Quantum Mechanics

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Contents

1 Fundamentals

1.1 Dimensional Analysis and Quantum Mechanics

The fundamental constants in quantum theory, expressed in terms of Planck's length (L), mass (M), and time (T) are the speed of light c (LT^{-1}), Planck's reduced constant $\hbar = h/2\pi$ (ML^2T^{-1}), the squared electron charge $e^2/(4\pi\epsilon_0)$ (ML^3T^{-2}), and the electron mass m (M).

Problem 1

Determine x, y, and z such that $\hbar^x c^y m^z$ has dimensions of length. This is called the *reduced Compton wavelength* λ_c, which evaluates to roughly $0.386 \times 10^{-12}\ m$.

Problem 2

From the combination $\hbar^x c^y (e^2/4\pi\epsilon_0)^z$, obtain a dimensionless quantity. To make it unique, choose $y = -1$, corresponding to the fine structure constant α. Give the formula for α and evaluate it numerically.

Problem 3

Determine the Bohr radius a_0 by dividing the result from part (1) by the result of part (2). State the numerical value of the Bohr radius in meters.

Solution 1

From dimensional analysis, we have three equations

$$x + z = 0 \qquad 2x + y = 1 \qquad x + y = 0\,,$$

solved by $x = 1$ and $y = z = -1$, telling us that $\lambda_c = \hbar/mc$.

Solution 2

To attain a dimensionless quantity, the same game gives three equations

$$x + z = 0 \qquad 2x - 1 + 3z = 0 \qquad -x + 1 - 2z = 0\,,$$

solved by $x = -1$, $z = 1$. The fine structure constant is evidently:

$$\alpha = \frac{e^2/4\pi\epsilon_0}{\hbar c} \approx \frac{1}{137} \approx 0.00730$$

Solution 3

The Bohr radius evaluates to

$$a_0 = \frac{\lambda_c}{\alpha} = \frac{\hbar^2}{m\,(e^2/4\pi\epsilon_0)} \approx 137 \times \lambda_c \approx 5.29 \times 10^{-11}\ m$$

1.2 Finding Linear Combinations

Problem

Let $|\psi_1\rangle$ and $|\psi_2\rangle$ be normalized eigenfunctions that correspond to the same eigenvalue. If $\langle\psi_1|\psi_2\rangle$ is a real number d, find a normalized linear combination of $|\psi_1\rangle$ and $|\psi_2\rangle$ that is orthogonal to $|\psi_1\rangle$. Also find a normalized linear combination that is orthogonal to $|\psi_1\rangle+|\psi_2\rangle$.

Solution

Let $|\chi_1\rangle = A\,|\psi_1\rangle + B\,|\psi_2\rangle$ and $|\chi_2\rangle = C\,|\psi_1\rangle + D\,|\psi_2\rangle$ be the linear combinations we're looking for, and the task is reduced to finding A, B, C, and D. These are given by, respectively

$$\langle\chi_1|\psi_1\rangle = 0 \qquad\qquad \langle\chi_2|\left(|\psi_1\rangle + |\psi_2\rangle\right) = 0\,.$$

Blooming out the algebra, find $A + Bd = 0$ and $C + D = 0$, and by the normalization requirement $\langle\chi_n|\chi_n\rangle = 1$, arrive at:

$$\chi_1 = \frac{d\,|\psi_1\rangle - |\psi_2\rangle}{\sqrt{1-d^2}} \qquad\qquad \chi_2 = \frac{|\psi_1\rangle - |\psi_2\rangle}{\sqrt{2-2d}}$$

1.3 Measurement and Probability

Problem

An operator $\hat{A}$, corresponding to and observable α, has two normalized eigenfunctions $|\psi_1\rangle$ and $|\psi_2\rangle$, with eigenvalues a_1 and a_2. An operator $\hat{B}$, corresponding to and observable β, has two normalized eigenfunctions $|\phi_1\rangle$ and $|\phi_2\rangle$, with eigenvalues b_1 and b_2. The eigenfunctions are related by

$$|\psi_1\rangle = \frac{2\,|\phi_1\rangle + 3\,|\phi_2\rangle}{\sqrt{13}} \qquad\qquad |\psi_2\rangle = \frac{3\,|\phi_1\rangle - 2\,|\phi_2\rangle}{\sqrt{13}}\,.$$

Suppose the system is measured to be in the state $|\psi_1\rangle$ with $\alpha = a_1$. If β is measured, and then α again, show that the probability of obtaining a_1 again is 97/169.

Solution

First solve for the second set of eigenfunctions:

$$|\phi_1\rangle = \frac{2\,|\psi_1\rangle + 3\,|\psi_2\rangle}{\sqrt{13}} \qquad\qquad |\phi_2\rangle = \frac{3\,|\psi_1\rangle - 2\,|\psi_2\rangle}{\sqrt{13}}$$

When operator $\hat{B}$ acts on the inital state $|\chi_0\rangle = |\psi_1\rangle$, the resultant state must assume one of $|\phi_{1,2}\rangle$. The respective probabilities are given by

$$P_{a_1\to b_1} = |\langle\phi_1|\chi_0\rangle|^2 = \frac{4}{13} \qquad\qquad P_{a_1\to b_2} = |\langle\phi_2|\chi_0\rangle|^2 = \frac{9}{13}\,.$$

Finally, operator $\hat{A}$ must act on whichever of the $|\phi_{1,2}\rangle$ was the result of the previous measurement, and the outcome will be one of $|\psi_{1,2}\rangle$. Since we were asked about the probability of getting $|\psi_1\rangle$ again, the two relevant probabilites can be written,

$$P_{a_1\to b_1\to a_1} = \frac{4}{13}\cdot|\langle\psi_1|\phi_1\rangle|^2 \qquad\qquad P_{a_1\to b_2\to a_1} = \frac{9}{13}\cdot|\langle\psi_1|\phi_2\rangle|^2\,,$$

which evaluate to $(4/13)^2$ and $(9/13)^2$, respectively. The total probability of measuring a_1 again is the sum of the two numbers above, which comes to 97/169.

2 Wavefunction

2.1 Time-Independent Schrodinger Equation

Problem

The time evolution of a single nonrelativistic particle is determined by the time-dependent Schrodinger equation, which reads

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x},t)\right]|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle \ ,$$

and is solved by the complex wavefunction $\Psi(\vec{x},t) = |\Psi(t)\rangle$. The Hamiltonian operator in square brackets is abbreviated by $\hat{H}$. By separation of variables, we break the wavefunction into time- and space-components as in $|\Psi(t)\rangle = f(t)|\psi\rangle$. Since a linear combination of solutions to a differential equation must also be a solution, the most general wavefunction is

$$|\Psi(t)\rangle = \sum_{n=0}^{\infty} f_n(t)|\psi_n\rangle \ .$$

Establish the time-independent Schrodinger equation $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ by finding $f_n(t)$ explicitly, and then write an expression for the initial conditions $f_n(0)$.

Solution

$$\sum_{n=0}^{\infty}\left[E_n f_n(t) - i\hbar\frac{\partial}{\partial t}f_n(t)\right]|\psi_n\rangle = 0 \qquad\qquad f_n(t) = f_n(0)\,e^{-iE_nt/\hbar}$$

$$f_n(0) = \langle\psi_n|\Psi(0)\rangle$$

2.2 Momentum Operator and Momentum Eigenstates

In one dimension, the expectation value of the position of a particle is given by

$$\langle x\rangle = \langle\Psi|\hat{x}|\Psi\rangle \ .$$

Problem 1

Take a time derivative of both sides, and then integrate by parts (like mad) to show that the momentum operator must be:

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

Be sure to use the Schrodinger equation

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\partial_{xx}\Psi + V\Psi$$

and its complex conjugate.

Problem 2

For the momentum observable p, determine the eigenstates $|p\rangle$ of the operator $\hat{p}$.

Solution 1

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m} = \frac{\hbar}{2mi}\int_{-\infty}^{\infty} dx\ \left(\frac{d\Psi^*}{dt}x\Psi + \Psi^* x\frac{d\Psi}{dt} + \Psi^*\frac{dx}{dt}\Psi\right)$$

$$\langle p\rangle = \frac{\hbar}{2i}\int_{-\infty}^{\infty} dx\ \left(\Psi^*\left(\partial_x\Psi\right) - \left(\partial_x\Psi^*\right)\Psi + 0\right) = -i\hbar\int_{-\infty}^{\infty} dx\ \Psi^*\left(\frac{\partial}{\partial x}\right)\Psi$$

Solution 2

$$\hat{p}\,|p\rangle = -i\hbar\frac{\partial}{\partial x}\,|p\rangle = p\,|p\rangle \qquad\qquad |p\rangle = Ae^{ipx/\hbar}\,|e_p\rangle$$

2.3 Position Space and Momentum Space

Problem 1

Consider a particle moving in one dimension. The 'ket' position representation of a wavefunction, $|\psi\rangle$, is not simply equivalent to $\psi(x)$, but is actually defined by

$$|\psi\rangle = \int dx\,\psi\left(x\right)|x\rangle\ ,$$

where $\psi(x)$ is given by $\langle x|\psi\rangle$. The quantity $|\psi(x)|^2$ is understood as the probability density of finding the particle at some point x. Show the inner product $\langle x|x'\rangle$ must equal the Dirac delta function $\delta(x-x')$.

Problem 2

The momentum representation of a wavefunction is

$$|\psi\rangle = \int \frac{dp}{2\pi\hbar}\,\psi\left(p\right)|p\rangle\ ,$$

where there is a factor of $(2\pi\hbar)^{-1}$ for each spatial dimension. Using another representation of the Dirac delta function given by $\langle p|p'\rangle = 2\pi\hbar\delta(p-p')$, derive the relation

$$1 = \int \frac{dp}{2\pi\hbar}\,|\psi(p)|^2\ ,$$

which tells us the probability density of finding the particle with momentum p has the $2\pi\hbar$ factor in the denominator.

