of H and degeneracies of each.
- (b) Show that the sum is zero.
- (c) Determine a CSCO.

Solution

(a) Let's rewrite H a little bit. Let $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3$, and let $\mathbf{S}_{12} = \mathbf{S}_1 + \mathbf{S}_2$.

$$H = A(\mathbf{S}_1 + \mathbf{S}_2) \cdot \mathbf{S}_3 = A\mathbf{S}_{12} \cdot \mathbf{S}_3 = \frac{A}{2} ((S_{12} + S_3)^2 - S_{12}^2 - S_3^2) = \frac{A}{2}(S^2 - S_{12}^2 - S_3^2) = \frac{A}{2} \left(S^2 - S_{12}^2 - \frac{3\hbar^2}{4} \right)$$

$$\text{Possible values: } S = (3/2, 1/2, 1/2) \quad S_{12} = (1, 0) \quad S_3 = 1/2$$

Let $S = 3/2$, which requires that $S_{12} = 1$. 4 such states.

$$E = \frac{A\hbar^2}{2} \left(\frac{15}{4} - 2 - \frac{3}{4} \right) = \frac{A\hbar^2}{2}$$

Let $S = 1/2$ and $S_{12} = 1$. 2 such states.

$$E = \frac{A\hbar^2}{2} \left(\frac{3}{4} - 2 - \frac{3}{4} \right) = -A\hbar^2$$

Let $S = 1/2$ and $S_{12} = 0$. 2 such states.

$$E = \frac{A\hbar^2}{2} \left(\frac{3}{4} - 0 - \frac{3}{4} \right) = 0$$

(b) We take the sum (weighted by degeneracy), to verify that the trace of H will be zero. (We haven't found the eigenbasis of H , but we know that an eigenbasis in which H is diagonal must exist, and that this would be the trace in that basis.)

$$\text{Tr}(H) = 4 \left(\frac{A\hbar^2}{2} \right) + 2(-A\hbar^2) + 2(0) = 0$$

(c) We expect that we will require 6 operators to define a CSCO for this system. Again it is more interesting to consider a CSCO including H . Consider:

$$\{H, S_z, S_{3z}, S^2, S_{12}^2, S_3^2\}$$

Problem 67

Two protons are located on the z -axis, separated by a distance d , and subjected to a magnetic field $\mathbf{B} = B_0\hat{z}$. The magnetic moment of the i^{th} proton is $\mu_i = 2\mu_0\mathbf{S}_i/\hbar$.

- (a) Ignoring proton-proton interaction, find the energy levels and states of the system.
- (b) The dipole-dipole magnetic interaction energy between the protons is

$$H_1 = \frac{1}{r^3} \left(\mu_1 \cdot \mu_2 - 3 \frac{(\mu_1 \cdot \mathbf{r})(\mu_2 \cdot \mathbf{r})}{r^2} \right)$$

where \mathbf{r} is the separation vector. Calculate the Energy levels.

- (c) Determine a CSCO for parts (a) and (b) which includes H .

Solution

(a) Ignoring the proton-proton interaction, the Hamiltonian is given by

$$H_0 = -\boldsymbol{\mu} \cdot \mathbf{B} = -\frac{2\mu_0}{\hbar}(\mathbf{S}_1 + \mathbf{S}_2) \cdot \mathbf{B} = -\frac{2\mu_0}{\hbar}B_0(S_{1z} + S_{2z})$$

The states are those for the coupling of two spin- $\frac{1}{2}$ objects, and the usual states $\{|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\}$ in the uncoupled basis happen to be eigenstates of this Hamiltonian. (These are the states which are eigenstates of the z-components of each of the two individual spin operators.) The matching energies are:

$$E = \{-2\mu_0 B_0, 0, 0, 2\mu_0 B_0\}$$

(b) We now have a Hamiltonian $H = H_0 + H_1$ in order to account for the proton-proton interaction. Note that the separation vector $\mathbf{r} = d\hat{z}$. Then:

$$H_1 = \frac{4\mu_0^2}{d^3\hbar^2}(\mathbf{S}_1 \cdot \mathbf{S}_2 - 3S_{1z}S_{2z}) = \frac{4\mu_0^2}{d^3\hbar^2} \left(\frac{S^2 - S_1^2 - S_2^2}{2} - 3S_{1z}S_{2z} \right)$$

We note that we have one term which is evaluated naturally in the coupled basis, and one term which is evaluated naturally in the uncoupled basis.

$$H_1|11\rangle = H_1|++\rangle = \frac{4\mu_0^2}{d^3\hbar^2} \left(\frac{1}{2} \left[2\hbar^2 - \frac{3}{2}\hbar^2 \right] - \left[\frac{\hbar}{2} \right]^2 \right) |11\rangle = -\frac{2\mu_0^2}{d^3\hbar^2} |11\rangle$$

$$H_1|1-1\rangle = H_1|--\rangle = -\frac{2\mu_0^2}{d^3\hbar^2} |1-1\rangle$$

$$H_1|10\rangle = H_1 \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) = \frac{4\mu_0^2}{d^3\hbar^2} \left(\frac{\hbar^2}{4} + 3 \cdot 2 \left[\frac{\hbar}{2} \right]^2 \right) |10\rangle = \frac{4\mu_0^2}{d^3\hbar^2} |10\rangle$$

$$H_1|00\rangle = H_1 \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) = 0$$

