Solutions to Quantum Mechanics by Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloe

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September 21, 2020

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Chapter 1

Waves and Particles. Introduction to the Fundamental Ideas of Quantum Mechanics

1.1 Multiple-Slit Experiment

A beam of neutrons of constant velocity, mass $M_n(M_n \approx 1.67x10^{-27}$ kg) and energy E, is incident on a linear chain of atomic nuclei, arranged in a regular fashion as shown in the figure (these nuclei could be, for example, those of a long, linear molecule). We call l the distance between two consecutive nuclei, and d, their size ($d \ll l$). A neutron detector D is placed far away, in a direction which makes an angle of θ with the direction of the incident neutrons.

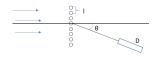


Figure 1.1: Multiple-slit Experiment

1.1.a Describe qualitatively the phenomena observed at D when the energy E of the incident neutrons is varied.

From Complement D_I , the fringe separation of the double-slit experiment is given by $\frac{\lambda D}{l}$. Using the Planck-Einstein relations(A-1), we know that as energy increases, the wavelength decreases. Thus, the distance between successive peaks decreases as well, so we end up seeing more

peaks in a given area.

1.1.b The counting rate, as a function of E, presents a resonance about $E = E_1$. Knowing that there are no other resonances for $E < E_1$, show that one can determine l. Calculate l for $\theta = 30^{\circ}$ and $E_1 = 1.3 \times 10^{-20}$ joule.

From complement D_I , for a double slit experiment,

$$l\sin(\theta) = m\lambda$$

Since we are looking at the first interference, we set m = 1. Using the Planck-Einstein relations(A-1), we can rewrite the right-side of the equation,

$$l\sin(\theta) = \frac{hc}{E}$$
$$l = \frac{hc}{E\sin(\theta)}$$

Plugging in the given variables and constants, we find $l = 1.61 \times 10^{-14}$ m. Note that we ignore d, the diameter of each nuclei since we assumed $d \ll l$.

1.1.c At about what value of *E* must we begin to take the finite size of the nuclei into account?

Using Heisenburg's uncertainty relation(C-23), and rewriting the momentum in terms of energy,

$$\Delta x \cdot \Delta p \ge \frac{\hbar}{2}$$
$$\Delta x \cdot \frac{h}{\lambda} \ge \frac{\hbar}{2}$$
$$\Delta x \ge \frac{hc}{4\pi E}$$
$$E \ge \frac{hc}{4\pi \cdot \Delta x}$$

The size of atomic nuclei are on the order of fermi, 10^{-15} m, so plugging in those numbers, we get something on the order of 8×10^{-21} J.

1.2 Bound State of a Particle in a "Delta Function Potential"

Consider a particle whose Hamiltonian \mathcal{H} [operator defined by formula (D-10) is:

$$\mathscr{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \alpha\delta(x)$$

where α is a positive constant whose dimensions are to be found.

1.2.a Integrate the eigenvalue equation of \mathscr{H} between $-\epsilon$ and $+\epsilon$. Letting ϵ approach 0, show that the derivative of the eigenfunction $\phi(x)$ presents a discontinuity at x = 0 and determine it in terms of α , m, and $\phi(0)$.

Nothing doing, let's do as the question asks,

,

$$\int_{-\epsilon}^{\epsilon} \mathscr{H} \left| \phi \right\rangle \ dx = \int_{-\epsilon}^{\epsilon} E \left| \phi \right\rangle \ dx$$

$$\int_{-\epsilon}^{\epsilon} -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi(x) \, dx - \int_{-\epsilon}^{\epsilon} \alpha \delta(x) \phi(x) \, dx = E \int_{-\epsilon}^{\epsilon} \phi(x) \, dx$$

On the right, the integral disappears as $\epsilon \to 0$. The delta function only turns on if the integral includes x = 0, and it picks out that value in that integral,

$$-\frac{\hbar^2}{2m}\frac{d\phi(x)}{dx}\Big|_{x=-\epsilon}^{x=\epsilon} -\alpha\phi(0) = 0$$

$$\left. \frac{d\phi(x)}{dx} \right|_{x=\epsilon} - \left. \frac{d\phi(x)}{dx} \right|_{x=-\epsilon} = -\frac{2m\alpha\phi(0)}{\hbar^2}$$

As $\epsilon \to 0$, the left side would disappear unless there were a discontinuity. Since the right side is not equal to zero, there must be a discontinuity in the derivative of $\phi(x)$.

1.2.b Assume that the energy *E* of the particle is negative(bound state). $\phi(x)$ can then be written:

$$\begin{cases} x < 0 \quad \phi(x) = A_1 \exp(\rho x) + A'_1 \exp(-\rho x) \\ x > 0 \quad \phi(x) = A_2 \exp(\rho x) + A'_2 \exp(-\rho x) \end{cases}$$

Express the constant ρ in terms of E and m. Using the results of the preceding question, calculate the matrix M defined by:

$$\begin{pmatrix} A_2 \\ A'_2 \end{pmatrix} = M \begin{pmatrix} A_1 \\ A'_1 \end{pmatrix}$$

Then, using the condition that $\phi(x)$ must be square-integrable, find the possible values of the energy. Calculate the corresponding normalized wave functions.

We can find ρ by using the Schrödinger equation(B-8),

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) = E\phi(x)$$

We only need to look at $\phi(x)$ at a single time, so lets look at the case x < 0,

$$-\frac{\hbar^2}{2m}(A_1\rho^2\exp(\rho x) + A_1'\rho^2\exp(-\rho x)) = E(A_1\exp(\rho x) + A_1'\exp(-\rho x))$$

$$-\frac{\hbar^2 \rho^2}{2m} = E$$

$$\rho^2 = -\frac{2mE}{\hbar^2}$$

To calculate the required matrix, we use the discontinuity in the derivative,

$$\left. \frac{d\phi(x)}{dx} \right|_{x=\epsilon} - \left. \frac{d\phi(x)}{dx} \right|_{x=-\epsilon} = -\frac{2m\alpha\phi(0)}{\hbar^2}$$

The first term we will need to use the x > 0 case and x < 0 for the second,

$$\rho A_2 \exp(\rho \epsilon) - A_2' \rho \exp(-\rho \epsilon) - A_1 \rho \exp(\rho \epsilon) + A_1' \rho \exp(-\rho \epsilon) = -\frac{2m\alpha}{\hbar^2} (A_1 + A_1')$$

Note that we chose an arbitrary case for x = 0. Because $\phi(x)$ must be continuous, $A_1 + A'_1 = A_2 + A'_2$. Letting $\epsilon \to 0$, we have,

$$A_2 - A'_2 - A_1 + A'_1 = -\frac{2m\alpha}{\rho\hbar^2}(A_1 + A'_1)$$

$$A_2 = -\frac{2m\alpha}{\rho\hbar^2}(A_1 + A_1') + A_1 - A_1' + A_2'$$

Using the continuity of the wavefunction,

$$2A_2 = A_1 \left(-\frac{2m\alpha}{\rho\hbar^2} + 2 \right) - \frac{2m\alpha}{\rho\hbar^2} A_1'$$

$$2A'_{2} = \frac{2m\alpha}{\rho\hbar^{2}}A_{1} + A'_{1}\left(2 + \frac{2m\alpha}{\rho\hbar^{2}}\right)$$
$$\begin{pmatrix}A_{2}\\A'_{2}\end{pmatrix} = \begin{pmatrix}-\frac{m\alpha}{\rho\hbar^{2}} + 1 & -\frac{m\alpha}{\rho\hbar^{2}}\\\\\frac{m\alpha}{\rho\hbar^{2}} & \frac{m\alpha}{\rho\hbar^{2}} + 1\end{pmatrix}\begin{pmatrix}A_{1}\\A'_{1}\end{pmatrix}$$

Let's now normalize the wavefunction,

$$\int_{-\infty}^{\infty} |\phi(x)|^2 \, dx = 1$$

If we have a particle coming from the left, we want to set $A_2 = 0$. Furthermore, since we want this to be square-integrable, we must set $A'_1 = 0$. Since the wavefunction must be continuous, $A_1 = A'_2$.

$$\int_{-\infty}^{0} A_1^2 \exp(2\rho x) \, dx + \int_{0}^{\infty} A_1^2 \exp(-2\rho x) \, dx = 1$$
$$A_1^2 \left(\frac{1}{2\rho} + \frac{1}{2\rho}\right) = 1$$
$$A_1^2 = \rho$$

Our normalized wavefunction is given,

$$\begin{cases} x < 0 \quad \phi(x) = \sqrt{\rho} \exp(\rho x) \\ x > 0 \quad \phi(x) = \sqrt{\rho} \exp(-\rho x) \end{cases}$$

To find the allowed energy, we go back to the discontinuity equation

$$\frac{d\phi(x)}{dx}\Big|_{x=\epsilon} - \frac{d\phi(x)}{dx}\Big|_{x=-\epsilon} = -\frac{2m\alpha A_1}{\hbar^2}$$
$$\rho A_1 + \rho A - 1 = -\frac{2m\alpha A_1}{\hbar^2}$$
$$\rho \hbar^2 = -m\alpha$$

Squaring both sides then substituting in our value of ρ ,

$$\rho^{2}\hbar^{4} = m^{2}\alpha^{2}$$
$$-2mE\hbar^{2} = m^{2}\alpha^{2}$$
$$E = -\frac{m\alpha^{2}}{2\hbar^{2}}$$

1.3 Transmission of a "delta function" potential barrier"

Consider a particle placed in the same potential as in the preceding exercise. The particle is now propagating from left to right along the x axis, with a positive energy E.