Problem 3

Let us define momentum eigenstates as plane waves, given by

$$|p\rangle = \int dx\, e^{ipx/\hbar}\,|x\rangle\ .$$

Show that the Dirac delta function can be represented by the integral:

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

Problem 4

The position eigenstates have the form

$$|x\rangle=\int dp\;f\left(x,p\right)|p\rangle\;\;.$$

Determine $f(x,p)$.

Solution 1

$$\langle x'|\psi\rangle=\int dx\;\psi\left(x\right)\langle x'|x\rangle=\int dx\;\psi\left(x\right)\delta\left(x-x'\right)=\psi\left(x'\right)$$

Solution 2

$$1=\langle\psi|\psi\rangle=\int\int\frac{dp\,dp'}{\left(2\pi\hbar\right)^2}\left(\psi^*\left(p'\right)\psi\left(p\right)\right)\langle p'|p\rangle=\int\frac{dp}{2\pi\hbar}\,|\psi(p)|^2$$

Solution 3

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

Solution 4

$$|x\rangle=\int dx'\int dp\;f\left(x,p\right)e^{ipx'/\hbar}\,|x'\rangle\qquad\qquad f\left(x,p\right)=\frac{e^{-ipx/\hbar}}{2\pi\hbar}$$

2.4 Fourier Representation of the Wavefunction

Problem

In ‘ket’ notation, the position and momentum eigenstates of a particle moving in one dimension read:

$$|x\rangle=\int\frac{dp}{2\pi\hbar}\,e^{-ipx/\hbar}\,|p\rangle\qquad\qquad|p\rangle=\int dx\;e^{ipx/\hbar}\,|x\rangle$$

The wavefunction of the particle, in each representation respectively, is

$$|\psi\rangle=\int dx\;\psi\left(x\right)|x\rangle\qquad\qquad|\psi\rangle=\int\frac{dp}{2\pi\hbar}\,\psi\left(p\right)|p\rangle\;\;.$$

Attain the Fourier representations of ψ by solving for $\psi(x)$ in terms of $\psi(p)$, and vice-versa. There should be no explicit ‘ket’ states in the results.

Solution

$$|\psi\rangle=\int dp\int\frac{dx}{2\pi\hbar}\psi\left(x\right)e^{-ipx/\hbar}\,|p\rangle\qquad\qquad\psi\left(p\right)=\int dx\;\psi\left(x\right)e^{-ipx/\hbar}$$

$$|\psi\rangle=\int dx\int\frac{dp}{2\pi\hbar}\psi\left(p\right)e^{ipx/\hbar}\,|x\rangle\qquad\qquad\psi\left(x\right)=\int\frac{dp}{2\pi\hbar}\,\psi\left(p\right)e^{ipx/\hbar}$$

3 Commutation

3.1 Commutation with the Hamiltonian

Problem

The *commutation* is a construction that tells us what terms are 'left over' when two operators are interchanged:

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

Use the Schrodinger equation $\hat{H}\left|\Psi\right\rangle = i\hbar\partial_t\left|\Psi\right\rangle$ to show that an observable Q obeys

$$\frac{d}{dt}\left\langle Q\right\rangle = -\frac{i}{\hbar}\left\langle\left[\hat{Q}, \hat{H}\right]\right\rangle .$$

Note if the above equation yields zero, we say that the operator $\hat{Q}$ *commutes* with the Hamiltonian, and the observable is a constant over time.

Solution

$$\frac{d}{dt}\left\langle Q\right\rangle = \left\langle\partial_t\Psi|\hat{Q}|\Psi\right\rangle + \left\langle\Psi|\hat{Q}|\partial_t\Psi\right\rangle = -\frac{1}{i\hbar}\left\langle\Psi|\hat{H}\hat{Q}|\Psi\right\rangle + \frac{1}{i\hbar}\left\langle\Psi|\hat{Q}\hat{H}|\Psi\right\rangle$$

$$\frac{d}{dt}\left\langle Q\right\rangle = -\frac{i}{\hbar}\left\langle\Psi\right|\left[\hat{Q}, \hat{H}\right]\left|\Psi\right\rangle = -\frac{i}{\hbar}\left\langle\left[\hat{Q}, \hat{H}\right]\right\rangle$$

3.2 Time Evolution and Non-Commuting Operator

For a certain system, the operator corresponding to the physical quantity A does not commute with the Hamiltonian. It has eigenvalues a_1 and a_2, corresponding to eigenfunctions

$$\left|\phi_1\right\rangle = \frac{\left|\psi_1\right\rangle + \left|\psi_2\right\rangle}{\sqrt{2}} \qquad \left|\phi_2\right\rangle = \frac{\left|\psi_1\right\rangle - \left|\psi_2\right\rangle}{\sqrt{2}} ,$$

where $\left|\psi_1\right\rangle$ and $\left|\psi_2\right\rangle$ are the eigenfunctions of the Hamiltonian, with energy eigenvalues E_1 and E_2.

Problem 1

If the system has initial state $\left|\Psi(0)\right\rangle = \left|\phi_1\right\rangle$, determine the expectation value of the observable A using the formula:

$$\left\langle A\right\rangle = \left\langle\Psi\left(t\right)|\hat{A}|\Psi\left(t\right)\right\rangle = \sum_{n=1,2}\left|\tilde{f}_n\left(t\right)\right|^2\left\langle\phi_n|\hat{A}|\phi_n\right\rangle$$

Problem 2

Verify the time evolution of $\left\langle A\right\rangle$ using the formula:

$$\frac{d}{dt}\left\langle A\right\rangle = -\frac{i}{\hbar}\left\langle\left[\hat{A}, \hat{H}\right]\right\rangle$$

Solution 1

$$|\Psi(t)\rangle = \sum_{n=1,2} \langle\psi_n|\Psi(0)\rangle\, e^{-iE_nt/\hbar}\,|\psi_n\rangle = \frac{e^{-iE_1t/\hbar}\,|\psi_1\rangle + e^{-iE_2t/\hbar}\,|\psi_2\rangle}{\sqrt{2}}$$

$$|\Psi(t)\rangle = \frac{1}{2}\left(e^{-iE_1t/\hbar} + e^{-iE_2t/\hbar}\right)|\phi_1\rangle + \frac{1}{2}\left(e^{-iE_1t/\hbar} - e^{-iE_2t/\hbar}\right)|\phi_2\rangle$$

$$\langle A\rangle = \frac{a_1+a_2}{2} + \frac{a_1-a_2}{2}\cos\left(\frac{(E_1-E_2)\,t}{\hbar}\right)$$

Solution 2

$$|\Psi\rangle = \beta_1(t)\,|\psi_1\rangle + \beta_2(t)\,|\psi_2\rangle \qquad\qquad \langle\Psi| = \frac{\beta_1^*+\beta_2^*}{\sqrt{2}}\langle\phi_1| + \frac{\beta_1^*-\beta_2^*}{\sqrt{2}}\langle\phi_2|$$

$$i\hbar\frac{d}{dt}\langle A\rangle = \langle\Psi|\hat{O}\hat{H}|\Psi\rangle - \langle\Psi|\hat{H}\hat{O}|\Psi\rangle = -\frac{1}{2}(a_1-a_2)(E_1-E_2)(\beta_1^*\beta_2+\beta_2^*\beta_1)$$

$$i\hbar\frac{d}{dt}\langle A\rangle = -\left(\frac{a_1-a_2}{2}\right)(E_1-E_2)\sin\left(\frac{(E_1-E_2)\,t}{\hbar}\right)$$

3.3 Position, Momentum, Hamiltonian Commutations

In one dimension, the position and momentum operators, respectively, are written

$$\hat{x} = x \qquad\qquad \hat{p} = -i\hbar\frac{\partial}{\partial x}\,.$$

Problem 1

Derive the following relations:

$$[\hat{x},\hat{p}] = i\hbar \qquad\qquad \left[\hat{x},\hat{p}^2\right] = \hat{x}\hat{p}^2 - \hat{p}^2\hat{x} = 2i\hbar\hat{p}$$

Problem 2

Calculate the commutation relation between the position operator $\hat{x}$ and the Hamiltonian $\hat{H} = \hat{p}^2/2m + \hat{V}(x)$, and show that

$$\frac{d}{dt}\langle x\rangle = \frac{\langle p\rangle}{m}\,.$$

Problem 3

Calculate the commutation relation between the momentum operator $\hat{p}$ and the Hamiltonian to show that

$$\frac{d}{dt}\langle p\rangle = -\frac{\partial}{\partial x}\langle V(x)\rangle\ ,$$

which is Newton's second law.

Problem 4

Derive again the result from part (3) without using any results from commutation relations. That is, take the time derivative of

$$\langle p\rangle = \int_{-\infty}^{\infty} dx\ \Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi$$

and integrate by parts. Use only the Schrodinger equation $i\hbar\partial_t\Psi = -(\hbar^2/2m)\partial_{xx}\Psi + V(x)\Psi$.

Solution 1

$$[\hat{x},\hat{p}]\,\Psi = \hat{x}\hat{p}\Psi - \hat{p}\hat{x}\Psi = -i\hbar\partial_x\left(x\Psi\right) + i\hbar x\partial_x\Psi = i\hbar\Psi$$
$$2i\hbar\hat{p} = \hat{p}\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right) + \left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)\hat{p}$$

Solution 2

$$\left[\hat{x},\hat{H}\right] = \frac{1}{2m}\left(\hat{x}\hat{p}^2 - \hat{p}^2\hat{x}\right) = i\hbar\frac{\hat{p}}{m}$$
$$i\hbar\frac{d}{dt}\left\langle x\right\rangle = \left\langle\left[\hat{x},\hat{H}\right]\right\rangle = i\hbar\frac{\left\langle p\right\rangle}{m}$$

Solution 3

$$\left[\hat{p},\hat{H}\right] = \left[\hat{p},\hat{p}^2/2m + \hat{V}\right] = \left[\hat{p},\hat{V}\right]$$
$$i\hbar\frac{d}{dt}\left\langle p\right\rangle = \left\langle\left[\hat{p},\hat{V}\right]\right\rangle = -i\hbar\left\langle\left[\partial_x,\hat{V}\right]\right\rangle = -i\hbar\left\langle\frac{\partial V}{\partial x}\right\rangle$$

Solution 4

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3.4 Commuting Operators and Basis Vectors

Problem

Prove that two commuting physical operators can share the same non-degenerate basis set.