Recombining this with $H = H_0 + H_1$ the complete spectrum for this problem can be effectively summarized as:

$$E = \begin{pmatrix} \langle 11|H|11\rangle \\ \langle 1-1|H|1-1\rangle \\ \langle 10|H|10\rangle \\ \langle 00|H|00\rangle \end{pmatrix} = 2\mu_0 B_0 \begin{pmatrix} -1 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \frac{2\mu_0^2}{d^3} \begin{pmatrix} -1 \\ -1 \\ 2 \\ 0 \end{pmatrix}$$

(c) H_0 is not a CSCO due to degeneracy, but H has no degeneracy left once the two-particle interaction is taken into account. Therefore H is a CSCO by itself in the coupled problem (part (b)).

Problem 68

A particle is in the potential

$$V(r) = \begin{cases} 0 & a \leq r \leq b \\ \infty & \text{else} \end{cases}$$

(a) Determine the ground state wavefunction and energy.

(b) Consider the perturbation (linear Stark effect) $H_1 = Az$, which effectively transitions the particle to another state. What are the smallest possible measurements of L^2 and L_z .

Solution

(a) We begin with the radial Schrodinger equation, where $U = r\psi_R$:

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} - \frac{\ell(\ell+1)}{r^2} \right) U + VU = EU \quad \rightarrow \quad \text{Ground State } \ell = 0 \quad \rightarrow \quad -\frac{\hbar^2}{2m} \frac{\partial^2 U}{\partial r^2} = EU$$

This last expression is what we want to solve in the well region. Clearly the wavefunction is zero where the potential is infinite. We have the following solutions for U :

$$U(r) = \sqrt{\frac{2}{b-a}} \sin\left(\frac{n\pi(r-a)}{b-a}\right) \rightarrow n = 1 \text{ for ground state}$$

And the spectrum:

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{\pi}{b-a}\right)^2$$

In order to construct the complete ground state wavefunction we would need to add the angular distribution:

$$\psi_{gs} = \psi_R Y_0^0 = \frac{1}{r} \sqrt{\frac{2}{b-a}} \sin\left(\frac{n\pi(r-a)}{b-a}\right) Y_0^0 = \frac{1}{r\sqrt{4\pi}} \sqrt{\frac{2}{b-a}} \sin\left(\frac{n\pi(r-a)}{b-a}\right)$$

(b) The Stark effect Hamiltonian $H_1 \propto z$ is odd, so we need $\Delta\ell = \text{odd}$ for a transition. Since z has no φ dependence in spherical coordinates, it has a selection rule $\Delta m = 0$. We are starting in $\ell = 0$ for the ground state, so the transition would have to leave $L_z = 0$ unchanged, and the lowest possible value of L^2 after this transition would be $2\hbar^2$, corresponding to $\ell = 1$.

Problem 69

Calculate the p^4 relativistic correction to the energy spectrum of Hydrogen to first-order. Follow these steps:

- Write p^4 in terms of H , V , and $1/r^2$
- Evaluate each of the terms using Virial theorem or HF theorem.
- Write the correction in terms of the fine structure constant $\alpha = e^2/\hbar c \approx 1/137$.

Solution

(a) Recall that energy is given in relativity by $E^2 = p^2 c^2 + (mc^2)^2$. Kinetic energy would be what is left after subtracting the rest-mass energy, or $T = \sqrt{(pc)^2 + (mc^2)^2} - mc^2$. We expand this:

$$T = mc^2 \left(\sqrt{1 + \frac{p^2}{m^2 c^2}} - 1 \right) \approx mc^2 \left(1 + \frac{p^2}{2m^2 c^2} - \frac{p^4}{8m^4 c^4} - 1 \right) = \frac{p^2}{2m} - \frac{p^4}{8m^3 c^2} \rightarrow H_1 = -\frac{p^4}{8m^3 c^2}$$

We can take this second term containing p^4 to be a first relativistic correction. We're going to do something a little unusual that will let us calculate expectation values of p^4 in Hydrogen. consider the Hydrogen Hamiltonian:

$$H = \frac{p^2}{2m} - \frac{e^2}{r} \rightarrow p^2 = 2m \left(H + \frac{e^2}{r} \right) \rightarrow p^4 = 4m^2 \left(H^2 + H \frac{e^2}{r} + \frac{e^2}{r} H + \frac{e^4}{r^2} \right)$$

We note that $[p^4, L^2] = 0$, that p^4 does not affect m (the projection of ℓ) in any way, and that p^4 is an even operator. We conclude that in an expectation $\langle n\ell m' | p^4 | n\ell m \rangle$ that we must have $\ell = \ell'$ and $m = m'$ to get a result. Then we are effectively only looking at the diagonal of the first-order perturbative submatrix.