1.3.a Show that a stationary state of the particle can be written:

$$\begin{cases} x < 0 \quad \phi(x) = \exp(ikx) + A\exp(-ikx) \\ x > 0 \quad \phi(x) = B\exp(ikx) \end{cases}$$

where k, A, and B are constants which are to be calculated in terms of the energy E, of m and of α (watch out for the discontinuity in $\frac{d\phi}{dx}$ at x = 0. By observation, the given wavefunction is not dependent on time, and it follows the form given

By observation, the given wavefunction is not dependent on time, and it follows the form given by (D-7), so it is a stationary state. To determine the constants, we can look at the Schrödinger equation(B-8),

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) - \alpha\delta(x)\phi(x) = E\phi(x)$$

This holds true for all values of x, so let's look at x > 0. The delta function term dies,

$$-\frac{\hbar^2}{2m}(-Bk^2\exp(ikx)) = EB\exp(ikx)$$
$$\frac{\hbar^2k^2}{2m} = E$$
$$k^2 = \frac{2mE}{\hbar^2}$$

At x = 0, we use the wavefunction continuity,

$$B = 1 + A$$

1(0)

1// >1

as well as the discontinuity in the first derivative,

1 ()]

$$\frac{d\phi(x)}{dx}\Big|_{x=\epsilon} - \frac{d\phi(x)}{dx}\Big|_{x=-\epsilon} = -\frac{2m\alpha\phi(0)}{\hbar^2}$$
$$ikB - ik(1-A) = -\frac{2m\alpha B}{\hbar^2}$$
$$B(ik\hbar^2 + 2m\alpha) = ik\hbar^2(1-A)$$
$$B = \frac{ik\hbar^2}{ik\hbar^2 + m\alpha}$$
$$A = -\frac{m\alpha}{ik\hbar^2 + m\alpha}$$

1.3.b Set $-E_L = -m\alpha^2/2\hbar^2$ (bound state energy of the particle). Calculate, in terms of the dimensionless parameter E/E_L , the reflection coefficient R and the transmission coefficient T of the barrier. Study their variations with respect to E; what happens when $E \to \infty$? How can this be interpreted? Show that, if the expression of T is extended for negative values of E, it diverges when $E \to E_L$, and discuss this result.

To find the reflection coefficient, we look at the parameters of incoming and outgoing particles. A particle moving to the right has magnitude 1, while a particle moving to the left has magnitude A,

$$R = |A|^2 = \frac{m^2 \alpha^2}{k^2 \hbar^4 + m^2 \alpha^2}$$
$$= \frac{m^2 \alpha^2}{m^2 \alpha^2 (1 + E/E_L)}$$
$$R = \frac{1}{1 + E/E_L}$$

Similarly, a particle moving to the right after passing through the barrier has magnitude B,

$$T = |B|^2 = \frac{k^2 \hbar^4}{k^2 \hbar^4 + m^2 \alpha^2}$$
$$T = \frac{E/E_L}{1 + E/E_L}$$

We see that T + R = 1. As $E \to \infty$, $T \to 1$ and $R \to 0$, which means the wavefunction has more and more energy to overcome the barrier. As energy increases, the probability that the particle will go through the barrier increases. At $E = -E_L$, it has the same energy as the barrier, which is why we see that discontinuity. Classically, think of this as a ball hitting the top edge of a wall. Small variations around this point determine if the ball is reflected or transmitted.

1.4 Delta potential, Fourier transform

Return to exercise 2, using, this time, the Fourier transform.

1.4.a Write the eigenvalue equation of \mathscr{H} and the Fourier transform of this equation. Deduce directly from this the expression for $\overline{\phi}(p)$, the Fourier transform of $\phi(x)$, in terms of p, E, α , and $\phi(0)$. Then show that only one value of E, a negative one, is possible. Only the bound state of the particle, and not the ones in which it propagates, is found by this method; why? Then calculate $\phi(x)$ and show that one can find in this way all the results of exercise 2.

Looking at Appendix I, the Fourier transform of the eigenvalue equation is

$$-\frac{\hbar^2}{2m}\left(\frac{ip}{\hbar}\right)^2\bar{\phi}(p) - \mathscr{F}[\alpha\delta(x)\phi(x)] = E\bar{\phi}(p)$$

We get this using

$$\bar{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-\frac{ipx}{\hbar}\right) \phi(x) \, dx$$
$$\phi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(\frac{ipx}{\hbar}\right) \bar{\phi}(p) \, dp$$

We note that

$$\frac{d^2}{dx^2}\bar{\phi}(p) = \left(\frac{ip}{\hbar}\right)^2\bar{\phi}(p)$$

We need to be careful about the Fourier transform of the delta function.

$$\mathscr{F}[\alpha\delta(x)\phi(x)] = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left(-\frac{ipx}{\hbar}\right) \alpha\delta(x)\phi(x) \ dx$$
$$= \frac{1}{\sqrt{2\pi\hbar}} \alpha\phi(0)$$

Substituting this back in,

$$\frac{p^2}{2m}\bar{\phi}(p) - \frac{\alpha\phi(0)}{\sqrt{2\pi\hbar}} = E\bar{\phi}(p)$$

$$\bar{\phi}(p) = \frac{\alpha\phi(0)}{\sqrt{2\pi\hbar}} \frac{1}{(p^2/2m - E)}$$

1.4. DELTA POTENTIAL, FOURIER TRANSFORM

We can reverse our Fourier transform to get $\phi(x)$,

$$\phi(x) = \frac{\alpha\phi(0)}{2\pi\hbar} \int_{-\infty}^{\infty} \frac{\exp\left(\frac{ipx}{\hbar}\right)}{(p^2/2m - E)} dp$$
$$\phi(x) = \frac{\alpha\phi(0)m}{\hbar\sqrt{-2mE}} \exp\left(-\frac{\sqrt{-2mE}}{\hbar}x\right)$$

To determine the allowed energy, let's set x = 0 and match sides,

$$\phi(0) = \frac{\alpha m \phi(0)}{\hbar \sqrt{-2mE}}$$

In order for this to hold true,

$$\frac{\alpha m}{\hbar\sqrt{-2mE}} = 1$$
$$E = -\frac{\alpha^2 m}{2\hbar^2}$$

1.4.b The average kinetic energy of the particle can be written (cf. chap. III):

$$E_k = \frac{1}{2m} \int_{-\infty}^{\infty} p^2 |\bar{\phi}(p)|^2 dp$$

Show that, when $\bar{\phi}(p)$ is a "sufficiently smooth" function, we also have:

$$E_k = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \phi^*(x) \frac{d^2\phi}{dx^2} dx$$

These formulas enable us to obtain, in two different ways, the energy E_k for a particle in the bound state calculated in (a). What result is obtained? Note that, in this case $\phi(x)$ is not "regular" at x = 0, where its derivative is discontinuous. It is then necessary to differentiate $\phi(x)$ in the sense of distributions, which introduces a contribution of the point x = 0 to the average value we are looking for. Interpret this contribution physically: consider a square well, centered at x = 0, whose width *a* approaches 0 and whose depth V_0 approaches infinity (so that $aV_0 = \alpha$), and study the behaviour of the wave function in this well.

Starting with the second equation and substituting in the definitions from Appendix I,

$$\phi^*(x)\frac{d^2\phi}{dx^2} = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \exp\left(-\frac{ipx}{\hbar}\right) \bar{\phi}(p) \left(\frac{ipx}{\hbar}\right)^2 \exp\left(\frac{ipx}{\hbar}\right) \ dp$$

$$E_k = \frac{1}{4m\pi\hbar} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p^2 |\bar{\phi}(p)|^2 \, dp \, dx$$

The constants in front disappear when we integrate over all x,

$$E_k = \frac{1}{2m} \int_{-\infty}^{\infty} p^2 |\bar{\phi}(p)|^2 \ dp$$

1.5 Well consisting of two delta functions

Consider a particle of mass m whose potential energy is

$$V(x) = -\alpha\delta(x) - \alpha\delta(x-l) \quad \alpha > 0$$

where l is a constant length.

1.5.a Calculate the bound states of the particle, setting $E = -\frac{\hbar^2 \rho^2}{2m}$. Show that the possible energies are given by the relation

$$\exp(-\rho l) = \pm \left(1 - \frac{2\rho}{\mu}\right)$$

where μ is defined by $\mu = \frac{2m\alpha}{\hbar^2}$. Give a graphical solution of this equation. We can divide this into three regions,

$$\phi(x) = \begin{cases} A \exp(\rho x) & x < 0\\ B(\exp(-\rho x) + \exp(\rho(x-l))) & 0 < x < l\\ A \exp(-\rho(x-l)) & x > l \end{cases}$$

We get this because we know that the wavefunction corresponding to a delta function is exponential on both sides, so we can reasonable expect the wavefunction corresponding to two delta functions is going to more exponential functions.