Solution

Let the pair of operators, basis states, and eigenvalues be defined as

$$\hat{A}\left|\psi_n\right\rangle = a_n\left|\psi_n\right\rangle \qquad\qquad \hat{B}\left|\phi_n\right\rangle = b_n\left|\phi_n\right\rangle\ .$$

In the most general case, the basis states relate to each other by

$$\left|\psi_n\right\rangle = \sum_m \gamma_{mn}\left|\phi_n\right\rangle \qquad\qquad \left|\phi_n\right\rangle = \sum_m \tilde{\gamma}_{mn}\left|\psi_n\right\rangle\ ,$$

where γ and $\tilde{\gamma}$ are unknown matrices of coefficients. Next, let the operator $\hat{A}\hat{B}$ act on $\left|\psi_n\right\rangle$, and also let $\hat{B}\hat{A}$ act on $\left|\psi_n\right\rangle$.

$$\hat{A}\hat{B}\left|\psi_n\right\rangle = \sum_{mm'} a_{m'}b_m\gamma_{mn}\tilde{\gamma}_{m'n}\left|\psi_{m'}\right\rangle$$

$$\hat{B}\hat{A}\left|\psi_n\right\rangle = \sum_{mm'} a_m b_m\gamma_{mn}\tilde{\gamma}_{m'm}\left|\psi_{m'}\right\rangle$$

Since $\hat{A}$ and $\hat{B}$ are commuting, the two expressions must be equal, and we deduce that $m' = m$ and also $m = n$. Therefore, the matrices γ and $\tilde{\gamma}$ must be purely diagonal and the sums vanish. It's now clear that states $|\phi_n\rangle$ are eigenfunctions of *both* operators $\hat{A}$ and $\hat{B}$, and the same can be said for states $|\psi_n\rangle$, completing the proof (for the nondegenerate case). Explicitly (and similarly for $\hat{B}$):

$$\hat{A}\,|\phi_n\rangle = \hat{A}\tilde{\gamma}_{nn}\,|\psi_n\rangle = \tilde{\gamma}_{nn}a_n\,|\psi_n\rangle = a_n\,|\phi_n\rangle$$

4 Approximations

4.1 Time-Independent Non-Degenerate Perturbation Theory

Introduction

Consider a Hamiltonian operator $\hat{H}^{(0)}$ that takes on a first-order correction $\hat{H}'$. The eigenvectors and eigenvalues of $\hat{H}$ take on correction terms of all orders, and the total system is determined by

$$\hat{H} = \hat{H}^{(0)} + \lambda\hat{H}'$$
$$|\Psi_n\rangle = |\Psi_n^{(0)}\rangle + \lambda\,|\Psi_n^{(1)}\rangle + \lambda^2\,|\Psi_n^{(2)}\rangle + \cdots$$
$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\ ,$$

where λ is a tool for keeping track of order and can be set to 1 at any stage.

Problem 1

Verify that the zero-order equation in λ gives the unperturbed case,

$$\hat{H}^{(0)}\,|\Psi_n^{(0)}\rangle = E_n^{(0)}\,|\Psi_n^{(0)}\rangle\ .$$

Problem 2

Prove that the first-order correction to the energy eigenvalues is given by

$$E_n^{(1)} = \langle\Psi_n^{(0)}|\hat{H}'|\Psi_n^{(0)}\rangle\ .$$

Problem 3

Prove that the first-order correction to the wavefunction is given by

$$|\Psi_n^{(1)}\rangle = -\sum_{m\neq n}\frac{\langle\Psi_m^{(0)}|\hat{H}'|\Psi_n^{(0)}\rangle}{E_m^{(0)} - E_n^{(0)}}\,|\Psi_m^{(0)}\rangle\ .$$

Problem 4

Prove that the second-order correction to the energy eigenvalues is given by the always-negative term

$$E_n^{(2)} = \langle\Psi_n^{(0)}|\hat{H}'|\Psi_n^{(1)}\rangle = -\sum_{m\neq n}\frac{\left|\langle\Psi_m^{(0)}|\hat{H}'|\Psi_n^{(0)}\rangle\right|^2}{E_m^{(0)} - E_n^{(0)}}\ .$$

Problem 5

Denoting $\hat{H}'_{ab} = \langle\Psi_a^{(0)}|\hat{H}'|\Psi_b^{(0)}\rangle$, prove that the second-order correction to the wavefunction is given by

$$|\Psi_n^{(2)}\rangle = \sum_{l\neq n}\left(\sum_{k\neq n}\frac{\hat{H}'_{lk}\hat{H}'_{kn}}{\left(E_l^{(0)}-E_n^{(0)}\right)\left(E_k^{(0)}-E_n^{(0)}\right)} - \frac{\hat{H}'_{nn}\hat{H}'_{ln}}{\left(E_l^{(0)}-E_n^{(0)}\right)^2}\right)|\Psi_l^{(0)}\rangle\ .$$

Problem 6

Prove that the third-order correction to the energy eigenvalues is

$$E_n^{(3)} = \sum_{l,k\neq n}\frac{\hat{H}'_{nl}\hat{H}'_{lk}\hat{H}'_{kn}}{\left(E_l^{(0)}-E_n^{(0)}\right)\left(E_k^{(0)}-E_n^{(0)}\right)} - \sum_{l\neq n}\frac{\hat{H}'_{nn}\left|\hat{H}'_{nl}\right|^2}{\left(E_l^{(0)}-E_n^{(0)}\right)^2}\ .$$

Problem 7

Explain why non-degenerate perturbation theory fails if two or more eigenvalues (energy levels) of the Hamiltonian are equal, or nearly equal.

Solution 1

The statement $\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$, accounting for all above-stated corrections, delivers an infinite number of equations in powers of λ. The $\lambda = 0$ case delivers the unperturbed Schrodinger equation.

Solution 2

Taking the first-order term in λ and projecting $\langle\Psi_l^{(0)}|$ onto both sides, we get

$$\langle\Psi_l^{(0)}|\hat{H}'|\Psi_n^{(0)}\rangle + \langle\Psi_l^{(0)}|\hat{H}^{(0)}|\Psi_n^{(1)}\rangle = E_n^{(0)}\langle\Psi_l^{(0)}|\Psi_n^{(1)}\rangle + E_n^{(1)}\delta_{ln}\ .$$

For the case $l = n$, the two terms adjacent to the equal sign cancel, and we recover the desired expression.

Solution 3

Take $l \neq n$ to find

$$\langle\Psi_l^{(0)}|\hat{H}'|\Psi_n^{(0)}\rangle + \left(E_l^{(0)} - E_n^{(0)}\right)\langle\Psi_l^{(0)}|\Psi_n^{(1)}\rangle = 0\ .$$

Meanwhile, the first-order correction to the wavefunction is a sum over the unperturbed states with 'unknown' coefficients A_{mn}, as in $|\Psi_n^{(1)}\rangle = \sum_m A_{mn}|\Psi_m^{(0)}\rangle$. The A_{mn} aren't unknown at all; the're identically equal to $\langle\Psi_m^{(0)}|\Psi_n^{(1)}\rangle$, which is the inner product that occurs in the equation above.

Solution 4

The second-order terms in λ read

$$\hat{H}^0|\Psi_n^{(2)}\rangle + \hat{H}'|\Psi_n^{(1)}\rangle = E_n^{(1)}|\Psi_n^{(1)}\rangle + E_n^{(0)}|\Psi_n^{(2)}\rangle + E_n^{(2)}|\Psi_n^{(0)}\rangle\ .$$

Projecting $\langle\Psi_l^{(0)}|$ onto both sides and letting $l = n$ gives the desired result.

Solution 5

For the $l \neq n$ case, we find

$$\left(E_l^{(0)} - E_n^{(0)}\right) \langle\Psi_l^{(0)}|\Psi_n^{(2)}\rangle + \langle\Psi_l^{(0)}|\hat{H}'|\Psi_n^{(1)}\rangle = E_n^{(1)} \langle\Psi_l^{(0)}|\Psi_n^{(1)}\rangle \ ,$$

and proceeding as we did for the first-order case, it follows that

$$|\Psi_n^{(2)}\rangle = \sum_{l\neq n} \frac{-\langle\Psi_l^{(0)}|\hat{H}'|\Psi_n^{(1)}\rangle + E_n^{(1)} \langle\Psi_l^{(0)}|\Psi_n^{(1)}\rangle}{\left(E_l^{(0)} - E_n^{(0)}\right)} |\Psi_l^{(0)}\rangle \ ,$$

where plugging in the formulae for $|\Psi_n^{(1)}\rangle$, $E_n^{(1)}$, and $\langle\Psi_l^{(0)}|\Psi_n^{(1)}\rangle$ gives the desired result.

Solution 6

You should find

$$E_n^{(3)} = \langle\Psi_n^{(0)}|\hat{H}'|\Psi_n^{(2)}\rangle \ .$$

Solution 7

For equal or near-equal eigenvalues, each correction term involves division by zero.