(b) Let's take expectation values using the above:

$$\langle n\ell m | p^4 | n\ell m \rangle = 4m^2 \left(E_n^2 + E_n \left\langle n\ell m \left| \frac{e^2}{r} \right| n\ell m \right\rangle + \left\langle n\ell m \left| \frac{e^2}{r} \right| n\ell m \right\rangle E_n + \left\langle n\ell m \left| \frac{e^4}{r^2} \right| n\ell m \right\rangle \right)$$

The middle two terms contain $\langle e^2/r \rangle = -\langle V \rangle$. Recall from the Virial Theorem that for the Hydrogen atom $\langle V \rangle = -2\langle T \rangle$, $-\langle T \rangle = E_n$, and $\langle V \rangle = 2E_n$. We apply this simplification to the above:

$$\langle n\ell m | p^4 | n\ell m \rangle = 4m^2 \left(E_n^2 + E_n(-2E_n) + (-2E_n)E_n + \left\langle n\ell m \left| \frac{e^4}{r^2} \right| n\ell m \right\rangle \right) = 4m^2 \left(-3E_n^2 + \left\langle n\ell m \left| \frac{e^4}{r^2} \right| n\ell m \right\rangle \right)$$

In order to deal with the term $e^4 \langle 1/r^2 \rangle$ we'll use the HF theorem. Consider:

$$\frac{dE}{d\lambda} = \langle \psi | \partial_\lambda H | \psi \rangle \rightarrow \frac{d}{d\lambda} \left(-\frac{m e^4}{2\hbar^2 n^2} \right) = \left\langle \frac{d}{d\lambda} \left(\frac{p_r^2}{2m} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} - \frac{e^2}{r} \right) \right\rangle$$

We let $\lambda \rightarrow \ell$ and note that $n = n_r + \ell + 1$. Then:

$$\frac{d}{d\ell} \left(-\frac{me^4}{2\hbar^2(n_r + \ell + 1)^2} \right) = \left\langle \frac{(2\ell + 1)\hbar^2}{2mr^2} \right\rangle \rightarrow \frac{me^4}{\hbar^2 n^3} = \frac{(2\ell + 1)\hbar^2}{2m} \left\langle \frac{1}{r^2} \right\rangle \rightarrow \left\langle \frac{1}{r^2} \right\rangle = \frac{2m^2 e^4}{\hbar^4 n^3 (2\ell + 1)}$$

Then using this result in our calculation of $\langle p^4 \rangle$:

$$\langle p^4 \rangle = 4m^2 \left(\frac{2m^2 e^8}{\hbar^4 (2\ell + 1)n^3} - 3E_n^2 \right) = 4m^2 E_n^2 \left(\frac{8n}{2\ell + 1} - 3 \right) = \frac{m^4 e^8}{\hbar^4 n^4} \left(\frac{8n}{2\ell + 1} - 3 \right) = \frac{\alpha^4 m^4 c^4}{n^4} \left(\frac{8n}{2\ell + 1} - 3 \right)$$

(c) Given our expectation value for p^4 , we can return the relativistic correction we set out to calculate.

$$E_{n\ell}^{(1)} = -\frac{1}{8m^3 c^2} \langle p^4 \rangle = -\frac{\alpha^4 m c^2}{8n^4} \left(\frac{8n}{2\ell + 1} - 3 \right) = -\frac{\alpha^2 |E_n|}{4n^2} \left(\frac{8n}{2\ell + 1} - 3 \right)$$

Note that since $\alpha \approx 1/137$, we can get the order of this correction. For $E_1 = -13.6\text{eV}$, we would expect $E_{10}^{(1)} \approx 10^{-3}\text{eV}$. The total corrected energy (to first order) is given by $E = E_n + E_{n\ell}^{(1)}$.

Problem 70

When placed in a magnetic field, the Hydrogen energy spectrum is given by

$$H = H_0 + H_{FS} + H_B$$

where H_0 is the unperturbed Hamiltonian, H_{FS} is the fine structure correction (which includes a first order relativistic correction and spin-orbit interaction), and H_B is the interaction from the magnetic field.

In the presence of a strong-field, $H_B \gg H_{FS}$ (Paschen-Back effect – or strong-field Zeeman effect), determine the energy levels for $n = 1$ and $n = 2$.

Solution

Let's consider the last term H_B in the Hamiltonian. The orbital angular momentum and spin could both interact with a magnetic field. Note the two introduced on the spin term (this is the Landé g factor).

$$H_B = -\mu_L \cdot \mathbf{B} - \mu_s \cdot \mathbf{B} = \frac{e}{2mc} (\mathbf{L} \cdot \mathbf{B} + 2\mathbf{S} \cdot \mathbf{B}) = \frac{eB}{2mc} (L_z + 2S_z)$$

We expect both this Zeeman term and the fine-structure term to have very small effects relative to the original Hamiltonian H_0 , and will therefore treat them perturbatively. Specifically for the Paschen-Back effect, we are looking at a regime in which H_B overwhelms H_{FS} , and we will consequently neglect it. (If you wanted to include it, you would need the result from the previous problem, along with a spin-orbit coupling term. It would be a good exercise to compute either if you are not sure you would be able to do so.) So we let $H = H_0 + H_B$ for the remainder of the problem. We note that $[H_B, H_0] = 0$, and that we can therefore diagonalize them in a common set of states $|n\ell m_\ell m_s\rangle$.

$$H|n\ell m_\ell m_s\rangle = \left[H_0 + \frac{eB}{2mc} (L_z + 2S_z) \right] |n\ell m_\ell m_s\rangle = E|n\ell m_\ell m_s\rangle \rightarrow E = -\frac{e^2}{2a_0 n^2} + \frac{eB\hbar}{2mc} (m_\ell + 2m_s)$$

It is then easy to list out the energies for $n = 1$ ($\ell = 0 \rightarrow m_\ell = 0$, and $m_s = \pm\frac{1}{2}$), and $n = 2$ ($\ell = 0, 1 \rightarrow m_\ell = 0, \pm 1$, and $m_s = \pm\frac{1}{2}$).