To solve for the bound states, let's start by looking at x = 0. From continuity,

$$A = B(1 + \exp(-\rho l))$$

From problem 2, we know there is a discontinuity in the derivative,

$$\begin{aligned} \left. \frac{d\phi}{dx} \right|_{x=\epsilon} &- \left. \frac{d\phi}{dx} \right|_{x=-\epsilon} = -\mu\phi(0) \\ &-\rho B + \rho B \exp(-\rho l) - \rho A = -\mu A \\ &-\rho + \rho \exp(-\rho l) - \rho - \rho \exp(-\rho l) = -\mu(1 + \exp(-\rho l)) \\ &-2\rho = -\mu(1 + \exp(-\rho l)) \\ &\exp(-\rho l) = 1 - \frac{2\rho}{\mu} \end{aligned}$$

The bound states are given by

$$\exp(-\rho l) = \pm \left(1 - \frac{2\rho}{\mu}\right)$$

(i) Ground State. Show that this state is even (invariant with respect to reflection about the point x = l/2), and that its energy E_s is less than the energy $-E_L$ introduced in problem 3. Interpret this result physically. Represent graphically the corresponding wave function.

1.6 Square Well Potential

Consider a square well potential of width a and depth V_0 (in this exercise, we shall use systematically the notation of 2-c- α of complement H_I). We intend to study the properties of the bound state of a particle in a well when its width a approaches zero.

1.6.a Show that there indeed exists only one bound state and calculate its energy $E\left(\text{we find } E \approx -\frac{mV_0a^2}{2\hbar^2}, \text{ that is, an energy which varies}\right)$ with the square of the area aV_0 of the well).

18CHAPTER 1. WAVES AND PARTICLES. INTRODUCTION TO THE FUNDAMENTAL IDEAS OF QUANTU

Chapter 2

The Mathematical Tools of Quantum Mechanics

2.1 Hermitian Operator

 $|\phi_n\rangle$ are the eigenstates of a Hermitian operator H (H is, for example, the Hamiltonian of an arbitrary physical system). Assume that the states $|\phi_n\rangle$ form a discrete orthonormal basis. The operator U(m,n) is defined by:

 $U(m,n) = \left|\phi_m\right\rangle \left\langle\phi_n\right|$

2.1.a Calculate the adjoint $U^{\dagger}(m,n)$ of U(m,n)

Using the definition of the adjoint,

$$U^{\dagger}(m,n) = |\phi_n\rangle \langle \phi_m|$$

2.1.b Calculate the commutator [H, U(m, n)]

Let's act the commutator on a vector (looking ahead, we'll set the vector as $|\phi_n\rangle$,

$$[H, U] |\phi_n\rangle = HU |\phi_n\rangle - UH |\phi_n\rangle$$

$$= H \left| \phi_m \right\rangle \left\langle \phi_n \right| \phi_n \right\rangle - \left| \phi_m \right\rangle \left\langle \phi_n \right| H \left| \phi_n \right\rangle$$

Since H has eigenkets ϕ_n and ϕ_m , i.e.,

$$\begin{cases} H |\phi_m\rangle = m |\phi_m\rangle \\ H |\phi_n\rangle = n |\phi_n\rangle \end{cases}$$
$$[H, U(m, n)] = m - n$$

2.1.c Prove the relation

$$U(m,n)U^{\dagger}(p,q) = \delta_{nq}U(m,p)$$

Writing this out,

$$U(m,n)U^{\dagger}(p,q) = |\phi_m\rangle \langle \phi_n | \phi_q \rangle \langle \phi_p |$$

The middle section dies unless n = q, leaving us the delta function,

$$=\delta_{nq}\left|\phi_{m}\right\rangle\left\langle\phi_{p}\right|$$

$$U(m,n)U^{\dagger}(p,q) = \delta_{nq}U(m,p)$$

2.1.d Calculate $Tr{U(m,n)}$, the trace of the operator U(m,n)

By definition, the trace is given by

$${\rm Tr}\, U = \sum_\alpha \left< \alpha |U| \alpha \right>$$

where α are the basis states.

$$=\sum_{\alpha}\left\langle \alpha|\phi_{m}\right\rangle \left\langle \phi_{n}|\alpha\right\rangle$$

Since $|\phi_n\rangle$ form a basis, and since we sum over the basis states, at least one part dies unless m = n,

$$\operatorname{Tr} U = \delta_{mn}$$

2.1.e Let A be an operator, with matrix elements $A_{mn} = \langle \phi_m | A | \phi_n \rangle$. Prove the relation:

$$A = \sum_{m,n} A_{mn} U(m,n)$$

Let's start from the right side. Acting it on $|\phi_n\rangle$, we only need to sum over m since we can use orthonormality for n,

$$\sum_{m,n} A_{mn} U(m,n) \left| \phi_n \right\rangle = \sum_m \left\langle \phi_m | A | \phi_n \right\rangle \left| \phi_m \right\rangle \left\langle \phi_n | \phi_n \right\rangle$$

 A_{mn} is a scalar, so we can move that around for free,

$$=\sum_{m}\left|\phi_{m}\right\rangle\left\langle\phi_{m}\right|A\left|\phi_{n}\right\rangle$$

Performing the sum, the first part becomes identity, so we can remove it,

$$\sum_{m,n} A_{mn} U(m,n) \left| \phi_n \right\rangle = A \left| \phi_n \right\rangle$$

2.1. HERMITIAN OPERATOR

2.1.f Show that $A_{pq} = \text{Tr}\{AU^{\dagger}(p,q)\}$

We start with the right side. We can write the part inside the trace using the relation we found in part (e),

$$AU^{\dagger}(p,q) = \sum_{m,n} A_{mn}U(m,n)U^{\dagger}(p,q)$$

Using the relation from (c),

$$=\sum_{m,n}A_{mn}\delta_{nq}U(m,p)$$

$$=\sum_{m}A_{mq}U(m,p)$$

Taking the trace and using the result from (d),

$$\operatorname{Tr}\{AU^{\dagger}(p,q)\} = \sum_{m} A_{mq} \delta_{mp}$$

$$\operatorname{Tr}\{AU^{\dagger}(p,q)\} = A_{pq}$$

2.2 Pauli Matrices

In a two-dimensional vector space, consider the operator whose matrix, in an orthonormal basis $\{|1\rangle, |2\rangle\}$, is written:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

2.2.a Is σ_y Hermitian? Calculate its eigenvalues and eigenvectors (giving their normalized expansion in terms of the $\{|1\rangle, |2\rangle\}$ basis).

 σ_y is Hermitian from observation (1.13). Solving the characteristic equation (1.20), we get two eigenvalues, $\lambda = \pm 1$. The eigenvectors are,

$$|\lambda = 1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} -i \\ 1 \end{bmatrix}; \quad |\lambda = -1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} i \\ 1 \end{bmatrix}$$

In the $\{|1\rangle, |2\rangle\}$ basis,

$$\begin{cases} |\lambda = 1\rangle = 1/\sqrt{2}(-i |1\rangle + |2\rangle) \\ |\lambda = -1\rangle = 1/\sqrt{2}(i |1\rangle + |2\rangle) \end{cases}$$

2.2.b Calculate the matrices which represent the projectors onto these eigenvectors. Then verify that they satisfy the orthogonality and closure relations.

The projection operator (1.16) for $\lambda = 1$,

$$\begin{split} A &= \left| \lambda = 1 \right\rangle \left\langle \lambda = 1 \right| \\ &= \frac{1}{2} \left(-i \left| 1 \right\rangle + \left| 2 \right\rangle \right) \left(i \left\langle 1 \right| + \left\langle 2 \right| \right) \\ &A &= \frac{1}{2} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \end{split}$$

Similarly, for $\lambda = -1$,

$$B = \left| \lambda = -1 \right\rangle \left\langle \lambda = -1 \right|$$

$$B = \frac{1}{2} \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}$$

We can show that they are orthonormal by multiplying the two together, AB = BA = 0. We can show completeness by adding them together, A + B = I.

2.3 Kets and Operators

The state space of a certain physical system is three-dimensional. Let $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ be an orthonormal basis of this space. The kets $|\psi_0\rangle$ and $|\psi_1\rangle$ are defined by:

$$\begin{cases} |\psi_0\rangle = 1/\sqrt{2} \ |u_1\rangle + i/2 \ |u_2\rangle + 1/2 \ |u_3\rangle \\ |\psi_1\rangle = 1/\sqrt{3} \ |u_1\rangle + i/\sqrt{3} \ |u_3\rangle \end{cases}$$

2.3.a Are these kets normalized?

,

To tell if these kets are normalized, we need to find the norm (1.4). Let's start with $|\psi_0\rangle$,

$$\langle \psi_0 | \psi_0 \rangle = \left(\frac{1}{\sqrt{2}} \langle u_1 | -\frac{i}{2} \langle u_2 | +\frac{1}{2} \langle u_3 | \right) \left(\frac{1}{\sqrt{2}} | u_1 \rangle + \frac{i}{2} | u_2 \rangle + \frac{1}{2} | u_3 \rangle \right)$$

Since the basis kets are orthonormal, we ignore most of the terms,

$$= \frac{1}{2} \langle u_1 | u_1 \rangle + \frac{1}{4} \langle u_2 | u_2 \rangle + \frac{1}{4} \langle u_3 | u_3 \rangle = 1$$

For $|\psi_1\rangle$,

$$\langle \psi_1 | \psi_1 \rangle = (1/\sqrt{3} \ \langle u_1 | -i/\sqrt{3} \ \langle u_3 |) (1/\sqrt{3} \ | u_1 \rangle + i/\sqrt{3} \ | u_3 \rangle)$$
$$= 1/3 \ \langle u_1 | u_1 \rangle + 1/3 \ \langle u_3 | u_3 \rangle = 2/3$$

 $|\psi_0\rangle$ is normalized, but $|\psi_1\rangle$ is not.

