Quantum Mechanics Exercises Notes

Elijan Mastnak

Winter Semester 2020-2021

About These Notes

These are my notes from the Exercises portion of the class *Kvanta Mehanika* (Quantum Mechanics), a required course for third-year physics students at the Faculty of Math and Physics in Ljubljana, Slovenia. The exact problem sets herein are specific to the physics program at the University of Ljubljana, but the content is fairly standard for an late-undergraduate Quantum Mechanics course. I am making the notes publicly available in the hope that they might help others learning the same material.

Navigation: For easier document navigation, the table of contents is "clickable", meaning you can jump directly to a section by clicking the colored section names in the table of contents. Unfortunately, the clickable links do not work in most online or mobile PDF viewers; you have to download the file first.

On Authorship: The exercises are led by Asst. Prof. Tomaž Rejec, who has curated the problem sets and guides us through the solutions. Accordingly, credit for the problems in these notes goes to Prof. Rejec. I have merely typeset the problems and provided additional explanations where I saw fit.

Disclaimer: Mistakes—both trivial typos and legitimate errors—are likely. Keep in mind that these are the notes of an undergraduate student in the process of learning the material himself—take what you read with a grain of salt. If you find mistakes and feel like telling me, by Github pull request, email or some other means, I'll be happy to hear from you, even for the most trivial of errors.

Contents

1 First Section

1.1 First Exercise Set

1.1.1 Theory: Basic Concepts in Quantum Mechanics

- The fundamental quantity in quantum mechanics is the wave function. In one dimension, this is $\psi(x,t)$. Any measurable quantity can be derived from the wave function, e.g. probability density

  $$\rho(x,t) = |\psi(x,t)|^2 = \frac{\mathrm{d}p}{\mathrm{d}x}$$

  $\mathrm{d}p$ represents the probability of finding particle with wave function $\psi(x,t)$ in the x interval $\mathrm{d}x$ at time t.

- The Hamiltonian operator is

  $$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) \qquad \text{where} \qquad \hat{p} = -i\hbar\frac{\partial}{\partial x}$$

  Notation: By convention, we usually write operators without the hat symbol and distinguish between operators and scalar quantities based on context.

- We will often solve the stationary Schrödinger equation, which reads

  $$H\psi_n(x) = E_n\psi_n(x)$$

  Note that there is no time dependence of ψ here, and that this is an eigenvalue equation, where E_n are the eigenvalues of the Hamiltonian operator and ψ_n are the corresponding eigenfunctions.

  We then use the solutions $\psi_n(x)$ of the stationary Schrödinger equation to get the time-dependent wave function $\psi(x,t)$. This process is called *time evolution.*

- The time evolution procedure goes as follows: Start with an initial wavefunction $\psi(x,0)$ at time $t=0$. Expand $\psi(x,0)$ over a basis of the eigenfunctions $\psi_n(x)$.

  $$\psi(x,0) = \sum_n c_n\psi_n(x)$$

  The time-dependent wave function is then

  $$\psi(x,t) = \sum_n c_n e^{-\frac{iE_n}{\hbar}t}\psi_n(x)$$

  We have essentially replaced the constant coefficients c_n in the stationary expansion with the time-dependent coefficients $\tilde{c}_n = c_n e^{-\frac{iE_n}{\hbar}t}$.

- Next, on to a particle's energy eigenvalues. A particle or quantum system typically has many eigenvalues as the dimension of the Hilbert space containing the system's wave functions. Often this is infinite! The set of all energy eigenvalues is $\{E_n\}$, and is often called the spectrum.

  The number of linearly independent eigenfunctions a system has at a given energy eigenvalue E_n is the eigenvalue's degeneracy.

- Next, on to the eigenfunctions. Consider a non-degenerate energy level with eigenfunction ψ_n satisfying

$$H\psi_n(x) = E_n\psi_n(x)$$

If ψ_n solves the eigenvalue problem, then mathematically $\lambda\psi_n$ also solves the eigenvalue problem for all $\lambda \in \mathbb{C}$. But physically, there is a restriction: the probability density must be normalized to unity, i.e.

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, \mathrm{d}x = 1$$

The normalization condition requires $|\lambda| = 1$, often written $\lambda = e^{i\alpha}$ where $\alpha \in \mathbb{R}$. This result is important: essentially, any eigenfunction ψ_n is undetermined up to a constant phase factor $\lambda = e^{i\alpha}$ of magnitude $|\lambda| = 1$.