Problem 71

(a) Two spin-one half particles are in the state

$$|\psi\rangle = A|++\rangle + B|--\rangle$$

where $|A|^2 + |B|^2 = 1$. Determine the possible values of S^2 and S_z and the probabilities of each.

(b) Extend this to Hydrogen, where the angular wavefunction and state ket of the electron is,

$$AY_1^0|-\rangle + BY_1^1|+\rangle$$

No need to determine the probabilities this time.

Solution

(a) Recall the CG coefficients to get between the coupled and uncoupled basis. We plug those in to obtain:

$$|\psi\rangle = A|11\rangle + \frac{B}{\sqrt{2}}(|10\rangle - |00\rangle)$$

Then the possible measurements and probabilities of the operators in question are as follows:

$$S^2 = \begin{cases} 2\hbar^2 \\ 0 \end{cases} \quad \text{With Probabilities:} \quad \begin{array}{l} |A|^2 + |B|^2/2 \\ |B|^2/2 \end{array} \quad S_z = \begin{cases} \hbar \\ 0 \end{cases} \quad \text{With Probabilities:} \quad \begin{array}{l} |A|^2 \\ |B|^2 \end{array}$$

(b) This is not physically a two-particle system, but it works just like one. We have $\mathbf{J} = \mathbf{L} + \mathbf{S}$, where the orbital angular momentum and spin are coupled. Thus we can rewrite the wavefunction in question as:

$$AY_1^0|-\rangle + BY_1^1|+\rangle = A|10\rangle|\frac{1}{2} - \frac{1}{2}\rangle + B|11\rangle|\frac{1}{2} \frac{1}{2}\rangle$$

The first term has $J_z = -1/2$ and the second $J_z = 3/2$. We then apply the same kind of arguments to measure J^2 and J_z as above.

Problem 72

Consider a particle in the potential,

$$V = \frac{m}{2} (\omega_1^2 x^2 + \omega_2^2 y^2)$$

where $\omega_1 \neq \omega_2$. What condition on ω_1 and ω_2 makes H a CSCO?

Solution

We can see that we can write an energy spectrum E_1 in x and E_2 in y , where the overall spectrum is $E = E_1 + E_2$. Then $E_1 = \hbar\omega_1(n_1 + 1/2)$ and $E_2 = \hbar\omega_2(n_2 + 1/2)$. The key observation here is that H is not a CSCO when there is degeneracy in the system. Degeneracy occurs when:

$$\hbar\omega_1(n_1 - n'_1) = \hbar\omega_2(n'_2 - n_2)$$

Thus we may write

$$\frac{\omega_1}{\omega_2} = \frac{n_1 - n'_1}{n_2 - n'_2}$$

where $n_1, n'_1, n_2,$ and n'_2 are all integers. There is no possibility of degeneracy if we cannot satisfy this equation. Thus, if we require that one or both of ω_1 and ω_2 are irrational (such that their ratio is irrational), we will not get degenerate states and H alone can be a CSCO.

17 New Problems

17.1

(a) Show that for any time-independent operator Ω the relationship $\partial_t \langle \Omega \rangle = 0$ holds, where the expectation value is taken between eigenstates of the Hamiltonian.

(b) Consider the Hamiltonian:

$$H = \frac{p^2}{2m} + kx^n = T + V$$

Derive the quantum Virial theorem for such a system, i.e. show that for the above system $2\langle T \rangle = n\langle V \rangle$. (Hint: Choose $\Omega = xp$.)

Solution

(a) We have $H|\psi\rangle = E|\psi\rangle$ and notate $\langle \Omega \rangle = \langle \psi | \Omega | \psi \rangle$. We invoke Heisenberg's equation of motion,

$$\frac{d\Omega}{dt} = \frac{1}{i\hbar} [\Omega, H] \quad \rightarrow \quad \frac{d\langle \Omega \rangle}{dt} = \frac{1}{i\hbar} \langle \psi | [\Omega, H] | \psi \rangle = \frac{1}{i\hbar} (\langle \Omega H \rangle - \langle H \Omega \rangle)$$

and note that since H is Hermitian $\langle \psi | H = \langle \psi | H^\dagger = E \langle \psi |$. This implies:

$$\frac{d\langle \Omega \rangle}{dt} = \frac{1}{i\hbar} (E \langle \Omega \rangle - E \langle \Omega \rangle) = 0 \quad \rightarrow \quad \therefore \quad \dot{\langle \Omega \rangle} = 0 = \langle [\Omega, H] \rangle$$

(b) Let $\Omega = xp$; we have established from part (a) that $\langle [xp, H] \rangle = 0$. We consider the commutator in this expression:

$$[xp, H] = x[p, H] + [x, H]p = x[p, V] + [x, T]p = x[p, kx^n] + \frac{1}{2m}[x, p^2]p = kx(-ni\hbar x^{n-1}) + \frac{1}{2m}(2i\hbar p)p = i\hbar(2T - nV)$$

Therefore, using the result from part (a):

$$\langle [xp, H] \rangle = i\hbar \langle 2T - nV \rangle = i\hbar(2\langle T \rangle - n\langle V \rangle) = 0 \quad \rightarrow \quad 2\langle T \rangle = n\langle V \rangle$$

17.2

A canonical coherent state is an eigenstate of the 1D SHO annihilation operator. Let $|\alpha\rangle$ be a canonical coherent state with eigenvalue α such that $a|\alpha\rangle = \alpha|\alpha\rangle$.