2.3.b

Calculate the matrices ρ_0 and ρ_1 representing, in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis, the projection operators onto the state $|\psi_0\rangle$ and onto the state $|\psi_1\rangle$. Verify that these matrices are Hermitian.

Using equation (1.16),

$$\begin{aligned} \rho_0 &= |\psi_0\rangle \langle \psi_0| \\ &= (1/\sqrt{2} \ |u_1\rangle + i/2 \ |u_2\rangle + 1/2 \ |u_3\rangle)(1/\sqrt{2} \ \langle u_1| - i/2 \ \langle u_2| + 1/2 \ \langle u_3| \end{aligned}$$

We can define our orthonormal basis however we want, but for ease, let's use,

$$|u_1\rangle = \begin{bmatrix} 1\\0\\0 \end{bmatrix}; |u_2\rangle = \begin{bmatrix} 0\\1\\0 \end{bmatrix}; |u_3\rangle = \begin{bmatrix} 0\\0\\1 \end{bmatrix}$$

In this basis,

$$\rho_0 = \begin{bmatrix} 1/2 & -i/2\sqrt{2} & 1/2\sqrt{2} \\ i/2\sqrt{2} & 1/4 & i/4 \\ 1/2\sqrt{2} & -i/4 & 1/4 \end{bmatrix}$$

We use the Hermitian condition (1.13) to see that ρ_0 is Hermitian. Similarly,

$$\rho_1 = \left| \psi_1 \right\rangle \left\langle \psi_1 \right|$$

$$= (1/\sqrt{3} |u_1\rangle + i/\sqrt{3} |u_3\rangle)(1/\sqrt{3} \langle u_1| - i/\sqrt{3} \langle u_3|)$$

$$\rho_1 = \begin{bmatrix} 1/3 & 0 & -i/3\\ 0 & 0 & 0\\ i/3 & 0 & 1/3 \end{bmatrix}$$

Again, we see that ρ_1 is Hermitian.

2.4 Operators

Let K be the operator defined by $K = |\phi\rangle \langle \psi|$, where $|\phi\rangle$ and $|\psi\rangle$ are two vectors of the state space.

$\mathbf{2.4.a}$

Under what condition is K **Hermitian** Following the Hermitian condition, we want to show

$$K = K^{\dagger}$$

Under dual correspondence (1.1), this translates to,

$$|\phi\rangle \langle \psi| = |\psi\rangle |\phi\rangle$$

This is true for $|\phi\rangle = |\psi\rangle$.

$\mathbf{2.4.b}$

Calculate K^2 . Under what condition is K a projector?

$$K^{2} = \left|\phi\right\rangle \left\langle\psi\right|\phi\right\rangle \left\langle\psi\right|$$

Comparing to equation (1.16), K is a projector if $|\phi\rangle = |\psi\rangle$.

2.4.c

Show that K can always be written in the form $K = \lambda P_1 P_2$ where λ is a constant to be calculated and P_1 and P_2 are projectors

We set P_1 to be the $|\phi\rangle$ projector and P_2 to be the $|\psi\rangle$ projector (1.16)

.

$$\begin{cases} P_1 = |\phi\rangle \langle \phi| \\ P_2 = |\psi\rangle \langle \psi| \end{cases}$$

Multiplying them together,

$$P_1 P_2 = \left|\phi\right\rangle \left\langle\phi\right|\psi\right\rangle \left\langle\psi\right|$$

The middle part is just a scalar, so if we want to get rid of it, we need to multiply by a constant,

$$\lambda = \frac{1}{\langle \phi | \psi \rangle}$$

Combining all of this,

$$\lambda P_1 P_2 = \left|\phi\right\rangle \left\langle\psi\right| = K$$

2.5 Orthogonal Projector

Let P_1 be the orthogonal projector onto the subspace \mathscr{E}_1 , P_2 be the orthogonal projector onto the subspace \mathscr{E}_2 . Show that, for the product P_1P_2 to be an orthogonal projector as well, it is necessary and sufficient that P_1 and P_2 commute. In this case, what is the subspace onto which P_1P_2 projects?

Let's say

$$\begin{cases} P_1 = |\phi\rangle \langle \phi| \\ P_2 = |\psi\rangle \langle \psi| \end{cases}$$

where $|\phi\rangle$ and $|\psi\rangle$ are in \mathscr{E}_1 and \mathscr{E}_2 respectively. The product is thus,

$$P_1 P_2 = \left|\phi\right\rangle \left\langle\phi\right|\psi\right\rangle \left\langle\psi\right|$$

To show that this is an orthogonal projection, we assume $|\phi\rangle$ and $|\psi\rangle$ are normalized. We can then use the property of orthogonal projectors that $P_1 = P_1^*$ and $P_2 = P_2^*$,

$$P_1P_2 = P_1^*P_2^*$$

Using equation (1.12),

$$= (P_2 P_1)^*$$

If P_1P_2 is an orthogonal projection, then $P_1P_2 = P_2P_1$. Alternatively, if we assume P_1P_2 commutes,

$$(P_1P_2)^2 = (P_1P_2)(P_1P_2)$$

= $P_1P_2P_2^*P_1^*$
= $P_1P_2P_1$

Since P_1P_2 commutes,

$$=P_1P_1P_2 (2.5.1)$$

$$(P_1 P_2)^2 = P_1 P_2$$

 P_1P_2 projects onto the overlap of \mathscr{E}_1 and \mathscr{E}_2 . I'm not entirely sure how to rigorously prove this, but imagine that \mathscr{E}_1 is the x - y plane and \mathscr{E}_2 is the y - z plane. If we apply P_2 to a vector, it projects onto that plane. Then, if we apply P_1 to that projection, it must project onto the y-axis (the overlap) since the vector should have no x component after being projected. We can do the same for the inverse.

2.6 Pauli Matrices

The σ_x matrix is defined by:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Prove the relation:

$$\exp(i\alpha\sigma_x) = I\cos(\alpha) + i\sigma_x\sin(\alpha)$$

where I is the 2×2 unit matrix.

We can expand the left side using a Taylor expansion,

$$\exp(i\alpha\sigma_x) = I + i\alpha\sigma_x + \frac{1}{2} (i\alpha)^2 \sigma_x^2 + \dots$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + i\alpha \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{\alpha^2}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \dots$$
$$= \begin{pmatrix} 1 - \frac{\alpha^2}{2} + \dots & i\alpha + \dots \\ i\alpha + \dots & 1 - \frac{\alpha^2}{2} + \dots \end{pmatrix}$$

Similarly, if we expand the right side,

$$I\cos(\alpha) = \begin{pmatrix} 1 - \alpha^2/2 + \dots & 0\\ 0 & 1 - \alpha^2/2 + \dots \end{pmatrix}$$
$$i\sigma_x \sin(\alpha) = \begin{pmatrix} 0 & i\alpha + \dots\\ i\alpha + \dots & 0 \end{pmatrix}$$

You can do this out to an arbitrary number of terms until you convince yourself that this relation holds true.

2.7 Pauli Matrices

Establish for the σ_y matrix given in exercise 2, a relation analogous to the one proved for σ_x in the preceding exercise. Generalize for all matrices of the form:

$$\sigma_u = \lambda \sigma_x + \mu \sigma_y$$

with

$$\lambda^2 + \mu^2 = 1$$

Calculate the matrices representing $\exp(2i\sigma_x)$, $(\exp(i\sigma_x))^2$ and $\exp(i(\sigma_x + \sigma_y))$ Is $\exp(2i\sigma_x)$ equal to $(\exp(i\sigma_x))^2$? $\exp(i(\sigma_x + \sigma_y))$ to $\exp(i\sigma_x)\exp(i\sigma_y)$?

Following the methodology in question 6, we expand the exponential,

$$\exp(i\alpha\sigma_y) = I + i\alpha\sigma_y + \frac{1}{2} (i\alpha)^2 \sigma_y^2 + \dots$$

$$= \begin{pmatrix} 1 - \alpha^2/2 + \dots & \alpha + \dots \\ -\alpha + \dots & 1 - \alpha^2/2 + \dots \end{pmatrix}$$

We can convince ourselves that this is

$$\exp(i\alpha\sigma_y) = I\cos(\alpha) + i\sigma_y\sin(\alpha)$$

For σ_u , we can't use the normal rules of exponential multiplication (which answers the last part of this question). Expanding,

$$\exp(i\alpha(\lambda\sin_x+\mu\sigma_y)) = I + i\alpha(\lambda\sigma_x+\mu\sigma_y) + \frac{1}{2}(i\alpha)^2(\lambda^2\sigma_x^2 + \mu^2\sigma_y^2 + \lambda\mu\sigma_x\sigma_y + \lambda\mu\sigma_y\sigma_x)$$

$$\exp(i\alpha(\lambda\sigma_x + \mu\sigma_y)) = I\cos(\alpha) + i\sigma_x\sin(\alpha\lambda) + i\sigma_y\sin(\alpha\mu)$$

Using the relation found in question 6,

$$\exp(2i\sigma_x) = I\cos(2) + i\sigma_x\sin(2)$$

$$(exp(i\sigma_x))^2 = I(\cos^2(1) - \sin^2(1)) + 2i\sigma_x \cos(1)\sin(1)$$

These are equal using angle addition formulas.