- In other words, suppose we have two eigenfunctions

$$\psi_n(x) \qquad \text{and} \qquad e^{i\alpha}\psi_n(x)$$

Physically, the two wave functions are the same! We can't distinguish between the two in experiments, because the phase factor $e^{i\alpha}$ is lost during the process of finding the probability density when squaring the absolute value! *All wave functions are determined only up to a constant phase factor of magnitude one.*

As an example, consider the infinite potential well from 0 to a. The energy eigenvalues are

$$E_n = \frac{\hbar^2\pi^2 n^2}{2ma^2} \qquad \text{and} \qquad \psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}, \qquad n \in \mathbb{N}^+$$

However, e.g. $\tilde{\psi}_n(x) = i\sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}, n \in \mathbb{N}^+$ represents the same physical information as ψ_n.

1.1.2 Bound States in a Finite Potential Well

Find the energy eigenvalues of the bound states of a particle with energy E in a finite potential well of depth $V_0 > 0$ and width a. Assume $|E| < V_0$; note that bound states have negative energies.

- Split the x axis into three regions: to the left of the well, inside the well, and to the right of the well, e.g. regions 1, 2 and 3, respectively. The potential energy is

$$V(x) = \begin{cases} 0, & x \in \text{region } 1 \\ -V_0, & x \in \text{region } 2 \\ 0, & x \in \text{region } 3 \end{cases}$$

- The Schrödinger equation for region 1 is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + 0 \cdot \psi = E\psi$$

remember that $V = 0$ in region 1. The general solution is a linear combination of exponential functions:

$$\psi_1(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

To find κ, insert ψ_1 into the Schrödinger equation for region 1. Differentiating, canceling the wave function terms from both sides, and rearranging gives

$$-\frac{\hbar^2}{2m}\kappa^2\left(Ae^{i\kappa x}+Be^{-i\kappa x}\right)=E\left(Ae^{i\kappa x}+Be^{-i\kappa x}\right)\implies\kappa^2=\frac{2mE_0}{\hbar^2}$$

where $E_0=-E$ is a positive quantity.

- The Schrödinger equation for region 2 is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-V_0\cdot\psi=E\psi$$

We use a plane wave ansatz:

$$\psi_2(x)=Ce^{ikx}+De^{-ikx}$$

To find k, insert ψ_2 into the Schrödinger equation for region 2. The result after differentiation is

$$+\frac{\hbar^2}{2m}k^2\left(Ce^{ikx}+De^{-ikx}\right)-V_0\left(Ce^{ikx}+De^{-ikx}\right)=E\left(Ce^{ikx}+De^{-ikx}\right)$$

The wave functions terms in parentheses cancel, leading to $k^2=\frac{2m(V_0-E_0)}{\hbar^2}$ where $E_0=-E$ is a positive quantity.

- The Schrödinger equation for region 3 is analogous to the equation for region 1. Following a similar procedure, we would get

$$\psi_3=Fe^{\kappa x}+Ge^{-\kappa x}\qquad\text{where}\qquad\kappa^2=\frac{2mE_0}{\hbar^2}$$

- Next, to find energy, we apply boundary conditions, namely that the wave function is continuous and continuously differentiable at the boundaries between regions and that the functions vanishes at $\pm\infty$, meaning there is no probability of finding the particle infinitely far away from the well. The conditions are:

Region	Condition 1	Condition 2
1/2	$\psi_1(0)=\psi_2(0)$	$\frac{\partial\psi_1}{\partial x}(0)=\frac{\partial\psi_2}{\partial x}(0)$
2/3	$\psi_2(a)=\psi_3(a)$	$\frac{\partial\psi_2}{\partial x}(a)=\frac{\partial\psi_3}{\partial x}(a)$
$\pm\infty$	$\psi_1(-\infty)=0$	$\psi_3(\infty)=0$

The last two conditions at $\pm\infty$ require that $B=0$ and $F=0$, respectively; otherwise ψ_1 and ψ_3 would diverge.

The continuity conditions (in the Condition 1 column) require

$$A=C+D\qquad\text{and}\qquad Ce^{ika}+De^{-ika}=Ge^{-\kappa a}$$

The continuous differentiability conditions require

$$A\kappa=ik(C-D)\qquad\text{and}\qquad ik(Ce^{ika}-De^{-ika})=-\kappa Ge^{-\kappa a}$$

- We could then write the four equations in a 4×4 coefficient matrix

$$\begin{bmatrix} \cdots \\ \cdots \\ \cdots \\ \cdots \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

  To proceed, we would require the matrix's determinant be zero for a unique solution. The determinant of the coefficient matrix is a function of κ and k, which are in turn functions of energy. We then view the matrix's determinant as a function of energy and try to find its zeros. Each zero is an energy eigenvalue of the particle in a finite potential well. However, this involves solving the above system of four equations for the four unknowns A, B, C and D. That's tedious! We will stop here and solve the same problem more elegantly in the next exercise. But first, we'll need some theoretical machinery.