(a) Write $|\alpha\rangle$ as a linear combination of stationary states $|n\rangle$ of the 1D SHO.

(b) Normalize the result from part (a).

(c) Let $|\psi_\alpha\rangle$ be the time-dependent form of the state $|\alpha\rangle$, obtained by using the time evolution operator. Write and simplify $|\psi_\alpha\rangle$ using the results from the previous parts.

(d) Calculate the time-dependent expectation values $\langle x \rangle_t = \langle \psi_\alpha | x | \psi_\alpha \rangle$ and $\langle p \rangle_t = \langle \psi_\alpha | p | \psi_\alpha \rangle$. (Do not do the whole calculation twice. Once you obtain one, you should be able to obtain the other with relatively little work.)

(e) What do you notice about the results from part (d) / How does the behavior of this system compare with that of a classical SHO?

Solution

(a) We begin by expanding $|\alpha\rangle$ in terms of the energy eigenstates of the SHO.

$$|\alpha\rangle = \sum_n |n\rangle \langle n|\alpha\rangle = \sum_n C_n |n\rangle \quad \rightarrow \quad \text{Determine Coefficients } C_n = \langle n|\alpha\rangle$$

We use the property that $a|\alpha\rangle = \alpha|\alpha\rangle$ to proceed.

$$\begin{aligned} a|\alpha\rangle &= \sum_n C_n a|n\rangle = \sum_{n=1}^{\infty} C_n \sqrt{n} |n-1\rangle = \sum_{n=0}^{\infty} C_{n+1} \sqrt{n+1} |n\rangle \\ &= \alpha|\alpha\rangle = \alpha \sum_n C_n |n\rangle \end{aligned}$$

We obtain the recursion relation $\alpha C_n = \sqrt{n+1}C_{n+1}$. If we begin with C_0 and apply this repeatedly, we see that $C_n = \frac{\alpha^n}{\sqrt{n!}}C_0$. Therefore:

$$|\alpha\rangle = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle$$

(b) We determine C_0 by normalization.

$$\begin{aligned} \langle\alpha|\alpha\rangle = 1 &= \left(\sum_m \langle m | \frac{(\alpha^*)^m}{\sqrt{m!}} C_0^* \right) \left(\sum_n \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle \right) = \sum_{n,m} |C_0|^2 \frac{(\alpha^*)^m \alpha^n}{\sqrt{m!n!}} \delta_{nm} = |C_0|^2 \sum_n \frac{|\alpha|^{2n}}{n!} \\ \rightarrow |C_0|^2 &= \left(\sum_n \frac{|\alpha|^{2n}}{n!} \right)^{-1} \end{aligned}$$

(c) The evolution operator is $U = e^{-iHt/\hbar}$. We want to calculate $|\psi_\alpha\rangle = U|\alpha\rangle$.

$$|\psi_\alpha\rangle = e^{-iHt/\hbar} \sum_n \frac{\alpha^n}{\sqrt{n!}} C_0 |n\rangle = C_0 \sum_n \frac{\alpha^n}{\sqrt{n!}} e^{-iE_n t/\hbar} |n\rangle = C_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t(n+1/2)} |n\rangle$$

(d) We calculate $\langle x \rangle_t$ first.

$$\langle\psi_\alpha|x|\psi_\alpha\rangle = |C_0|^2 \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m \alpha^n}{\sqrt{n!m!}} e^{i\omega t(m-n)} \langle m|x|n\rangle$$

The term $\langle m|x|n\rangle$ is of interest.

$$x = \sqrt{\frac{\hbar}{2M\omega}}(a + a^\dagger) \rightarrow \langle m|x|n\rangle = \sqrt{\frac{\hbar}{2M\omega}}(\langle m|a|n\rangle + \langle m|a^\dagger|n\rangle) = \sqrt{\frac{\hbar}{2M\omega}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})$$

We plug this result into the first expression above and simplify:

$$\begin{aligned} \langle x \rangle_t &= |C_0|^2 \sum_{m,n=0}^{\infty} \frac{(\alpha^*)^m \alpha^n}{\sqrt{n!m!}} e^{i\omega t(m-n)} \sqrt{\frac{\hbar}{2M\omega}} (\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \left(\sum_{n=1}^{\infty} \frac{(\alpha^*)^{n-1} \alpha^n}{\sqrt{n!(n-1)!}} e^{i\omega t((n-1)-n)} \sqrt{n} + \sum_{n=0}^{\infty} \frac{(\alpha^*)^{n+1} \alpha^n}{\sqrt{n!(n+1)!}} e^{i\omega t((n+1)-n)} \sqrt{n+1} \right) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \left(\sum_{n=1}^{\infty} \frac{\alpha|\alpha|^{2(n-1)}}{(n-1)!} e^{-i\omega t} + \sum_{n=0}^{\infty} \frac{\alpha^*|\alpha|^{2n}}{n!} e^{i\omega t} \right) \\ &= |C_0|^2 \sqrt{\frac{\hbar}{2M\omega}} \sum_{n=0}^{\infty} \frac{|\alpha|^n}{n!} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) = \sqrt{\frac{\hbar}{2M\omega}} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) \end{aligned}$$