2.8. 2.8

2.8 2.8

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2.9 2.9

2.10. 2.10

$2.10 \quad 2.10$

2.11 Commuting Observables and CSCOs

Consider a physical system whose three-dimensional state space is spanned by the orthonormal basis formed by the three kets $|u_1\rangle$, $|u_2\rangle$, $|u_3\rangle$. In the basis of these three vectors, taken in this order, the two operators H and B are defined by

$$H = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1 \end{pmatrix}; \quad B = b \begin{pmatrix} 1 & 0 & 0\\ 0 & 0 & 1\\ 0 & 1 & 0 \end{pmatrix}$$

where ω_0 and b are real constants.

2.11.a Are *H* and *B* Hermitian?

By observation, yes.

2.11.b Show that H and B commute. Give a basis of eigenvectors common to H and B.

To show they commute,

$$HB = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$
$$BH = \hbar\omega_0 b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$$

For the eigenvectors, let's go ahead and solve the characteristic equation (1.20). Doing so gives eigenvalues $\lambda = \hbar\omega_0, -\hbar\omega_0, -\hbar\omega_0$. We have a degeneracy for $-\hbar\omega_0$, but we can find the easiest eigenvectors for the other eigenvalues,

$$|\lambda = \hbar\omega_0\rangle = \begin{bmatrix} 1\\0\\0 \end{bmatrix}; \quad |(\lambda = -\hbar\omega_0)_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0\\1\\1 \end{bmatrix}$$

Since we want this basis to be orthonormal,

$$|(\lambda = -\hbar\omega_0)_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0\\1\\-1 \end{bmatrix}$$

We can show that these are a common basis,

$$\begin{cases} H \mid \lambda = \hbar\omega_0 \rangle = \hbar\omega_0 \mid \lambda = \hbar\omega_0 \rangle \\ H \mid (\lambda = -\hbar\omega_0)_1 \rangle = -\hbar\omega_0 \mid (\lambda = -\hbar\omega_0)_1 \rangle \\ H \mid (\lambda = -\hbar\omega_0)_2 \rangle = -\hbar\omega_0 \mid (\lambda = -\hbar\omega_0)_2 \rangle \end{cases}$$

$$\begin{cases} B \mid \lambda = \hbar\omega_0 \rangle = b \mid \lambda = \hbar\omega_0 \rangle \\ B \mid (\lambda = -\hbar\omega_0)_1 \rangle = b \mid (\lambda = -\hbar\omega_0)_1 \rangle \\ B \mid (\lambda = -\hbar\omega_0)_2 \rangle = -b \mid \lambda = -\hbar\omega_0)_2 \rangle \end{cases}$$

2.11.c Of the set of operators $\{H\}$, $\{B\}$, $\{H,B\}$, $\{H^2,B\}$, which form a CSCO?

For $\{H\}$ and $\{B\}$, these cannot be CSCO since they are degenerate, which means that some eigenvectors must have the same eigenvalue.

 $\{H, B\}$ is a CSCO since no two eigenvectors have the same set of eigenkets.

 H^2 is the identity matrix multiplied by some scalar constant, so we can easily convince ourselves that it commutes with H and B, which means that the eigenvectors of H are shared with H^2 . Further, since H^2 is basically the identity matrix, all the eigenvalues are going to be the same $(\lambda = (\hbar\omega_0)^2)$. This means that $\{H^2, B\}$ is not a CSCO since there are two eigenvectors which have the same eigenvalues.

2.12 Spin Operators

In the same state space as that of the preceding exercise, consider two operators L_z and S defined by:

$$\begin{cases} L_{z} |u_{1}\rangle = |u_{1}\rangle; & L_{z} |u_{2}\rangle = 0; & L_{z} |u_{3}\rangle = -|u_{3}\rangle \\ S |u_{1}\rangle = |u_{3}\rangle; & S |u_{2}\rangle = |u_{2}\rangle; & S |u_{3}\rangle = |u_{1}\rangle \end{cases}$$

2.12.a Write the matrices which represent, in the $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ basis, the operators L_z, L_z^2, S, S^2 . Are these operators observables?

From observation,

$$L_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$S = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

From this,

$$L_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$S^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

These are all Hermitian (1.13) and observables.

2.12.b Give the form of the most general matrix which represents an operator which commutes with L_z . Same question for L_z^2 , then for S^2 .

Let's say we have some matrix,

$$M = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix}$$

In order for M to commute, it must be diagonal.

2.12. SPIN OPERATORS

Acting L_z on it,

$$L_z M = \begin{pmatrix} m_{11} & m_{12} & m_{13} \\ 0 & 0 & 0 \\ -m_{31} & -m_{32} & -m_{33} \end{pmatrix}$$
$$ML_z = \begin{pmatrix} m_{11} & 0 & -m_{13} \\ 0 & 0 & 0 \\ m_{31} & 0 & -m_{33} \end{pmatrix}$$

In order for these to commute, only m_{11} and m_{33} can be non-zero, and we can add a term in the middle since m_{22} is unrestrained,

$$M = \begin{pmatrix} m_{11} & 0 & 0\\ 0 & m_{22} & 0\\ 0 & 0 & m_{33} \end{pmatrix}$$

We can repeat the process for L_z^2 ,

$$L_z^2 M = \begin{pmatrix} m_{11} & 0 & m_{13} \\ 0 & 0 & 0 \\ m_{31} & 0 & m_{33} \end{pmatrix}$$
$$ML_z^2 = \begin{pmatrix} m_{11} & 0 & m_{13} \\ 0 & 0 & 0 \\ m_{31} & 0 & m_{33} \end{pmatrix}$$

All four corners survive, and we can again add a term in the middle,

$$M = \begin{pmatrix} m_{11} & 0 & m_{13} \\ 0 & m_{22} & 0 \\ m_{31} & 0 & m_{33} \end{pmatrix}$$

Since S^2 is the identity matrix, any matrix will commute with it.

2.12.c Do L_z^2 and S form a CSCO? Give a basis of common eigenvectors.

We'll solve the characteristic equation (1.20) for L_z^2 , giving us eigenvalues $\lambda = 0, 0, 1$. Two eigenvectors,

$$|\lambda = 1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\0\\1 \end{bmatrix}; \quad |(\lambda = 0)_1\rangle = \begin{bmatrix} 0\\1\\0 \end{bmatrix}$$

By orthonormality,

$$|(\lambda=0)_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1\\ 0\\ -1 \end{bmatrix}$$

To see if they form a CSCO, let's look at the eigenvalues,

$$\begin{cases} L_z^2 |\lambda = 1\rangle = |\lambda = 1\rangle \\ L_z^2 |(\lambda = 0)_1\rangle = 0 |(\lambda = 0)_1\rangle \\ L_z^2 |(\lambda = 0)_2\rangle = 0 |(\lambda = 0)_2\rangle \end{cases}$$
$$\begin{cases} S |\lambda = 1\rangle = |\lambda = 1\rangle \\ S |(\lambda = 0)_1\rangle = |(\lambda = 0)_1\rangle \\ S |(\lambda = 0)_2\rangle = - |(\lambda = 0)_2\rangle \end{cases}$$

Since all the eigenvectors have different pairs of eigenvalues, L^2_z and S form a CSCO.

Chapter 3

The Postulates of Quantum Mechanics

3.1 Wave Function

In a one-dimensional problem, consider a particle whose wave function is:

$$\psi(x) = N \frac{\exp\left(\frac{ip_0 x}{\hbar}\right)}{\sqrt{x^2 + a^2}}$$

where a and p_0 are real constants and N is a normalization coefficient.

3.1.a Determine N so that $\psi(x)$ is normalized

To normalize the wavefunction,

$$\int_{-\infty}^{\infty} \psi^*(x)\psi(x) \, dx = 1$$
$$N^2 \int_{-\infty}^{\infty} \frac{1}{x^2 + a^2} \, dx = 1$$

Looking up this integral,

$$N^2 = \frac{a}{\pi}$$

3.1.b The position of the particle is measured. What is the probability of finding a result between $-a/\sqrt{3}$ and $+a/\sqrt{3}$?

Using (C-1),

$$\int_{-a/\sqrt{3}}^{a/\sqrt{3}} \psi^*(x)\psi(x) \ dx$$

$$= \frac{a}{\pi} \left[\arctan\left(\frac{1}{\sqrt{3}}\right) - \arctan\left(-\frac{1}{\sqrt{3}}\right) \right]$$
$$P = \frac{1}{3}$$

3.1.c Calculate the mean value of the momentum of a particle which has $\psi(x)$ for its wave function.