1.1.3 Theory: Wavefunctions of a Particle in an Even Potential

Theorem: The eigenfunctions of a particle in an even potential are either even or odd.

- First, recall the superpositio principle: if two eigenfunctions ψ_1 and ψ_2 have the same eigenvalue E, than any linear combination of ψ_1 and ψ_2 is also an eigenfunction with eigenvalue E. In equation form, if $H\psi_1(x) = E\psi_1(x)$ and $H\psi_2(x) = E\psi_2(x)$ then

$$H\left(\alpha\psi_1(x) + \beta\psi_2(x)\right) = E\left(\alpha\psi_1(x) + \beta\psi_2(x)\right)$$

  We'll use the superposition principle later in the proof when considering degenerate states.

- To prove the even/odd theorem for particles in an even potential $V(x) = V(-x)$, we start with the stationary Schrödinger equation

$$H\psi(x) = E\psi(x)$$

  We make the parity transformation $x \to -x$ and note the Hamiltonian is invariant under parity transformation if V is even, since $\frac{\partial}{\partial(-x)} = -\frac{\partial}{\partial x}$, and $\frac{\partial^2}{\partial(-x)^2} = \frac{\partial^2}{\partial x^2}$. Under the transformation $x \to -x$, the Schrödinger equation reads

$$H\psi(-x) = E\psi(-x)$$

  This means that if $\psi(x)$ is an eigenfunction of H for the energy eigenvalue E, then $\psi(-x)$ is also an eigenfunction for the same energy eigenvalue.

- Next, two options: either the eigenvalue E is degenerate or not.

  If E is not degenerate, then $\psi(-x)$ and $\psi(x)$ are equal up to a constant phase factor. In other words, if E is not degenerate and V is even, then $\psi(x)$ and $\psi(-x)$ are linearly dependent. In equation form,

$$\psi(x) = e^{i\alpha}\psi(-x) = e^{2i\alpha}\psi(x) \implies e^{2i\alpha} = 1 \implies e^{i\alpha} = \pm 1$$

  If $e^{i\alpha} = 1$, then ψ is even, and if $e^{i\alpha} = -1$, then ψ is odd. There are no other options. In other words, the eigenfunctions corresponding to the non-degenerate states of a particle in an even potential are either even or odd, as we wanted to show.

- Next, if E is degenerate, then $\psi(x)$ and $\psi(-x)$ are by definition linearly independent. By the superposition principle, we can create two more linear combinations of $\psi(x)$ and $\psi(-x)$: a sum and a difference, e.g.

$$\psi_+(x) = \psi(x) + \psi(-x) \qquad \text{and} \qquad \psi_-(x) = \psi(x) - \psi(-x)$$

  Note that, by construction, ψ_+ is even and ψ_- is odd. In other words, even though ψ_1 and ψ_2 may not be even or odd themselves, we can always combine the two into a valid eigenfunction that is either even or odd.

- The general takeaway is: if our problem's potential has reflection symmetry about the origin, we can a priori search for only even or odd functions, because we know there exists a basis of the surrounding Hilbert space formed of only odd and even eigenfunctions.

1.1.4 Finite Potential Well Take 2

Continued from the previous problem: find the energy eigenvalues of the bound states of a particle with energy E in a finite potential well of depth $V_0 > 0$ and width a.

- Here's how to proceed: First, note the problem has reflection symmetry if we place the center of the well at the origin. The well then spans from $x = -\frac{a}{2}$ to $x = \frac{a}{2}$. In this case $V(x) = V(-x)$, i.e. the potential is an even function of x.

  Why is this useful? It reduces the number of wave functions we have to find by one. Namely, if the eigenfunctions are even, then ψ_3 is a copy of ψ_1. If the eigenfunctions are odd, then $\psi_3 = -\psi_1$. In both cases, we only need to find ψ_1.

  We then only need to solve the problem on half of the real axis.

- First, assuming the solution is an even function. Reusing results from the earlier treatment of the finite potential well, for region 3 we have

$$\psi_3 = Ge^{-\kappa x} \qquad \text{where} \qquad \kappa^2 = \frac{2mE_0}{\hbar^2}$$

  and for region 2, inside the well, the even wavefunctions take the form

$$\psi_2 = A\cos(kx) \qquad \text{where} \qquad k^2 = \frac{2m(V_0 - E_0)}{\hbar^2}$$

  A few notes: we switched from plane waves to sinusoidal functions, where are better suited to odd/even symmetry. And we dropped the $B\sin(kx)$ term and kept only the cosine because we're solving for an even function a priori.