We then note that $\langle p \rangle_t = M\partial_t \langle x \rangle_t$, such that we may write the following:

$$\langle p \rangle_t = i\sqrt{\frac{\hbar M\omega}{2}} (\alpha^* e^{i\omega t} - \alpha e^{-i\omega t})$$

(e) We may rearrange this into real and imaginary parts to write it purely in terms of sinusoidal functions. In analogy with a classical system, the “spring” begins at its equilibrium position for a purely imaginary α , and begins at the end of its range of motion for a purely real α . We can thereby see that the real and imaginary parts of α determine the initial conditions of the system at $t = 0$, and that the expectation values of position and momentum then oscillate as in a classical oscillator. This is however still a quantum system, and with further analysis one can show that the Heisenberg uncertainty principle is satisfied here; instead of two known values of position and momentum oscillating in time, we have two distributions (Gaussian) whose centroids are oscillating as shown above.

17.3

Prove the following (Dirac notation recommended):

- (a) A hermitian operator has real eigenvalues.
- (b) Eigenvectors of a Hermitian operator with distinct eigenvalues are orthogonal.
- (c) The operator which transforms an orthonormal set of basis vectors into another is unitary.
- (d) If A is a Hermitian matrix, then there exists a unitary matrix U such that $U^\dagger A U$ is diagonal.
- (e) If Ω and Λ are two commuting matrices/operators, they can be simultaneously diagonalized.

Solution

(a) Let A be a Hermitian operator, such that $A = A^\dagger$. Let $|a\rangle$ be an eigenvector/eigenstate of A with eigenvalue a . Then:

$$A|a\rangle = a|a\rangle \rightarrow \langle a|A|a\rangle = a\langle a|a\rangle \quad \text{and} \quad \langle a|A^\dagger = \langle a|A = a^*\langle a| \rightarrow \langle a|A|a\rangle = a^*\langle a|a\rangle$$

By subtracting the results of each expression we obtain $(a - a^*)\langle a|a\rangle = 0$. Since the inner product of a vector with itself is positive semi-definite (i.e. $\langle a|a\rangle \geq 0$), for the relationship to hold for any $|a\rangle$ and a , we must have $a = a^*$, meaning that a is real.

(b) Let A be a hermitian operator and $|a_1\rangle$ and $|a_2\rangle$ be eigenstates of A with eigenvalues a_1 and a_2 , respectively. Since the eigenvalues are distinct, we require $a_1 \neq a_2$. Then we may do the following:

$$A|a_1\rangle = a_1|a_1\rangle \rightarrow \langle a_2|A|a_1\rangle = a_1\langle a_2|a_1\rangle \quad \text{and} \quad A|a_2\rangle = a_2|a_2\rangle \rightarrow \langle a_2|A = a_2\langle a_2| \rightarrow \langle a_2|A|a_1\rangle = a_2\langle a_2|a_1\rangle$$

We again take the difference of the results, to obtain the equation $(a_1 - a_2)\langle a_2|a_1\rangle = 0$. Since $a_1 \neq a_2$ by assumption, we must have $\langle a_2|a_1\rangle = 0$.

(c) We define a set of orthonormal basis vectors $|e_i\rangle$, and let U be the operator which takes it to another set of orthonormal basis vectors $|a_i\rangle$. Then:

$$|a_i\rangle = U|e_i\rangle \rightarrow \langle a_j| = \langle e_j|U^\dagger \rightarrow \langle a_j|a_i\rangle = \langle e_j|U^\dagger U|e_i\rangle$$

Since both sets of vectors are orthonormal we have $\langle \omega_j|\omega_i\rangle = \delta_{ij} = \langle e_j|e_i\rangle$. Then the above is true when $U^\dagger U = \mathbb{I}$, or U is unitary.

(d) Let $|e_i\rangle$ be the standard orthonormal basis, and $|a_i\rangle$ be an orthonormal eigenbasis of the operator A . U is the matrix that transforms the standard basis to the eigenbasis. Then:

$$\begin{aligned} |a_i\rangle = U|e_i\rangle \text{ and } A|a_i\rangle = a_i|a_i\rangle &\rightarrow \langle a_j|A|a_i\rangle = a_i\langle a_j|a_i\rangle = a_i\delta_{ij} \\ &= \langle e_j|U^\dagger A U|e_i\rangle = a_i\delta_{ij} \end{aligned}$$

This shows that $U^\dagger A U$ is diagonal, with the eigenvalues of A as the matrix elements down the diagonal. Then U diagonalizes A .