From (C-4),

$$\langle p \rangle = \langle \psi | p | \psi \rangle$$

The momentum operator,

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

Let's act the momentum operator on our wave function,

$$p \left|\psi\right\rangle = -i\hbar N \frac{\partial}{\partial x} \left(\frac{\exp(ip_0 x/\hbar)}{\sqrt{x^2 + a^2}}\right)$$

$$= -i\hbar N \left[\frac{i^{p_0}/\hbar \exp}{\sqrt{x^2 + a^2}} - \frac{x \exp}{(x^2 + a^2)^{3/2}} \right]$$

$$\langle \psi | p | \psi \rangle = -i\hbar N^2 \int_{-\infty}^{\infty} \left[\frac{ip_0}{\hbar} \frac{1}{x^2 + a^2} - \frac{x}{(x^2 + a^2)^2} \right] \ dx$$

The second term dies since that is an odd function,

$$\langle p \rangle = -i\hbar \frac{a}{\pi} \frac{ip_0}{\hbar} \frac{a}{\pi} = \frac{p_0 a^2}{\pi^2}$$

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3.2 Measurement of a one-dimensional particle

Consider, in a one-dimensional problem, a particle of mass m whose wave function at time t is $\psi(x,t)$.

3.2.a At time t, the distance d of this particle from the origin is measured. Write, as a function of $\psi(x,t)$, the probability $\mathscr{P}(d_0)$ of finding a result greater than a given length d_0 . What are the limits of $\mathscr{P}(d_0)$ when $d_0 \to 0$ and $d_0 \to \infty$?

We already know how to write the probability of finding the particle within a certain range. Thus, in order to find the probability of the particle outside of that range, we subtract the probability of finding the particle within a certain range from the probability of finding the particle anywhere. For a normalized wave function, the probability of finding it somewhere is unity, so

$$\mathscr{P}(d_0) = 1 - \int_{-d_0}^{d_0} \psi^*(x)\psi(x) \, dx$$

As $d_0 \to 0$, the second term goes to zero, so we certain to find the particle outside of that range. As $d_0 \to \infty$, it becomes more difficult to find that particle outside of that range.

3.2.b Instead of performing the measurement of question a, one measures the velocity v of the particle at time t. Express, as a function of $\psi(x,t)$, the probability of finding a result greater than a given value v_0

The probability of finding the particle between $-p_0$ and p_0 , which are the momenta corresponding to v_0 ,

$$-i\hbar \int_{-p_0}^{p_0} \psi^*(x) \frac{\partial}{\partial x} \psi(x) \ dx$$

Since p = mv, we can easily convert to velocity,

$$\mathscr{P}(v_0) = -\frac{i\hbar}{m} \int_{-p_0}^{p_0} \psi^*(x) \frac{\partial}{\partial x} \psi(x) \, dx$$

3.3 Free Particle

The wave function of a free particle, in a one-dimensional problem, is given at time t = 0 by:

$$\psi(x,0) = N \int_{\infty}^{\infty} \exp(-|k|/k_0) \exp(ikx) dk$$

where k_0 and N are constants.

3.3.a What is the probability $\mathscr{P}(p_1, 0)$ that a measurement of the momentum, performed at time t = 0, will yield a result included between $-p_1$ and $+p_1$

We start by evaluating the integral,

$$\psi(x,0) = N \left[\int_{-\infty}^{0} \exp(k/k_0) \exp(ikx) \, dk + \int_{0}^{\infty} \exp(-k/k_0) \exp(ikx) \, dk \right]$$
$$\psi(x,0) = \frac{2Nk_0}{1 + k_0^2 x^2}$$

Solving for the normalization constant,

$$4N^{2}k_{0}^{2}\int_{-\infty}^{\infty}\frac{1}{(1+k_{0}^{2}x^{2})^{2}} dx = 1$$
$$4N^{2}k_{0}^{2}\frac{\pi}{2k_{0}} = 1$$
$$N = \sqrt{\frac{1}{2\pi k_{0}}}$$
$$\psi(x,0) = \sqrt{\frac{2k_{0}}{\pi}}\frac{1}{1+k_{0}^{2}x^{2}}$$

To find the probability,

$$\mathscr{P}(p_1,0) = \int_{-p_1}^{p_1} |\bar{\psi}(p,0)|^2 dp$$

Where $\bar{\psi}$ is the Fourier transform,

$$\bar{\psi}(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x,0) \exp(-ipx/\hbar) \ dx$$

3.3. FREE PARTICLE

If we compare to the original equation, we see that $\exp(ikx)$ cancels out,

$$\bar{\psi}(p,0) = \frac{1}{\sqrt{p_0}} \exp(-|p|/p_0)$$
$$\mathscr{P}(p_1,0) = \frac{1}{p_0} \int_{-p_1}^{p_1} \exp\left(-\frac{2|p|}{p_0}\right) dp$$
$$\mathscr{P}(p_1,0) = 1 - \exp\left(-\frac{2p_1}{p_0}\right)$$

3.3.b What happens to this probability $\mathscr{P}(p_1, t)$ if the measurement is performed at time t? Interpret.

The wave function is determined by the time evolution operator,

$$\psi(x,t) = U(t)\psi(x,0)$$

$$U(t) = \exp\left(-\frac{iP^2t}{2m\hbar}\right)$$

Transforming to momentum space is fairly straightforward, $P \rightarrow p$,

$$\bar{\psi}(p,t) = \exp\left(-\frac{ip^2t}{2m\hbar}\right)\bar{\psi}(p,0)$$

To find the probability,

$$\mathscr{P}(p_1,t) = \int_{-p_1}^{p_1} |\bar{\psi}(p,t)|^2 dp$$

Looking at this, we see

$$= \int_{-p_1}^{p_1} |\bar{\psi}(p,0)|^2 \ dp$$

Which is the same answer as we got in part (a). The probability is time-independent, which means the energy eigenstates are stationary states.

3.3.c What is the form of the wave packet at time t = 0? Calculate for this time the product $\Delta X \cdot \Delta P$; what is your conclusion? Describe qualitatively the subsequent evolution of the wave packet.

As we have found,

$$\psi(x,0) = \sqrt{\frac{2k_0}{\pi}} \frac{1}{1 + k_0^2 x^2}$$

The uncertainty,

$$\begin{cases} \Delta X = [\langle X^2 \rangle - \langle X \rangle^2]^{1/2}; \\ \Delta P = [\langle P^2 \rangle - \langle P \rangle^2]^{1/2} \end{cases}$$
$$\langle X \rangle = \int_{-\infty}^{\infty} x |\psi(x,0)|^2 \, dx = 0$$
$$\langle X^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x,0)|^2 \, dx = \frac{1}{k_0^2} \end{cases}$$
$$\langle P \rangle = \int_{-\infty}^{\infty} p |\bar{\psi}(p,0)|^2 \, dp = 0$$
$$\langle P^2 \rangle = \int_{-\infty}^{\infty} p^2 |\bar{\psi}(p,0)|^2 \, dp = \frac{p_0^2}{2}$$
$$\begin{cases} \Delta X = \frac{1}{k_0}; \\ \Delta P = \frac{\hbar k_0}{\sqrt{2}} \end{cases}$$
$$\Delta X \cdot \Delta P = \frac{\hbar}{\sqrt{2}} \end{cases}$$

which follows Heisenberg Uncertainty Principle.

3.4 Spreading of a Free Wave Packet

Consider a free particle

3.4.a Show, applying Ehrenfest's Theorem, that $\langle X \rangle$ is a linear function of time, the mean value $\langle P \rangle$ remaining constant

We apply (D-34) and (D-35),

$$\frac{d}{dt} \langle X \rangle = \frac{1}{m} \langle P \rangle$$
$$\frac{d}{dt} \langle P \rangle = - \langle V'(x) \rangle$$

For a free particle, the potential is constant, so we can see that $\langle P \rangle$ remains constant. Since $\langle P \rangle$ has a constant value, $\langle X \rangle$ must be linear in time in order to satisfy the above equations.

3.4.b Write the equations of motion for the mean values $\langle X^2 \rangle$ and $\langle XP + PX \rangle$. Integrate these equations.

In general, Ehrenfest's theorem is given by (D-27),

$$\frac{d}{dt}\left\langle A\right\rangle =\frac{1}{i\hbar}\left\langle \left[A,\mathscr{H}(t)\right]\right\rangle$$

For a free particle,

$$\mathscr{H} = \frac{P^2}{2m}$$

Let's start with the second mean value,

$$[XP + PX, P^{2}] = 4i\hbar P^{2}$$
$$\frac{d}{dt} \langle XP + PX \rangle = \frac{2}{m} \langle P^{2} \rangle = 0$$

We can see that $\langle P^2 \rangle = 0$ since if we plug this into Ehrenfest's theorem, we end up commuting P^2 with itself.

For $\langle X^2 \rangle$,

$$[X^2, P^2] = 2i\hbar(XP + PX)$$

$$\frac{d}{dt}\left\langle X^{2}\right\rangle =\frac{1}{m}\left\langle XP+PX\right\rangle$$

We can see that $\langle XP + PX \rangle$ is constant in time while $\langle X^2 \rangle$ varies linearly with time.