4.2 Two-Fold Degenerate Perturbation Theory

Consider a system in which exactly two eigenvalues (energy levels) of the Hamiltonian $\hat{H}^{(0)}$ are equal or nearly equal. If the two corresponding eigenstates are $|\Psi_a^{(0)}\rangle$ and $|\Psi_b^{(0)}\rangle$, we have

$$\hat{H}^{(0)} |\Psi_a^{(0)}\rangle = E^{(0)} |\Psi_a^{(0)}\rangle \qquad \hat{H}^{(0)} |\Psi_b^{(0)}\rangle = E^{(0)} |\Psi_b^{(0)}\rangle \qquad \langle\Psi_a^{(0)}|\Psi_b^{(0)}\rangle = 0 \ .$$

All is well until we introduce a perturbative term to the Hamiltonian such that $\hat{H} = \hat{H}^{(0)} + \hat{H}'$, as the non-degenerate technique leads to division by zero. To proceed, we'll work with the first-order approximations

$$\hat{H} = \hat{H}^{(0)} + \lambda\hat{H}'$$
$$|\Psi\rangle = |\Psi^{(0)}\rangle + \lambda |\Psi^{(1)}\rangle$$
$$E = E^{(0)} + \lambda E^{(1)} \ ,$$

where λ can be set to 1 at any stage. Next, notice that a linear combination of the two eigenstates, as in

$$|\Psi^{(0)}\rangle = \alpha |\Psi_a^{(0)}\rangle + \beta |\Psi_b^{(0)}\rangle \ ,$$

must also solve the Schrodinger equation with the same eigenvalue, where coefficients α and β obey $\alpha^*\alpha + \beta^*\beta = 1$.

Problem 1

Write the Schrodinger equation to first order, and then generate two equations for α and β by taking the inner product with $\langle\Psi_a^{(0)}|$ and $\langle\Psi_b^{(0)}|$, respectively. Defining $V_{ij} = \langle\Psi_i^{(0)}|\hat{H}'|\Psi_j^{(0)}\rangle$, write your result as a matrix that operates on the column vector $[\alpha, \beta]$.

Problem 2

Show that the first-order correction to the energy eigenvalue is equal to

$$E_{\pm}^{(1)} = \frac{1}{2}\left[V_{aa} + V_{bb} \pm \sqrt{(V_{aa} - V_{bb})^2 + 4\,|V_{ab}|^2}\right] .$$

Solution 1

$$\left(\hat{H}^{(0)} - E^{(0)}\right)|\Psi^{(1)}\rangle + \left(\hat{H}' - E^{(1)}\right)|\Psi^{(0)}\rangle = 0$$

$$\begin{bmatrix} V_{aa} - E^{(1)} & V_{ab} \\ V_{ba} & V_{bb} - E^{(1)} \end{bmatrix}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = \begin{bmatrix}0 \\ 0\end{bmatrix}$$

Solution 2

$$\begin{vmatrix} V_{aa} - E^{(1)} & V_{ab} \\ V_{ba} & V_{bb} - E^{(1)} \end{vmatrix} = 0$$

5 Wavepackets

5.1 Free Particle in One Dimension

A particle moving in one dimension has the normalized state function

$$\psi(x) = \left(2\pi a^2\right)^{-1/4} e^{-x^2/4a^2} ,$$

where a is a constant with units of length.

Problem 1
Solve for the momentum representation of the wavefunction, $\psi(p)$.

Problem 2
Find the probability $P(p)$ that the particle has momentum between p and $p + dp$.

Problem 3
The uncertainty in the variable is x defined as

$$\sigma_x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} ,$$

where an identical relation holds for p. Show that the product of uncertainties is

$$\sigma_x\,\sigma_p = \frac{\hbar}{2} .$$

Solution 1

$$\psi(p) = \left(2\pi a^2\right)^{-1/4}\int_{-\infty}^{\infty} dx\; e^{-x^2/4a^2 - ipx/\hbar} = \sqrt{2}\left(2\pi a^2\right)^{1/4} e^{-p^2a^2/\hbar^2}$$

Solution 2

$$\langle\psi|\psi\rangle = \int\int \frac{dp\, dp'}{(2\pi\hbar)^2} |\psi(p)|^2 \langle p'|p\rangle = \int dp \left[\sqrt{\frac{2}{\pi}}\frac{a}{\hbar}e^{-2p^2a^2/\hbar^2}\right] = \int dp\, P(p)$$

Solution 3

$$\sigma_x^2 = \left\langle x^2 \right\rangle - 0 = \frac{1}{\sqrt{2\pi a^2}}\int_{-\infty}^{\infty} dx\, x^2 e^{-x^2/2a^2} = \frac{a^3\sqrt{2\pi}}{\sqrt{2\pi a^2}} = a^2$$

$$\sigma_p^2 = \left\langle p^2 \right\rangle - 0 = \sqrt{\frac{2}{\pi}}\frac{a}{\hbar}\int_{-\infty}^{\infty} dp\, p^2 e^{-2p^2a^2/\hbar^2} = \sqrt{\frac{2}{\pi}}\frac{a}{\hbar}\sqrt{\frac{\pi}{32}}\frac{\hbar^3}{a^3} = \frac{\hbar^2}{4a^2}$$

$$\sigma_x\, \sigma_p = \sqrt{\frac{a^2\hbar^2}{4a^2}} = \frac{\hbar}{2}$$

5.2 Particle Flux Vector

Problem

For a system of particles of mass m in the state ψ, the formal expression for the flux vector (number per unit volume through init area perpendicular to the direction of motion) is

$$\vec{F} = \frac{-i\hbar}{2m}\left((\psi^*)\,\vec{\nabla}\psi - \psi\left(\vec{\nabla}\psi^*\right)\right) .$$

Show that, for a beam of particles of density ρ, the expression gives $F = v\rho$.

Solution

Identify ψ as Ae^{ikx} such that $\rho = A^2$. Also recall $mv = p = \hbar k$.

5.3 Free Particle in One Dimension

A free particle traveling in one dimension is represented by the wavevector $\psi(x) = Ae^{i(kx-\omega t)}$.

Problem 1

Calculate the group velocity using non-relativistic mechanics, and show that it equals the particle velocity u.

Problem 2

Show that the same result holds for relativistic mechanics.

Problem 3

Show that the phase velocity v_p is related to the group velocity by $v_p = v_g/2$ for non-relativistic mechanics.

Problem 4

Show that the phase velocity v_p is related to the group velocity by $v_p = c^2/v_g$ for relativistic mechanics.

Solution 1

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left(\frac{E}{\hbar}\right) = \frac{d}{dk}\left(\frac{\hbar^2 k^2}{2m\hbar}\right) = \frac{\hbar k}{m} = \frac{p}{m} = u$$

Solution 2

$$v_g = \frac{d\omega}{dk} = \frac{d}{dk}\left(\frac{E}{\hbar}\right) = \frac{d}{dk}\left(\frac{\sqrt{p^2c^2 + m^2c^4}}{\hbar}\right) = \frac{pc^2}{\gamma mc^2} = \frac{p}{\gamma m_{rest}} = \frac{p}{m_{rel}} = u$$

Solution 3

$$v_p = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{p^2}{2mp} = \frac{p}{2m} = \frac{u}{2}$$

Solution 4

$$v_p = \frac{\omega}{k} = \frac{\gamma mc^2}{\hbar k} = \frac{m_{rel}c^2}{p} = \frac{c^2}{u}$$

5.4 Wavepacket Spreading

Consider the Gaussian wavepacket:

$$\phi(p) = \left(4\pi\sigma^2\right)^{1/4} e^{-(p-p_0)^2\sigma^2/2\hbar^2}$$

Problem 1

Calculate $\psi(x,t)$ using

$$\psi(x,t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, \phi(p)\, e^{ipx/\hbar - itp^2/(2m\hbar)}\,.$$

Problem 2

Evaluate the mean position and width of the wavepacket via

$$\langle x \rangle = \int_{-\infty}^{\infty} dx\, x\, |\psi(x,t)|^2 \qquad \sigma_x^2 = \int_{-\infty}^{\infty} dx\, \left(x - \langle x \rangle\right)^2 |\psi(x,t)|^2$$

Problem 3

Show that the average value of the momentum $\langle p \rangle$ at $t = 0$ obeys the formula:

$$\langle p_{t=0} \rangle = -i\hbar \int dx\, \psi^*(x,0)\, \frac{\partial}{\partial x}\psi(x,0) = p_0$$

Solution 1

$$\psi(x,t) = e^{-p_0^2\sigma^2/2\hbar^2} \frac{\left(4\pi\sigma^2\right)^{1/4}}{2\pi\hbar} \sqrt{\frac{\pi}{\frac{\sigma^2}{2\hbar^2} + \frac{it}{2m\hbar}}}\, \exp\left[\frac{\left(\frac{p_0\sigma^2}{\hbar^2} + \frac{ix}{\hbar}\right)^2}{4\left(\frac{\sigma^2}{2\hbar^2} + \frac{it}{2m\hbar}\right)}\right]$$

Solution 2

Letting $v_0 = p_0/m$.

$$|\psi(x,t)|^2 = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} \exp\left[-\frac{\sigma^2 (x - v_0 t)^2}{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}\right]$$

Letting $q = x - v_0 t$.

$$\langle x \rangle = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} \left[\int_{-\infty}^{\infty} q\, e^{\frac{-\sigma^2 q^2}{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} dq + v_0 t \int_{-\infty}^{\infty} e^{\frac{-\sigma^2 q^2}{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} dq\right] = v_0 t$$

$$\sigma_x^2 = \frac{\sigma}{\sqrt{\pi}\sqrt{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} \int_{-\infty}^{\infty} dq\, q^2 e^{\frac{-\sigma^2 q^2}{\sigma^4 + \left(\frac{\hbar t}{m}\right)^2}} = \frac{\sigma^2 + \left(\frac{\hbar t}{\sigma m}\right)^2}{2}$$

Solution 3

...