(e) Let Ω and Λ be commuting operators ($[\Omega, \Lambda] = 0$), and $|\omega_i\rangle$ represent the complete set of eigenstates of Ω corresponding to eigenvalues ω_i . Since $[\Omega, \Lambda] = 0$, we may write $(\Omega\Lambda - \Lambda\Omega)|\omega_i\rangle = 0$. From here we do the following:

$$\Omega\Lambda|\omega_i\rangle = \Lambda\Omega|\omega_i\rangle = \omega_i(\Lambda|\omega_i\rangle)$$

Since $\Omega(\Lambda|\omega_i\rangle) = \omega_i(\Lambda|\omega_i\rangle)$ we see that $\Lambda|\omega_i\rangle$ is also an eigenvector of Ω with eigenvalue ω_i . This is only possible if $\Lambda|\omega_i\rangle = \lambda_i|\omega_i\rangle$. This means that all eigenstates of Ω are also eigenstates of Λ , and that the same matrix which diagonalizes Ω would diagonalize Λ .

17.4

The following are properties, definitions, and relationships which apply to n -dimensional (discrete) vector spaces for vectors $|a\rangle$ and $|b\rangle$. Write the infinite-dimensional (continuous) vector space analog of each of the following for functions $f(t)$ and $g(t)$ / states $|f\rangle$ and $|g\rangle$.

- (a) Projection over a basis: $|a\rangle = \sum_i |e_i\rangle \langle e_i|a\rangle$. (Hint: ask questions until you understand the notation $f(x) = \langle x|f\rangle$.)
- (b) Inner Product: $\langle a|b\rangle = \sum_i a_i^* b_i = \sum_i \langle a|e_i\rangle \langle e_i|b\rangle$.
- (c) Matrix transformations: $|a'\rangle = M|a\rangle \rightarrow a'_i = \sum_j M_{ij} a_j \leftrightarrow \langle e_i|a'\rangle = \sum_j \langle e_i|M|e_j\rangle \langle e_j|a\rangle$.
- (d) Unitary transformations: $U^\dagger U = \mathbb{I} \rightarrow \sum_i U_{ij}^* U_{ik} = \delta_{jk}$. (Note that for $|a'\rangle = U|a\rangle$ and $|b'\rangle = U|b\rangle$ this insures that $\langle a'|b'\rangle = \langle a|U^\dagger U|b\rangle = \langle a|b\rangle$.)
- (e) Use parts (c) and (d) to relate the fourier series and transform (what is the kernel?), and Parseval's theorem. What property of the Fourier transform does Parseval's theorem imply?

Solution

Finite-Dimensional / Discrete Expressions	Infinite-Dimensional / Continuous Expressions
Projection over a discrete basis: $ a\rangle = \sum_i e_i\rangle \langle e_i a\rangle$	Projection over a continuous basis: $ f\rangle = \int dt t\rangle \langle t f\rangle = \int dt f(t) t\rangle$
Inner/Dot Product generalized to complex vectors: $\langle a b\rangle = \mathbf{a}^\dagger \cdot \mathbf{b} = \sum_i a_i^* b_i$	Inner Product for complex functions: $\langle f g\rangle = \int dt \langle f t\rangle \langle t g\rangle = \int dt f^*(t)g(t)$
Matrix transformations: $ a'\rangle = M a\rangle$ $a'_i = \sum_j M_{ij} a_j \leftrightarrow \langle e_i a'\rangle = \sum_j \langle e_i M e_j\rangle \langle e_j a\rangle$	Integral Transformations: $ \tilde{f}\rangle = M f\rangle$ ($M \rightarrow$ Kernel) $\tilde{f}(\tau) = \langle \tau \tilde{f}\rangle = \int dt \langle \tau M t\rangle \langle t f\rangle = \int dt M(\tau, t)f(t)$
Unitary Transformations: $\langle a b\rangle = \langle a U^\dagger U b\rangle = \langle a' b'\rangle$ True iff $\sum_i U_{ij}^* U_{ik} = \delta_{jk}$ $\langle a' b'\rangle = \sum_i \langle a U^\dagger i\rangle \langle i U b\rangle$ $= \sum_i \left(\sum_j \langle a j\rangle \langle j U^\dagger i\rangle \right) \left(\sum_k \langle i U k\rangle \langle k b\rangle \right)$ $= \sum_i a_i^* b'_i = \sum_i \left(\sum_j (U_{ij} a_j)^* \sum_k (U_{ik} b_k) \right)$ $= \sum_{jk} a_j^* b_k \sum_i U_{ij}^* U_{ik} = \langle a b\rangle \text{ iff } U \text{ is Unitary.}$	Unitary Transformations: $\langle f g\rangle = \langle f U^\dagger U g\rangle = \langle \tilde{f} \tilde{g}\rangle$ True iff $\int d\tau U(\tau, t_1)^* U(\tau, t_2) = \delta(t_2 - t_1)$ $\langle \tilde{f} \tilde{g}\rangle = \int d\tau \langle f U^\dagger \tau\rangle \langle \tau U g\rangle$ $= \int d\tau \left(\int dt_1 \langle f t_1\rangle \langle t_1 U^\dagger \tau\rangle \right) \left(\int dt_2 \langle \tau U t_2\rangle \langle t_2 g\rangle \right)$ $= \int d\tau \left(\int dt_1 (U(\tau, t_1)f(t_1))^* \right) \left(\int dt_2 U(\tau, t_2)g(t_2) \right)$ $= \int dt_1 dt_2 f^*(t_1)g(t_2) \int d\tau U^*(\tau, t_1)U(\tau, t_2)$ $= \langle f g\rangle \text{ iff } U \text{ is Unitary.}$

(e)

17.5

(a) Consider an N -dimensional isotropic (all frequencies equal) SHO. Write down a general expression for the energy eigenvalues, and list the first five energies and the degeneracies of each.