3.4.c Show that with a suitable choice of time origin, the root-mean-square deviation ΔX is given by:

$$(\Delta X)^2 = \frac{1}{m^2} (\Delta P)_0^2 t^2 + (\Delta X)_0^2$$

where $(\Delta X)_0$ and $(\Delta P)_0$ are the root-mean-square deviations of the initial time. Using the definition of root mean square deviation,

$$(\Delta X)^2 = \langle X^2 \rangle - \langle X \rangle^2$$

The first term gives

$$\langle X^2 \rangle = (\Delta X)_0^2$$

The second term gives

$$\langle X \rangle = \frac{1}{m} \langle P \rangle t$$

Since $\langle P \rangle$ is constant in time, $\langle P \rangle = \Delta P$,

$$(\Delta X)^2 = \frac{1}{m^2} (\Delta P)_0^2 t^2 + (\Delta X)_0^2$$

3.5 Particle Subject to a Constant Potential

In a one-dimensional problem, consider a particle of potential energy V(X) = -fX, where f is a positive constant [V(X) arises, for example, from a gravity field or a uniform electric field].

3.5.a Write Ehrenfest's theorem for the mean values of the position X and the momentum P of the particle. Integrate these equations; compare with the classical motion.

As in the previous problem, we turn to (D-27),

$$\frac{d}{dt}\left\langle A\right\rangle =\frac{1}{i\hbar}\left\langle \left[A,\mathscr{H}(t)\right]\right\rangle$$

This time, because we are in a potential, the Hamiltonian is given by

$$\mathscr{H}(t) = \frac{P^2}{2m} - fX$$

Let's calculate some commutation relations,

$$\left[X, \frac{P^2}{2m} - fX\right] = \frac{1}{2m}[X, P^2] - f[X, X]$$
$$\left[P, \frac{P^2}{2m} - fX\right] = \frac{1}{2m}[P, P^2] - f[P, X]$$

The first term in each of these we recognize from the equations of motion for a free particle, so we can use (D-34) and (D-35).

$$\frac{d}{dt} \langle X \rangle = \frac{1}{m} \langle P \rangle$$
$$\frac{d}{dt} \langle P \rangle = f$$

Integrating $\langle P \rangle$,

$$\langle P \rangle = ft + \langle P \rangle_0$$

Substituting this in,

$$\langle X \rangle = \frac{1}{m} (1/2ft^2 + \langle P \rangle_0 + \langle X \rangle_0)$$

3.5.b Show that the root-mean-square deviation of ΔP does not vary over time.

Using the definition,

$$(\Delta P)^2 = \langle P^2 \rangle - \langle P \rangle^2$$

We need to calculate $\langle P^2 \rangle$, which involves calculating the commutation relation

$$\left[P^2, \frac{P^2}{2m} - fX\right] = f[X, P^2]$$
$$\frac{d}{dt} \langle P^2 \rangle = 2f \langle P \rangle$$

Substituting in $\langle P \rangle$ that was determined in the last part,

$$\frac{d}{dt} \langle P^2 \rangle = 2f(ft + \langle P \rangle_0)$$
$$\langle P^2 \rangle = f^2 t^2 + 2ft \langle P \rangle_0$$
$$\langle P^2 \rangle - \langle P \rangle^2 = f^2 t^2 + 2ft \langle P \rangle_0 - (f^2 t^2 + 2ft \langle P \rangle_0 + \langle P \rangle_0^2)$$
$$(\Delta P)^2 = - \langle P \rangle_0^2$$

3.5.c Write the Schrodinger equation in the $\{|p\rangle\}$ representation. Deduce from it a relation between $\frac{\partial}{\partial t} |\langle p|\psi(t)\rangle|^2$ and $\frac{\partial}{\partial p} |\langle p|\psi(t)\rangle|^2$. Integrate the equation thus obtained; give a physical interpretation.

The Schrodinger equation,

$$i\hbar \frac{\partial}{\partial t} \left| \psi(t) \right\rangle = \mathscr{H} \left| \psi(t) \right\rangle$$

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = \frac{P^2}{2m}\left|\psi(t)\right\rangle - i\hbar f\frac{\partial}{\partial p}\left|\psi(t)\right\rangle$$

Multiplying by $\langle p|$,

$$i\hbar\frac{\partial}{\partial t}\left\langle p|\psi(t)\right\rangle = \frac{p^2}{2m}\left\langle p|\psi(t)\right\rangle - i\hbar f\frac{\partial}{\partial p}\left\langle p|\psi(t)\right\rangle$$

3.6 Three-dimensional wave function

Consider the three-dimensional wave function

$$\psi(x, y, z) = N \exp\left[-\left(\frac{|x|}{2a} + \frac{|y|}{2b} + \frac{|z|}{2c}\right)\right]$$

where a, b, and c are three positive lengths.

3.6.a Calculate the constant N which normalizes ψ .

To normalize,

$$N^{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[-\left(\frac{|x|}{a} + \frac{|y|}{b} + \frac{|z|}{c}\right)\right] dxdydz = 1$$

Let's look at one of these integrals,

$$\int_{-\infty}^{\infty} \exp\left(-\frac{|x|}{a}\right) \, dx = \int_{-\infty}^{0} \exp(x/a) \, dx + \int_{0}^{\infty} \exp(-x/a) \, dx = 2a$$

Extrapolating this out, our integral gives

$$N^2(8abc) = 1$$

$$N^2 = \frac{1}{8abc}$$

3.6.b Calculate the probability that a measurement of X will yield a result included between 0 and a.

We can simplify this a little. Since we can have y and z values anywhere, we only need to evaluate

$$4N^{2}bc \int_{0}^{a} \exp(-|x|/a) dx$$
$$= \frac{1}{2a} \int_{0}^{a} \exp(-x/a) dx = \frac{1 - e^{-1}}{2}$$

3.6.c Calculate the probability that simultaneous measurements of Y and Z will yield results included respectively between -b and b, and -c and c.

The integral we need to evaluate simplifies to

$$\frac{1}{4bc} \int_{-b}^{b} \int_{-c}^{c} \exp\left(-\frac{|y|}{b}\right) \exp\left(-\frac{|z|}{c}\right) dydz$$

Let's evaluate one of these integrals,

$$\int_{-b}^{b} \exp\left(-\frac{|y|}{b}\right) dy = \int_{0}^{b} \exp(y/b) dy + \int_{0}^{b} \exp(-y/b) dy$$
$$= 2b\left(1 - \frac{1}{e}\right)$$

As expected, we get something twice as large as the integral in the previous part.

$$\mathscr{P} = \left(1 - \frac{1}{e}\right)^2$$

3.6.d Calculate the probability that a measurement of the momentum will yield a result included in the element $dp_x dp_y dp_z$ centered at the point $p_x = p_y = 0$; $p_z = \hbar/c$

The first thing to do is transform to momentum space,

$$\bar{\psi}(p_x, p_y, p_z) = \frac{N}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(x, y, z) \exp\left(-\frac{ip_x x}{\hbar}\right) \exp\left(-\frac{ip_y y}{\hbar}\right) \exp\left(-\frac{ip_z z}{\hbar}\right) dx dy dz$$

Let's evaluate part of this first,

$$\int_{-\infty}^{\infty} \exp\left(-\frac{|x|}{2a} - \frac{ip_x x}{\hbar}\right) dx$$

$$= \int_{-\infty}^{0} \exp\left[x\left(\frac{1}{2a} - \frac{ip}{\hbar}\right)\right] dx + \int_{0}^{\infty} \exp\left[-x\left(\frac{1}{2a} + \frac{ip}{\hbar}\right)\right] dx = \frac{4a\hbar^2}{\hbar^2 + 4a^2p^2}$$

Extrapolating,

$$\psi(p_x, p_y, p_z) = \frac{N}{(2\pi\hbar)^{3/2}} \frac{64abc\hbar^6}{(\hbar^2 + 4a^2p_x^2)(\hbar^2 + 4b^2p_y^2)(\hbar^2 + 4c^2p_z^2)}$$

For an element $dp_x dp_y dp_z$ centered at the required point, we set $p_x = p_y = 0$ and $p_z = \hbar/c$,

$$d\mathscr{P} = \frac{8}{5(2\pi\hbar)^{3/2}}$$

3.7 Measurements

Let $\psi(x, y, z) = \psi(\vec{r})$ be the normalized wave function of a particle. Express in terms of $\psi(\vec{r})$ the probability for:

3.7.a a measurement of the abscissa X, to yield a result included between x_1 and x_2

$$\mathscr{P} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{x_1}^{x_2} \psi^*(\vec{r}) \psi(\vec{r}) \ dxdydz$$

3.7.b a measurement of the component P_x of the momentum, to yield a result between $\vec{p_1}$ and $\vec{p_2}$

The first thing to do is Fourier transform to momentum space,

$$\bar{\psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(\vec{r}) \exp\left(-\frac{ip_x x}{\hbar}\right) \exp\left(-\frac{ip_y y}{\hbar}\right) \exp\left(-\frac{ip_z z}{\hbar}\right) dx dy dz$$
$$\mathscr{P} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{p_1}^{p_2} \bar{\psi}^*(\vec{p}) \bar{\psi}(\vec{p}) dp_x dp_y dp_z$$