5.5 Confined Particle in One Dimension

Problem

For the wavefunction $\psi(x) = 1/\sqrt{2a}$ on the interval $-a < x < a$ with $\psi(x) = 0$ elsewhere, show that the uncertainty in the momentum is infinite.

Solution

$$\psi(p) = \int_{-a}^{a} dx\, \psi(x)\, e^{-ipx/\hbar} = \frac{1}{2a}\int_{-a}^{a} dx\ \left(\cos(px/\hbar) + i \sin(px/\hbar)\right)) = \frac{\hbar}{pa} \sin\left(\frac{pa}{\hbar}\right)$$

$$\sigma_p^2 = \int_{-\infty}^{\infty} dp\ \left(p^2 - \langle p \rangle\right) \frac{|\psi(p)|^2}{2\pi\hbar} \propto \int_{-\infty}^{\infty} dp\, p^2 \sin^2\left(\frac{pa}{\hbar}\right) = \infty$$

6 Barriers

6.1 Step Barrier Reflection and Transmission

A beam of particles of energy E_0 traveling along the $+x$ direction encounters an energy barrier with magnitude V_0 that obeys

$$V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & x > 0 \end{cases}.$$

Write down the reflection and transmission coefficients for both (1) $E > V_0$ and (2) $E < V_0$. Check that $R + T = 1$ in each case.

Solution 1

Let $\psi_L(x)$ denote the wavefunction for $x \leq 0$, and let $\psi_R(x)$ be the wavefunction for $x > 0$. The wavefunction and its derivative must be continuous across the barrier, so we have the continuity conditions

$$\psi_L(0) = \psi_R(0) \qquad\qquad \partial_x \psi_L(0) = \partial_x \psi_R(0) \ .$$

For positions $x \leq 0$, the potential is zero, and the momentum of the particle relates to the energy by $E_0 = p^2/2m$ where $p = \hbar k$. To the right of $x = 0$, the energy is reduced by the barrier. Altogether, we have

$$k_L = \sqrt{\frac{2mE_0}{\hbar^2}} \qquad\qquad k_R = \sqrt{\frac{2m(E_0 - V_0)}{\hbar^2}} \ ,$$

and notice that if the particle beam energy is less than that of the barrier then k_R becomes imaginary. The most general solution to Schrodinger's equation $\partial_{xx}\psi(x) = -(2m/\hbar^2)(E - V)\psi(x)$ is

$$\psi_L(x) = Ae^{ik_L x} + Be^{-ik_L x} \qquad\qquad \psi_R(x) = Ce^{ik_R x} + De^{-ik_R x} \ .$$

The constant D is zero by the problem statement, as there is no wave traveling from $x = \infty$ toward the barrier's edge. It hurts nothing to set $A = 1$ to denote the incoming wave as having unit amplitude. Continuity in the wavefunction and continuity in the derivative of the wavefunction across $x = 0$ delivers

$$1 + B = C \qquad\qquad k_L(1 - B) = Ck_R \ .$$

The remaining unkowns are thus

$$B = \frac{k_L - k_R}{k_L + k_R} \qquad\qquad C = \frac{2k_L}{k_L + k_R} \ .$$

The flux of reflected and transmitted particles give the reflection and transmission coefficients, which read:

$$R = F_{refl} = |B|^2 \left(\frac{k_L}{m}\right) = |B|^2 F_{inc} = |B|^2 = \left(\frac{k_L - k_R}{k_L + k_R}\right)^2$$

$$T = F_{trans} = |C|^2 \left(\frac{k_R}{m}\right) = |C|^2 \left(\frac{k_R}{k_L}\right) F_{inc} = \frac{4k_L k_R}{(k_L + k_R)^2}$$

Solution 2

For $E_0 < V_0$, the k_R term becomes imaginary, so we denote $k_R \to i\kappa$, where κ is real. Since $x > 0$ corresponds to evanescent waves, the overall transmission into the barrier is zero. The reflection coefficient R evaluates to 1, which is also classically correct.

6.2 Step Barrier Reflection and Evanescent Waves

A beam of particles of energy $E_0 < V_0$ traveling along the $+x$ direction encounters an energy barrier

$$V\left(x\right) = \begin{cases} 0 & x \leq 0 \\ V_0 & x > 0 \end{cases} .$$

To left of the barrier ($x \leq 0$), the wavefunction is

$$\psi_L\left(x\right) = e^{ikx} + Be^{-ikx} ,$$

where the wavenumber k is given by $k^2 = 2mE_0/\hbar^2$. On the right of $x = 0$, the wavenumber becomes imaginary because $E_0 < V_0$, so we write $\kappa^2 = 2m\left(V_0 - E_0\right)/\hbar^2$ such that

$$\psi_R\left(x\right) = Ce^{-\kappa x} .$$

Problem 1

Letting $\tan\theta = \kappa/k$, show that the wavefunction to the left of $x = 0$ obeys

$$\psi_L\left(x\right) = 2e^{-i\theta}\cos\left(kx + \theta\right) .$$

Problem 2

Solve for ψ_R on the right of $x = 0$ and state the amplitude of the evanescent wave.

Solution 1

$$B = \frac{1 - i\tan\theta}{1 + i\tan\theta} = \frac{\cos\theta - i\sin\theta}{\cos\theta + i\sin\theta} = e^{-2i\theta}$$

Solution 2

$$\psi_R\left(x\right) = Ce^{-\gamma x} = \frac{2\cos\theta}{\cos\theta + i\sin\theta}e^{-\gamma x} = \left[2\cos\theta e^{-\gamma x}\right]e^{-i\theta} = A_{ev}e^{-i\theta}$$

6.3 Top Hat Barrier

A beam of particles of energy $E_0 < V_0$ traveling along the $+x$ direction encounters an energy barrier with magnitude V_0 that obeys

$$V\left(x\right) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \geq x \geq a \\ 0 & x > a \end{cases} .$$

Problem 1

Write down the wavefunction in the thre regions $\psi_L(x < 0)$, $\psi_M(0 \geq x \geq a)$, and $\psi_R(x > a)$ with unknown amplitude coefficients. State the conditions that allow one to solve for the unknown coefficients.

Problem 2

Solve for all unkown coefficients.

Problem 3

Calculate the transmission coefficient through the barrier, and also the reflection coefficient away from the barrier. Check that their sum is unity.

Problem 4

Repeat the previous three calculations for $E_0 > V_0$.

Problem 5

Calculate the transmission coefficient in the limit of a very tall barrier such that $V_0 \gg E_0$.

Solution 1

$$k = \sqrt{\frac{2mE_0}{\hbar^2}} \qquad \gamma = \sqrt{\frac{2m\left(V_0 - E_0\right)}{\hbar^2}}$$

$$\psi_L\left(x\right) = e^{ikx} + Be^{-ikx} \qquad \psi_M\left(x\right) = Ce^{\gamma x} + De^{-\gamma x} \qquad \psi_R\left(x\right) = Ee^{ikx}$$

$$\psi_L\left(0\right) = \psi_M\left(0\right) \qquad \psi_M\left(a\right) = \psi_R\left(a\right)$$

$$\partial_x\psi_L\left(0\right) = \partial_x\psi_M\left(0\right) \qquad \partial_x\psi_M\left(a\right) = \partial_x\psi_R\left(a\right)$$

Solution 2

$$\begin{bmatrix} 1 & -1 & -1 & 0 & -1 \\ ik & \gamma & -\gamma & 0 & ik \\ 0 & e^{\gamma a} & e^{-\gamma a} & -e^{iak} & 0 \\ 0 & \gamma e^{\gamma a} & -\gamma e^{-\gamma a} & -ike^{iak} & 0 \end{bmatrix}$$

$$B = \frac{-\left(\gamma^2+k^2\right)\sinh(\gamma a)}{-2i\gamma k\cosh(\gamma a)+(g-k)(g+k)\sinh(\gamma a)}$$

$$C = \frac{-2k(-i\gamma+k)}{-e^{2\gamma a}(\gamma-ik)^2+(\gamma+ik)^2}$$

$$D = \frac{-2e^{2\gamma a}(i\gamma+k)k}{e^{2\gamma a}(\gamma-ik)^2-(\gamma+ik)^2}$$

$$E = \frac{2i\gamma ke^{-iak}}{2i\gamma k\cosh(\gamma a)+(-\gamma^2+k^2)\sinh(\gamma a)}$$

Solution 3

$$R = \left|B\right|^2 = \frac{1}{1+\frac{4\gamma^2k^2}{(\gamma^2+k^2)^2\sinh(\gamma a)^2}} \qquad T = \left|E\right|^2 = \frac{1}{\cosh\left(\gamma a\right)^2 + \frac{(\gamma^2-k^2)^2\sinh(\gamma a)^2}{4\gamma^2k^2}}$$

$$R = \frac{1}{1+\frac{1}{\sinh(\gamma a)^2}\left(\frac{4E_0(V_0-E_0)}{V_0^2}\right)} \qquad T = \frac{1}{1+\sinh\left(\gamma a\right)^2\left(\frac{V_0^2}{4E_0(V_0-E_0)}\right)}$$

$$R + T = \frac{1}{1+x} + \frac{1}{1+1/x} = \frac{2+x+1/x}{2+x+1/x} = 1$$

Solution 4

$$k=\sqrt{\frac{2mE_0}{\hbar^2}} \qquad \beta=\sqrt{\frac{2m\left(E_0-V_0\right)}{\hbar^2}}$$

$$\psi_L\left(x\right)=e^{ikx}+Be^{-ikx} \qquad \psi_M\left(x\right)=Ce^{i\beta x}+De^{-i\beta x} \qquad \psi_R\left(x\right)=Ee^{ikx}$$

Replace $\gamma\to i\beta$ in part (2).

$$R=\frac{\left(\beta^2-k^2\right)^2\sin\left(\beta a\right)^2}{4\beta^2k^2\cos\left(\beta a\right)^2+\left(\beta^2+k^2\right)^2\sin\left(\beta a\right)^2} \qquad T=\frac{1}{\cos\left(\beta a\right)^2+\frac{\left(\beta^2+k^2\right)^2\sin\left(\beta a\right)^2}{4\beta^2k^2}}$$

$$R=\frac{1}{1+\frac{1}{\sin\left(\beta a\right)^2}\left(\frac{4E_0\left(E_0-V_0\right)}{V_0^2}\right)} \qquad T=\frac{1}{1+\sin\left(\beta a\right)^2\left(\frac{V_0^2}{4E_0\left(E_0-V_0\right)}\right)}$$

Solution 5

$$T_{\left(V_0\gg E_0\right)}\approx\frac{16\gamma^2k^2}{\left(\gamma^2+k^2\right)^2}e^{-2\gamma a}=\frac{16E_0\left(V_0-E_0\right)}{V_0^2}e^{-2\gamma a}\approx\frac{16E_0}{V_0}e^{-2\gamma a}$$

7 Wells

7.1 Trapped Particle

Problem

Suppose that the wavefunction for a given particle with zero energy is known to be

$$\psi\left(x\right)=Axe^{-x^2/L^2}\ .$$

Determine the shape of the potential well, $U(x)$, in which the particle must be trapped.