(b) Consider the 3-dimensional anisotropic oscillator described by the Hamiltonian:

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega^2(x^2 + 4y^2 + 9z^2)$$

Write down a general expression for the energy eigenvalues, and list the first eight energies and degeneracies of each.

Solution

(a)

$$E = \hbar\omega \left(\frac{N}{2} + \sum_i n_i \right)$$

We list the states below, and $C_k^n = \frac{n!}{k!(n-k)!}$ is the binomial coefficient which reads N choose k .

Energy	Ways to obtain E	Degeneracy (No. of Distinguishable states with E)
$\hbar\omega\frac{N}{2}$	all $n_i = 0$	1 (Non-degenerate)
$\hbar\omega(\frac{N}{2} + 1)$	(1,0...)	N
$\hbar\omega(\frac{N}{2} + 2)$	(2,0...),(1,1,0...)	$N + C_2^N$ for $N \geq 2$
$\hbar\omega(\frac{N}{2} + 3)$	(3,0...),(2,1,0...),(1,1,1,0...)	$N + 2C_2^N + C_3^N$ for $N \geq 3$
$\hbar\omega(\frac{N}{2} + 4)$	(4,0...)(3,1,0...),(2,2,0...),(2,1,1,0...),(1,1,1,1,0...)	$N + 2C_2^N + C_3^N + C_4^N$ for $N \geq 5$

(b)

$$E = \hbar\omega \left(n_x + 2n_y + 3n_z + \frac{3}{2} \right)$$

Energy	(n_x, n_y, n_z)	No. of combinations
$\frac{3\hbar\omega}{2}$	all 0	1
$\frac{5\hbar\omega}{2}$	(1,0,0)	1
$\frac{7\hbar\omega}{2}$	(2,0,0),(0,1,0)	2
$\frac{9\hbar\omega}{2}$	(3,0,0),(1,1,0),(0,0,1)	3
$\frac{11\hbar\omega}{2}$	(4,0,0),(0,2,0),(2,1,0),(1,0,1)	4
$\frac{13\hbar\omega}{2}$	(5,0,0),(3,1,0),(1,2,0),(2,0,1),(0,1,1)	5
$\frac{15\hbar\omega}{2}$	(6,0,0),(4,1,0),(2,2,0),(0,3,0),(1,1,1),(0,0,2),(3,0,1)	7
$\frac{17\hbar\omega}{2}$	(7,0,0),(5,1,0),(3,2,0),(1,3,0),(2,1,1),(1,0,2),(4,0,1),(0,2,1)	8

17.6

(a)

Solution

18 Old Problems (Retired)

18.1 Problem 2

Consider a particle with $E > 0$ moving to the right subject to the potential $V(x)$, where the constant $V > 0$.

$$V(x) = \begin{cases} 0 & x \in (-\infty, 0] \\ V & x \in (0, \infty) \end{cases}$$

Determine the transmission and reflection coefficients for the following cases:

- (a) $E > V$, (b) $E \gg V$, (c) $E < V$.
 (d) Repeat part (a) for a particle moving to the left.

Solution

Let region 1 be for $x < 0$, and region 2 be for $x > 0$.

(a) We define a ψ_1 and ψ_2 in each. (These are solutions to the Schrödinger equation for the the given potential. We have already normalized the incoming probability amplitude by setting that coefficient to be one.)

$$\psi_1(x) = e^{ik_1x} + Be^{-ik_1x} \quad \psi_2(x) = Ce^{ik_2x}$$

We require that the wavefunction be continuous and have a continuous derivative at the boundary, resulting in the following boundary conditions. (We take the derivative to be continuous here, unlike with the delta function potential, because the discontinuity in V is finite in this case.) We then solve the system of equations for the coefficients C and B .

$$1 + B = C, \quad k_1 - Bk_1 = Ck_2 \quad \rightarrow \quad k_1 - Bk_1 = (1 + B)k_2 \quad \rightarrow \quad B = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{and} \quad C = \frac{2k_1}{k_1 + k_2}$$

We then calculate the transmission coefficient T and reflection coefficient R from the coefficients.

$$T = \frac{k_2}{k_1} |C|^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad R = |B|^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

A good check that we have not made a mistake is verifying that $T + R = 1$.

(b) In the limit $E \gg V$ we have $k_1 \approx k_2$. We see that $T \rightarrow 1$ and $R \rightarrow 0$ in this case.

(c) Region 2 has a decaying solution, which forces $T = 0$ and $R = 1$.

(d) We now have:

$$\psi_1(x) = C e^{-ik_1 x} \quad \text{and} \quad \psi_2(x) = e^{-ik_2 x} + B e^{ik_2 x}$$

We set the usual boundary conditions to obtain:

$$C = 1 + B \quad -k_1 C = -k_2 + B k_2$$

We note that these are the same conditions as in part (a), except that we have just interchanged k_1 and k_2 . The results are therefore:

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad R = \frac{(k_2 - k_1)^2}{(k_1 + k_2)^2}$$