3.7.c simultaneous measurements of X and P_z to yield:

$$x_1 \le x \le x_2$$

$$p_z \ge 0$$

We can perform this simultaneous measurement because X and P_z commute (note that X and P_x would not). Let's first perform the measurement of X,

$$\mathscr{P}_x = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{x_1}^{x_2} \psi^*(\vec{r})\psi(\vec{r}) \, dxdydz$$

We now want to Fourier transform to momentum space,

$$\bar{\psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{x_1}^{x_2} \psi(\vec{r}) \exp\left(-\frac{ip_x x}{\hbar}\right) \exp\left(-\frac{ip_y y}{\hbar}\right) \exp\left(-\frac{ip_z z}{\hbar}\right) dx dy dz$$

Note the different integration bounds because we have made the measurement on X.

$$\begin{split} \mathscr{P}_p &= \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \bar{\psi}^*(\vec{p}) \bar{\psi}(\vec{p}) \ dp_x dp_y dp_z \\ \\ \mathscr{P} &= \mathscr{P}_x \mathscr{P}_p \end{split}$$

3.8 Probability current

3.9 Probability current

3.10 Virial Theorem

3.10.a In a one-dimensional problem, consider a particle with the Hamiltonian:

 $\mathscr{H} = \frac{P^2}{2m} + V(X)$

where

$$V(X) = \lambda X^n$$

Calculate the commutator $[\mathscr{H}, XP]$. If there exists one or several stationary states $|\phi\rangle$ in the potential V, show that the mean values $\langle T \rangle$ and $\langle V \rangle$ of the kinetic and potential energies in these states satisfy the relation: $2 \langle T \rangle = n \langle V \rangle$

Let's split this up into two parts,

$$T = \frac{1}{2m} [P^2, XP]$$
$$T = -\frac{i\hbar}{m} P^2$$
$$V = \lambda [X^n, XP]$$

To solve this, let's look at the first couple iterations,

$$= \lambda([X^n, X]P + X[X^n, P]) = \lambda X[X^n, P]$$
$$= \lambda X(X[X^{n-1}, P] + i\hbar X^{n-1})$$

Continuing, we notice a pattern,

$$[X^{n}, P] = i\hbar n X^{n-1}$$
$$V = i\hbar n \lambda X^{n}$$
$$[\mathscr{H}, XP] = -\frac{i\hbar}{m} P^{2} + i\hbar n \lambda X^{n}$$

Using Ehrenfest's Theorem, and expecting $\langle XP \rangle$ to be 0 for a stationary state, we can rewrite this in terms of $\langle T \rangle$ and $\langle V \rangle$.

$$\begin{split} \langle T \rangle &= \frac{P^2}{2m} \\ \langle V \rangle &= \lambda X^n \\ 0 &= -2i\hbar \left< T \right> + i\hbar n \left< V \right> \\ 2 \left< T \right> &= n \left< V \right> \end{split}$$

3.11 Two-particle wave function

In a one-dimensional problem, consider a system of two particles (1) and (2) with which is associated the wave function $\psi(x_1, x_2)$.

3.11.a What is the probability of finding, in a measurement of the positions X_1 and X_2 of the two particles, a result such that:

$$x \le x_1 \le x + dx$$
$$\alpha \le x_2 \le \beta$$

$$\mathscr{P} = \int_{\alpha}^{\beta} \int_{x}^{x+dx} \psi^*(x_1, x_2) \psi(x_1, x_2) \ dx_1 dx_2$$

3.12 Infinite one-dimensional well

3.13 Infinite two-dimensional well

3.14 Matrices

Consider a physical system whose state space, which is three-dimensional, is spanned by the orthonormal basis formed by the three kets $|u_1\rangle$, $|u_2\rangle$, $|u_3\rangle$. In this basis, the Hamiltonian operator \mathscr{H} of the system and the two observables A and B are written:

$$\mathcal{H} = \hbar\omega_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}; \quad A = a \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}; \quad B = b \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

where ω_0 , a, and b are positive real constants.

The physical system at time t = 0 is in the state:

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}|u_1\rangle + \frac{1}{2}|u_2\rangle + \frac{1}{2}|u_3\rangle$$

3.14.a At time t = 0, the energy of the system is measured. What values can be found, and with what probabilities? Calculate, for the system in the state $|\psi(0)\rangle$, the mean value $\langle \mathscr{H} \rangle$ and the root-mean-square deviation $\Delta \mathscr{H}$.

The possible energy values can be found by finding the eigenvalues of \mathscr{H} ,

$$\mathscr{H} \left| \psi \right\rangle = E \left| \psi \right\rangle$$

The eigenvalues are

$$\lambda = \hbar\omega_0, 2\hbar\omega_0, 2\hbar\omega_0$$

The corresponding eigenvectors are

$$\begin{split} |1\rangle &= |u_1\rangle \,; \quad |2\rangle = |u_2\rangle \,; \quad |2'\rangle = |u_3\rangle \\ \mathscr{P}(E &= \hbar\omega_0) = |\langle 1|\psi(0)\rangle|^2 = \frac{1}{2} \\ \mathscr{P}(E &= 2\hbar\omega_0) = |\langle 2|\psi(0)\rangle|^2 + |\langle 3|\psi(0)\rangle|^2 = \frac{1}{2} \end{split}$$

The mean value,

$$\langle \mathscr{H} \rangle = \langle \psi(0) | \mathscr{H} | \psi 0 \rangle$$

Let's start by writing $|\psi(0)\rangle$ in matrix form,

$$|\psi(0)\rangle = \begin{pmatrix} 1/\sqrt{2} \\ 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$$

$$\langle \mathscr{H} \rangle = \hbar \omega_0 \begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}$$

$$\langle \mathscr{H} \rangle = \frac{3\hbar\omega_0}{2}$$

To find the root-mean-square-deviation,

$$\Delta \mathscr{H} = \langle \mathscr{H}^2 \rangle - \langle \mathscr{H} \rangle^2$$

We need to calculate,

$$\langle \mathscr{H}^2 \rangle = \hbar^2 \omega^2 \begin{pmatrix} 1/\sqrt{2} & 1/2 & 1/2 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} \\ 1/2 \\ 1/2 \end{pmatrix} = \frac{5\hbar^2 \omega_0^2}{2}$$
$$\Delta \mathscr{H} = \frac{10\hbar^2 \omega_0^2}{4} - \frac{9\hbar^2 \omega_0^2}{4} = \frac{\hbar^2 \omega_0^2}{4}$$

3.14.b Instead of measuring \mathcal{H} at time t = 0, one measures A; what results can be found, and with what probabilities? What is the state vector immediately after the measurement?

The eigenvalues of A are

$$\lambda = a, a, -a$$

The corresponding eigenvectors,

$$|1\rangle = \frac{1}{\sqrt{2}}(|u_2\rangle + |u_3\rangle); \quad |1'\rangle = |u_1\rangle; \quad |-1\rangle = \frac{1}{\sqrt{2}}(|u_2\rangle - |u_3\rangle)$$

After the measurement, the state vector will be in $A |\psi(0)\rangle$,

$$A \left| \psi(0) \right\rangle = \begin{pmatrix} a/\sqrt{2} \\ a/2 \\ a/2 \\ a/2 \end{pmatrix}$$

3.14.c Calculate the state vector $|\psi(t)\rangle$ of the system at time t

The time evolution operator gives,

$$|\psi(t)\rangle = \exp\left(-\frac{i\mathscr{H}t}{\hbar}\right)|\psi(0)\rangle$$

To first order,

$$\begin{split} |\psi(t)\rangle &= |\psi(0)\rangle - \frac{it}{\hbar}\mathscr{H}|\psi(0)\rangle \\ |\psi(t)\rangle &= \frac{1}{\sqrt{2}}(1 - i\omega_0 t) \left|u_1\right\rangle + \left(\frac{1}{2} - i\omega_0 t\right) \left|u_2\right\rangle + \left(\frac{1}{2} - i\omega_0 t\right) \left|u_3\right\rangle \end{split}$$

3.14.d Calculate the mean values $\langle A \rangle(t)$ and $\langle B \rangle(t)$ of A and B at time t. What comments can be made?

$$\langle A \rangle (t) = a \begin{pmatrix} 1/\sqrt{2}(1+i\omega_0 t) & 1/2+i\omega_0 t & 1/2+i\omega_0 t \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2}(1-i\omega_0 t) \\ 1/2-i\omega_0 t \\ 1/2-i\omega_0 t \end{pmatrix}$$

$$\langle A \rangle (t) = a \begin{pmatrix} 1 + \frac{5\omega_0^2 t^2}{2} \end{pmatrix}$$

$$\langle B \rangle (t) = b \langle A \rangle (t) = a \begin{pmatrix} 1/\sqrt{2}(1+i\omega_0 t) & 1/2+i\omega_0 t & 1/2+i\omega_0 t \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2}(1-i\omega_0 t) \\ 1/2-i\omega_0 t \\ 1/2-i\omega_0 t \end{pmatrix}$$

$$\left\langle B\right\rangle (t) = \frac{1}{\sqrt{2}} + \frac{1}{4} + \left(1 + \frac{2}{\sqrt{2}}\right)\omega_0^2 t^2$$

As time goes to infinity, the mean values of A and B increase to infinity.