Solution

$$-\frac{\hbar^2}{2m}\partial_{xx}\psi\left(x\right)+U\left(x\right)\psi\left(x\right)=0 \qquad U\left(x\right)=\frac{2\hbar^2}{mL^2}\left(\frac{x^2}{L^2}-\frac{3}{2}\right)$$

8 SHO

8.1 SHO Energy Levels

Consider the time-independent Schrodinger equation in one dimension $(-\hbar^2/2m)\partial_{xx}\psi(x)+V(x)\psi(x)=E\psi(x)$, where $V(x)$ is specified by the harmonic oscillator potential, $V=(m/2)\omega^2x^2$, and ω is the angular frequency.

Problem 1

Introduce the dimensionless energy $\epsilon_n=(2/\hbar\omega)E_n$ and the dimensionless coordinate $\xi=x\sqrt{m\omega/\hbar}$ to show that the Schrodinger equation takes the form

$$\psi''\left(\xi\right)+\left(\epsilon_n-\xi^2\right)\psi\left(\xi\right)=0\ .$$

Problem 2

In the limit that $|\xi|$ is very large, show that $\psi_{(|\xi|\to\infty)} = e^{\pm\xi^2/2}$, so that the wavefunction may be written

$$\psi\left(\xi\right) = f\left(\xi\right) e^{-\xi^2/2} \, .$$

Show further that $f(\xi)$ is governed by

$$f'' - 2\xi f' + \left(\epsilon_n - 1\right) f = 0 \, .$$

Problem 3

Assume a power series solution to $f\left(\xi\right)$ as in

$$f\left(\xi\right) = \sum_{k=0}^{\infty} A_k \xi^k \, ,$$

and show that the coefficients A_k obey the recursion relation

$$A_{k+2} = \frac{1 + 2k - \epsilon_n}{\left(k+1\right)\left(k+2\right)} A_k \, ,$$

indicating that the coefficients for even k are separated from those of odd k. Observe (up to normalization constant) that symmetric solutions must begin with $A_0 = 1$ and $A_1 = 0$, where meanwhile antisymmetric solutions have $A_0 = 0$ and $A_1 = 1$.

Problem 4

For large values of k, observe that the ratio A_{k+2}/A_k approaches the value $2/k$. For k large enough, the function $f(\xi)$ grows exponentially in ξ^2 and becomes too large to be consistent with $\psi(x) = f(\xi)e^{-\xi^2/2}$, thus the infinite series in k has to be trunctated at some finite $k = n$. Use the recursion relation for A_k to show that the harmonic oscillator energy levels are given by

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \, .$$

Solution 1

This is a straightforward substitution.

Solution 2

Argue that $\psi(\xi) \sim e^{+\xi^2/2}$ corresponds to an infinite wavefunction, so keep only the minus case. The non-asymptotic behavior of the wavefunction is contained in $f(\xi)$.

Solution 3

Along the way, arrive at

$$\sum_{k=0}^{\infty} \left[\left(k+2\right)\left(k+1\right) A_{k+2} - 2kA_k + \left(\epsilon_n - 1\right) A_k\right] \xi^k = 0 \, ,$$

where the first term has its index shifted $k \to k+2$.

Solution 4

Given $A_k \neq 0$, we can only have $A_{k+2} = 0$ if $1 + 2k - \epsilon_n = 0$. Let $k = n$ and redimensionalize the ϵ_n in terms of E_n.

8.2 SHO Wavefunctions by Power Series

The simple harmonic oscillator in one dimension obeys the time-independent Schrodinger equation $(-\hbar^2/2m)\partial_{xx}\psi_n(x) + (m/2)\omega^2 x^2\psi_n(x) = E_n\psi_n(x)$.

Problem 1

Without normalizing, write down the wavefunctions

$$\psi_n(\xi) = \sum_{k\leq n} A_k \xi^k e^{-\xi^2/2} \qquad A_{k+2} = \frac{2k-2n}{(k+1)(k+2)} A_k$$

for the first four states $n = 0, 1, 2, 3$ by making use of the recursion relation for the coefficients A_k.

Problem 2

Verify by direct integration that the four wavefunctions $\psi_n(\xi)$ written in part (a) are orthogonal.

Problem 3

Multiply each wavefunction by a constant such that the non-exponential dependency in ξ matches one of the famous *Hermite* polynomials

$$H_0 = 1 \qquad H_1 = 2\xi \qquad H_2 = 4\xi^2 - 2 \qquad H_3 = 8\xi^3 - 12\xi$$

$$H_4 = 16\xi^4 - 48\xi^2 + 12 \qquad H_5 = 32\xi^5 - 160\xi^3 + 120\xi\ ,$$

such that the wavefunctions may be written

$$\psi_n(\xi) = N_n H_n(\xi)\, e^{\xi^2/2}\ ,$$

where N_n is the normalization constant for a given n. Calculate this constant for the first four wavefunctions ψ_0, ψ_1, ψ_2, and ψ_3. Note that

$$\int_{-\infty}^{\infty} dx\ |\psi(x)|^2 = \sqrt{\frac{\hbar}{m\omega}} \int_{-\infty}^{\infty} d\xi\ |\psi(\xi)|^2 = 1\ .$$

Solution 1

Recall that symmetric solutions must begin with $A_0 = 1$ and $A_1 = 0$, and antisymmetric solutions have $A_0 = 0$ and $A_1 = 1$. Thus:

$$\psi_0(\xi) = A_0 e^{-\xi^2/2} \qquad \psi_1(\xi) = A_1 \xi e^{-\xi^2/2}$$

$$\psi_2(\xi) = A_0\left(1 - 2\xi^2\right) e^{-\xi^2/2} \qquad \psi_3(\xi) = A_1\left(\xi - \frac{2}{3}\xi^3\right) e^{-\xi^2/2m}$$

Solution 2

(b)

$$\int_{-\infty}^{\infty} d\xi\ \psi_n(\xi)\,\psi_m(\xi) \propto \delta_{mn}$$

Solution 3

$$N_0 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \qquad N_1 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2}}$$

$$N_2 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{2\sqrt{2}} \qquad N_3 = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{4\sqrt{3}}$$

8.3 Hermite Polynomial Generating Function

Consider the *generating function* $F(\xi, s) = e^{\xi^2-(s-\xi)^2} = e^{-s^2+2s\xi}$.

Problem 1

First show that

$$\frac{\partial^2 F}{\partial \xi^2} - 2\xi \frac{\partial F}{\partial \xi} + 2s \frac{\partial F}{\partial s} = 0\,,$$

and then insert into the above equation the Taylor expansion of F, namely

$$F(\xi, s) = \sum_{n=0}^{\infty} \frac{a_n(\xi)}{n!} s^n\,,$$

to derive an analog to the expression $f'' - 2\xi f' + (\epsilon_n - 1)f = 0$ in terms of $a_n(\xi)$.

Problem 2

Since the coefficients $a_n(\xi)$ obey the same differential equation as do $f(\xi)$, along with the Hermite polynomials $H_n(\xi)$, we know $a_n(\xi)$ must relate to $H_n(\xi)$ by a linear factor for each n. The choice has already been made for us in the definition of $F(\xi, s)$. Indeed, it turns out that $a_n(\xi) = H_n(\xi)$ exactly, meaning

$$e^{\xi^2-(s-\xi)^2} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n\,.$$

Use the above identity to derive the normalization constant for the nth SHO wavefunction:

$$N_n = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{1}{\sqrt{2^n n!}}$$

Solution 1

$$\sum_n \left[a_n'' - 2\xi a_n' + 2n a_n\right] s^n = 0 \qquad \epsilon_n = 2n+1$$

Solution 2

$$\int_{-\infty}^{\infty} d\xi\, e^{-\xi^2} e^{\xi^2-(s-\xi)^2} e^{\xi^2-(t-\xi)^2} = \int_{-\infty}^{\infty} d\xi \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{s^n t^m}{n!m!} H_n(\xi) H_m(\xi) e^{-\xi^2}$$

$$\sqrt{\pi} e^{2st} = \sqrt{\pi} \sum_{n=0}^{\infty} \frac{2^n s^n t^n}{n!} = \sum_{n=0}^{\infty} \frac{s^n}{n!} \left(\sum_{m=0}^{\infty} \frac{t^m}{m!} \int_{-\infty}^{\infty} d\xi\, H_n(\xi) H_m(\xi) e^{-\xi^2} \right)$$

$$\sqrt{\pi}2^n t^n = \sum_{m=0}^{\infty} \frac{t^m}{m!} \int_{-\infty}^{\infty} d\xi \, H_n(\xi) \, H_m(\xi) \, e^{-\xi^2}$$
$$\sqrt{\pi}2^n n! = \int_{-\infty}^{\infty} d\xi \, H_n(\xi) \, H_n(\xi) \, e^{-\xi^2}$$

8.4 Creation, Annihilation, and Number Operator

The Hamiltonian and energy levels for the quantum simple harmonic oscillator system are, respectively,

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \qquad\qquad E_n = \hbar\omega \left(n + \frac{1}{2} \right) \; .$$

Problem 1

Introducing the *creation* and *annihilation* operators, respectively, as

$$\hat{a}^\dagger = \left(\frac{-i\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}} \hat{x} \right) \qquad\qquad \hat{a} = \left(\frac{i\hat{p}}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}} \hat{x} \right) \; ,$$

prove that the Hamiltonian operator can be written in terms of a *number* operator $\hat{N}$, given by:

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right) \qquad\qquad \hat{N} = \hat{a}^\dagger \hat{a}$$

Problem 2

Show that if $\hat{H} \left| \psi_n \right\rangle = E_n \left| \psi_n \right\rangle$ then $\hat{N} \left| \psi_n \right\rangle = n \left| \psi_n \right\rangle$.

Problem 3

Prove the relation $\hat{a}\hat{a}^\dagger = \hat{H}/\hbar\omega + 1/2$, and use this to show that the effect of the creation operator $\hat{a}^\dagger$ acting on state $\left| \psi_n \right\rangle$ is

$$\hat{a}^\dagger \left| \psi_n \right\rangle = \sqrt{n+1} \left| \psi_{n+1} \right\rangle \; .$$

Problem 4

Show that the effect of the annihilation operator $\hat{a}$ acting on state $\left| \psi_n \right\rangle$ is

$$\hat{a} \left| \psi_n \right\rangle = \sqrt{n} \left| \psi_{n-1} \right\rangle \; .$$

Solution 1

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

Solution 2

$$\hbar\omega \left(\hat{N} + \frac{1}{2} \right) \left| \psi_n \right\rangle = \hbar\omega \left(n + \frac{1}{2} \right) \left| \psi_n \right\rangle$$

Solution 3

$$\left(\hat{a}^\dagger \hat{a}\right) \hat{a}^\dagger |\psi_n\rangle = (n+1)\, \hat{a}^\dagger |\psi_n\rangle \qquad \hat{N}\, |\chi_n\rangle = (n+1)\, |\chi_n\rangle$$

$$\langle \chi_n | \hat{N} | \chi_n \rangle = (n+1) \qquad |\chi_n\rangle = \sqrt{n+1}\, |\psi_{n+1}\rangle$$

Solution 4

$$\hat{a}\hat{a}^\dagger |\psi_m\rangle = \left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2}\right) |\psi_m\rangle = (m+1)\, |\psi_m\rangle$$

$$\hat{a}\sqrt{m+1}\, |\psi_{m+1}\rangle = (m+1)\, |\psi_m\rangle \qquad m+1 = n$$

8.5 SHO Commutations and Identities

Problem 1

Prove three commutation relations for the quantum simple harmonic oscillator:

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1 \qquad \left[\hat{N}, \hat{a}\right] = -\hat{a} \qquad \left[\hat{N}, \hat{a}^\dagger\right] = \hat{a}^\dagger$$

Problem 2

Applying the annihilation operator k times, we write

$$\hat{a}^k |\psi_n\rangle = \sqrt{n(n-1)\cdots(n-k+1)}\, |\psi_{n-k}\rangle \ ,$$

which tells us that $n-k \geq 0$ to have real eigenvalues, and the ground state $|\psi_0\rangle$ corresponds to $k=n$. Verify that annihilation stops at the ground state and goes no deeper by showing that $\hat{a}\, |\psi_0\rangle = 0$.

Problem 3

The nth eigenstate can be built up from the ground state by applying the creation operator n times:

$$|\psi_n\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^\dagger\right)^n |\psi_0\rangle$$

Show that the above relation is both self-consistent and properly normalized.

Problem 4

Use $\hat{a}^\dagger$ to derive the recursion relation for the Hermite polynomials

$$-H_{n+1}(\xi) = \left(\frac{d}{d\xi} - 2\xi\right) H_n(\xi) \ ,$$

where $\xi = x\sqrt{m\omega/\hbar}$.

Problem 5

Solve for $\hat{x}$ and $\hat{p}$ in terms of the creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$.

Solution 1

$$\left[\hat{a}, \hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} - \hat{N} = 1$$

$$\left[\hat{N}, \hat{a}\right] = \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}\hat{a}^\dagger\hat{a} = \left(\hat{N} - \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)\hat{a} = -\hat{a}$$

$$\left[\hat{N}, \hat{a}^\dagger\right] = \hat{a}^\dagger\hat{a}\hat{a} - \hat{a}^\dagger\hat{a}^\dagger\hat{a} = \hat{a}^\dagger\left(\frac{\hat{H}}{\hbar\omega} + \frac{1}{2} - \hat{N}\right) = \hat{a}^\dagger$$

Solution 2

$$\hat{a}\left|\psi_0\right\rangle \sim \left[\frac{-i^2\hbar\partial_x}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}x\right] N_0 H_0 e^{-x^2 m\omega/2\hbar} = 0$$

Solution 3

$$\left|\psi_n\right\rangle = \frac{\sqrt{1}}{\sqrt{n!}}\hat{a}^{n-1}\left|\psi_{0+1}\right\rangle = \frac{\sqrt{1}\sqrt{2}}{\sqrt{n!}}\hat{a}^{n-2}\left|\psi_{0+2}\right\rangle = \frac{\sqrt{1\cdot 2\cdot 3\cdots n}}{\sqrt{n!}}\hat{a}^{n-n}\left|\psi_{0+n}\right\rangle = \left|\psi_n\right\rangle$$

$$\left\langle\psi_n|\psi_n\right\rangle = \frac{1}{n!}\left\langle\psi_0|(\hat{a})^n(\hat{a}^\dagger)^n|\psi_0\right\rangle = \frac{\sqrt{n!}}{n!}\left\langle\psi_0|\hat{a}^n|\psi_n\right\rangle = \frac{\sqrt{n!}\sqrt{n!}}{n!}\left\langle\psi_0|\psi_0\right\rangle = 1$$

Solution 4

$$\left(\frac{-\hbar\partial_x}{\sqrt{2m\hbar\omega}} + \sqrt{\frac{m\omega}{2\hbar}}x\right) N_n H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) e^{-x^2 m\omega/2\hbar} = \sqrt{n+1}N_{n+1}H_{n+1}\left(x\right)e^{-x^2 m\omega/2\hbar}$$

$$\left(-\frac{1}{\sqrt{2}}\partial_\xi + \frac{1}{\sqrt{2}}\xi\right) N_n H_n\left(\xi\right)e^{-\xi^2/2} = \sqrt{n+1}\left(\frac{N_n}{\sqrt{2\left(n+1\right)}}\right) H_{n+1}\left(\xi\right)e^{-\xi^2/2}$$

Solution 5

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right) \qquad\qquad \hat{p} = i\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right)$$

8.6 SHO and Classical Motion

Problem 1

Show that $\langle x\rangle = 0$ for any stationary SHO wavefunction.

Problem 2

Show that the simple harmonic oscillator obeys

$$\frac{d\left\langle x\right\rangle}{dt} = \frac{\left\langle p\right\rangle}{m}\ .$$

Problem 3

Suppose a SHO system has the following non-stationary wavefunction at $t = 0$:

$$\Psi(x, 0) = N\left[\psi_0(x) + 2\psi_1(x)\right]$$

Show that $\langle x \rangle$ is a function of time.

Problem 4

Evaluate the integral

$$I = \int_{-\infty}^{\infty} dx\, x\, \psi_0(x)\, \psi_1(x)$$

by two different methods. First substitute Hermite polynomials and evaluate the Gaussian integral. Second, express x in terms of $\hat{a}$ and $\hat{a}^\dagger$, and get the same result given by the first method.

Solution 1

$$\langle x \rangle = \langle \psi_n | \hat{x} | \psi_n \rangle \propto \langle \psi_n | (\hat{a} + \hat{a}^\dagger) | \psi_n \rangle \sim \langle \psi_n | \psi_{n-1} \rangle + \langle \psi_n | \psi_{n+1} \rangle = 0$$

Solution 2

$$\frac{d}{dt}\langle x \rangle = -\frac{i}{\hbar}\left\langle \left[\hat{x}, \hat{H}\right] \right\rangle = -\frac{i}{\hbar}\left\langle \left[\hat{x}, \frac{\hat{p}^2}{2m}\right] + \left[\hat{x}, \frac{1}{2}m\omega^2\hat{x}^2\right] \right\rangle = -\frac{i}{\hbar}\left\langle \frac{2i\hbar\hat{p}}{2m} + 0 \right\rangle = \frac{\langle p \rangle}{m}$$

Solution 3

$$\Psi(x, t) = Ne^{-iE_0 t/\hbar}\psi_0(x) + 2Ne^{-iE_1 t/\hbar}\psi_1(x)$$

$$\langle x \rangle = N^2 \int_{-\infty}^{\infty} dx\, x\left(\psi_0(x)^2 + 4\psi_1(x)^2 + 4\psi_0(x)\,\psi_1(x)\cos\left((E_0 - E_1)\, t/\hbar\right)\right)$$

$$\langle x \rangle = 0 + 0 + 4N^2\cos\left(\frac{(E_0 - E_1)\, t}{\hbar}\right)\int_{-\infty}^{\infty} dx\, x\, \psi_0(x)\, \psi_1(x)$$

Solution 4

$$I = \sqrt{\frac{m\omega}{\hbar\pi}}\sqrt{\frac{1}{2}\frac{2\hbar}{m\omega}}\int_{-\infty}^{\infty} d\xi\, \xi^2 e^{-\xi^2} = \sqrt{\frac{\hbar}{2m\omega}}$$

$$I = \langle \psi_0 | \hat{x} | \psi_1 \rangle = \sqrt{\frac{\hbar}{2m\omega}}\langle \psi_0 | \psi_0 \rangle$$

8.7 Prepared SHO System

A particle of mass m moving in the harmonic oscillator potential $V(x) = m\omega^2 x^2/2$ is prepared at $t = 0$ in the state

$$\Psi(x, 0) = Ne^{-m\omega x^2/2\hbar}\left[4\left(x\sqrt{m\omega/\hbar}\right)^3 + 2\left(x\sqrt{m\omega/\hbar}\right)^2 + i\left(x\sqrt{m\omega/\hbar}\right) + 2i\right].$$

Problem 1

Rewrite the initial state in terms of the dimensionless variable $\xi = x\sqrt{m\omega/\hbar}$ and the Hermite polynomials $H_n(\xi)$. Also solve for the normalization constant N.

Problem 2

Determine the wavefunction at all times, $\Psi(x,t)$.

Problem 3

At time t, a measurement of the system's energy is made. What is the probability of each possible outcome? Check that the sum of all probabilities is unity.

Problem 4

Determine $\langle x \rangle$.

Solution 1

$$H_0 = 1 \qquad H_1 = 2\xi \qquad H_2 = 4\xi^2 - 2 \qquad H_3 = 8\xi^3 - 12\xi$$
$$\Psi(x,0) = Ne^{-\xi^2/2}\left[AH_0(\xi) + BH_1(\xi) + CH_2(\xi) + DH_3(\xi)\right]$$
$$N = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\sqrt{\frac{2}{75}} \qquad A = 2i+1 \qquad B = \frac{i+6}{2} \qquad C = D = \frac{1}{2}$$

Solution 2

$$\psi_n(x,t) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right)e^{-x^2 m\omega/2\hbar}e^{-iE_n t/\hbar}$$
$$\Psi(x,t) = \sqrt{\frac{2}{75}}\left[A\psi_0(x,t) + \sqrt{2}B\psi_1(x,t) + 2\sqrt{2}C\psi_2(x,t) + 4\sqrt{3}D\psi_3(x,t)\right]$$

Solution 3

$$P_0 = \frac{2}{75}\left|2i+1\right|^2 \approx 13.33\% \qquad P_1 = \frac{2}{75}2\left|\frac{i+6}{2}\right|^2 \approx 49.33\%$$
$$P_2 = \frac{2}{75}8\left|\frac{1}{2}\right|^2 \approx 5.33\% \qquad P_3 = \frac{2}{75}48\left|\frac{1}{2}\right|^2 \approx 32.00\%$$

Solution 4

$$|\Psi(t)\rangle = \tilde{A}(t)|\psi_0\rangle + \tilde{B}(t)|\psi_1\rangle + \tilde{C}(t)|\psi_2\rangle + \tilde{D}(t)|\psi_3\rangle$$
$$\langle x \rangle = \langle \Psi(t)|\hat{x}|\Psi(t)\rangle = \tilde{A}^*\tilde{B} + \tilde{B}^*\left(\tilde{A} + \sqrt{2}\tilde{C}\right) + \tilde{C}^*\left(\sqrt{2}\tilde{B} + \sqrt{3}\tilde{D}\right) + \tilde{D}^*\sqrt{3}\tilde{C}$$
$$\langle x \rangle = \left(\tilde{A}^*\tilde{B} + \tilde{B}^*\tilde{A}\right) + \sqrt{2}\left(\tilde{B}^*\tilde{C} + \tilde{C}^*\tilde{B}\right) + \sqrt{3}\left(\tilde{C}^*\tilde{D} + \tilde{D}^*\tilde{C}\right)$$
$$\langle x \rangle = \left[\sqrt{\frac{4}{75}}\left(A^*B + B^*A\right)\epsilon_{AB} + \sqrt{\frac{64}{75}}\left(B^*C + C^*B\right)\epsilon_{BC} + 24\sqrt{\frac{4}{75}}\left(C^*D + D^*C\right)\epsilon_{CD}\right]$$
$$\langle x \rangle = \left[\sqrt{\frac{4}{75}}16 + \sqrt{\frac{64}{75}}6 + 24\sqrt{\frac{4}{75}}\right]\cos(\omega t)$$

8.8 Evolution of a Low-Energy SHO

A particle of mass m moving in the harmonic oscillator potential $V(x) = m\omega^2 x^2/2$ is prepared at $t = 0$ in the state

$$\Psi(x,0) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2} .$$

Problem 1

Calculate $\langle E \rangle$ for all times $t \geq 0$ by two methods. First, use direct integration by substituting $\hat{p} = -i\hbar\partial_x$ and $\hat{x} = x$. Second, make the assumption that $\sigma^2 = \hbar/2m\omega$ and proceed by representing $\hat{p}$ and $\hat{x}$ in terms of $\hat{a}$ and $\hat{a}^\dagger$.

Problem 2

Without assuming that $\sigma^2 = \hbar/2m\omega$, calculate the probability that a measurement of the system's energy equals $E_n = \hbar\omega(n + 1/2)$ for any integer $n \geq 0$. Hint: use the relation $\xi = x\sqrt{m\omega/\hbar}$ along with the Hermite polynomial generating function

$$e^{\xi^2-(s-\xi)^2} = \sum_{n=0}^{\infty} \frac{H_n(\xi)}{n!} s^n .$$

Solution 1

$$\langle E \rangle = \langle \Psi(t) | \left(\frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \right) | \Psi(t) \rangle = \frac{\hbar^2}{8m\sigma^2} + \frac{1}{2} m\omega^2\sigma^2 = \frac{\hbar\omega}{2}$$

Solution 2

$$\int_{-\infty}^{\infty} d\xi\; e^{\xi^2-(s-\xi)^2} e^{-\xi^2/2-\xi^2\hbar/4m\omega\sigma^2} = \sum_{n=0}^{\infty} \frac{s^n}{n!} \int_{-\infty}^{\infty} d\xi\; H_n(\xi)\, e^{-\xi^2/2-\xi^2\hbar/4m\omega\sigma^2}$$

$$\sqrt{\frac{4\pi m\omega\sigma^2/\hbar}{1+2m\omega\sigma^2/\hbar}}\; \mathrm{Exp}\left[s^2 \left(\frac{2m\omega\sigma^2/\hbar - 1}{2m\omega\sigma^2/\hbar + 1} \right) \right] = \sum_{n=\text{even}}^{\infty} \frac{s^n}{n!} \int_{-\infty}^{\infty} d\xi\; H_n(\xi)\, e^{-\xi^2/2-\xi^2\hbar/4m\omega\sigma^2}$$

$$b = \frac{2m\omega\sigma^2}{\hbar} \qquad\qquad \tilde{I}_n = \int_{-\infty}^{\infty} d\xi\; H_n(\xi)\, e^{-\xi^2/2-\xi^2\hbar/4m\omega\sigma^2}$$

$$\sqrt{\frac{2\pi b}{1+b}} \left(1 + s^2 \left(\frac{b-1}{b+1} \right) + \frac{s^4}{2!} \left(\frac{b-1}{b+1} \right)^2 + \cdots \right) = \tilde{I}_0 + \frac{s^2}{2!}\tilde{I}_2 + \frac{s^4}{4!}\tilde{I}_4 + \cdots$$

$$\Psi(x,t) = \sum_{n=0}^{\infty} \langle \psi_n | \Psi(0) \rangle\, \psi_n(x)\, e^{-iE_nt/\hbar} = \sum_{n=\text{even}}^{\infty} \frac{N_n\sqrt{\hbar/m\omega}\,\tilde{I}_n}{(2\pi\sigma^2)^{1/4}} \psi_n(x)\, e^{-iE_nt/\hbar}$$

$$P_n = \left| \frac{N_n\sqrt{\hbar/m\omega}\,\tilde{I}_n}{(2\pi\sigma^2)^{1/4}} \right|^2 = \frac{2}{2^n\,(n/2)!} \left(\frac{\sqrt{b}}{1+b} \right) \left(\frac{b-1}{b+1} \right)^{n/2}$$

8.9 Momentum Space SHO Wavefunctions

The Hamiltonian operator for a particle in a one-dimensional SHO potential is $\hat{H} = \hat{p}^2/2m + m\omega^2\hat{x}^2/2$.

Problem 1

Substituting

$$\xi = x\sqrt{m\omega/\hbar}\,,$$

find the corresponding transformation $\hat{\gamma}$ that non-dimensionalizes the momentum operator $\hat{p}$ in order to derive the dimensionless Hamiltonian:

$$\frac{\hat{H}}{\hbar\omega} = \frac{1}{2}\hat{\gamma}^2 + \frac{1}{2}\hat{\xi}^2$$

Problem 2

Due to the symmetry in the Hamiltonain above, it's evident that the mometum space wavefunctions $\psi_n(p)$ are identical in form to the position space wavefunction $\psi_n(x)$. They differ by normalization constant by virtue that $|\psi_n(p)|^2$ must have dimension $[p]^{-1}$, whereas $|\psi_n(x)|^2$ have dimension $[x]^{-1}$. Find this constant and write down the momentum wavefunctions $\psi_n(p)$.

Solution 1

$$\hat{\gamma} = \frac{\hat{p}}{\sqrt{m\hbar\omega}}$$

Solution 2

$$\psi_n\left(p\right) = \left[\sqrt{\frac{2\pi}{m\hbar\omega}}\right]\left(\frac{m\omega}{\hbar\pi}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{p}{\sqrt{m\hbar\omega}}\right)e^{-p^2/2m\hbar\omega}$$