  For region 1, because we're searching for even functions, the result is the same as for region 3:

$$\psi_1 = Ge^{\kappa x}$$

- If we assume an odd solution, we have

$$\psi_3(x) = Ge^{-\kappa x} \qquad \psi_2(x) = B\sin(kx) \qquad \psi_1(x) = -Ge^{\kappa x}$$

- On to boundary conditions. Because an even or odd function will have the same behavior (up to a minus sign for odd functions) at both region boundaries, we only need to consider one region; we'll consider $x = \frac{a}{2}$. The boundary conditions are

$$\psi_2\left(\frac{a}{2}\right) = \psi_3\left(\frac{a}{2}\right) \qquad \text{and} \qquad \frac{\partial \psi_2}{\partial x}\left(\frac{a}{2}\right) = \frac{\partial \psi_3}{\partial x}\left(\frac{a}{2}\right)$$

- For an even solution, the boundary conditions read:

$$A\cos\left(k\frac{a}{2}\right) = Ge^{-\frac{\kappa a}{2}} \qquad \text{and} \qquad -kA\sin\left(k\frac{a}{2}\right) = -\kappa Ge^{-\frac{\kappa a}{2}}$$

  Next, a trick: divide the equations and cancel like terms to get

$$k\tan\left(k\frac{a}{2}\right) = \kappa$$

- For an odd solution, the boundary conditions read:

$$B\sin\left(k\frac{a}{2}\right) = Ge^{-\frac{\kappa a}{2}} \qquad \text{and} \qquad kB\cos\left(k\frac{a}{2}\right) = -\kappa Ge^{-\frac{\kappa a}{2}}$$

  Dividing the equations and cancel like terms gives

$$k\cot\left(k\frac{a}{2}\right) = -\kappa$$

- The solutions of the two equations

$$\tan\left(\frac{ka}{2}\right) = \frac{\kappa}{k} \qquad \text{and} \qquad \cot\left(\frac{ka}{2}\right) = -\frac{\kappa}{k}$$

  will give the energy eigenvalues of the even and odd states, respectively.

  These are transcendental equations. They don't have analytic solutions, and we'll have to solve them graphically. First, we introduce the dimensionless variable $u = ka$. We then express κ in terms of u using

$$\kappa^2 + k^2 = \kappa^2 + \frac{u^2}{a^2} = \frac{2mV_0}{\hbar^2}$$

  Alternatively, to work in dimensionless quantities, we could define $u_0^2 = \frac{2mV_0a^2}{\hbar^2}$ which leads to

$$\kappa^2 = \frac{u_0^2 - u^2}{a^2}$$

- In terms of u and u_0, the two transcendental equations become

$$\tan\left(\frac{u}{2}\right) = \frac{\sqrt{u_0^2 - u^2}}{u} = \sqrt{\frac{u_0^2}{u^2} - 1} \qquad \text{and} \qquad \cot\left(\frac{u}{2}\right) = -\sqrt{\frac{u_0^2}{u^2} - 1}$$

  We then plot both sides of the equations and look for values of u where the left side equals the right side. These values of u give the energy eigenvalues, which are the solution to our problem.

  Finally, some notes:

  - The right sides of the equations are defined only for $u \leq u_0$ and diverge as $u \to 0$.
  - As u increases, k increases, E becomes more positive, and states become less bound. The ground state occurs at the smallest value of u.
  - The number of bound states increases as u_0 increases. This is achieved by increasing V_0 (well depth), a (well width), or m (particle mass). A finite potential well always has at least one bound state, near $u = 0$.

1.2 Second Exercise Set

1.2.1 Bound States in a Delta Potential Well Version 1

Find the energies and wave functions of the bound states of a quantum particle of mass m in a delta function potential well by reusing the results from a finite potential well.

- We will reuse our results from the previous problem set by interpreting a delta potential as a finite potential well in the limit

$$a \to 0, \qquad V_0 \to \infty \qquad \text{and} \qquad aV_0 = \text{constant} \equiv \lambda$$

where then write the potential as $V(x) = -\lambda\delta(x)$.

- Recall from the previous exercise set that even bound states in a finite potential well of width a and depth V_0 obey

$$\tan\frac{u}{2} = \sqrt{\left(\frac{u_0}{u}\right)^2 - 1} \qquad \text{where} \qquad u_0^2 = \frac{2mV_0a^2}{\hbar^2} \qquad \text{and} \qquad u = ak$$

The wave numbers k and κ inside and outside the well are

$$k = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} \qquad \text{and} \qquad \kappa = \sqrt{\frac{2mE_0}{\hbar^2}}$$

- The limit $a \to 0$ forces $u_0 \to 0$. In the limit $u_0 \to 0$, we expect at most one, even bound state. For small u and u_0, we expect u and u_0 to be very close, so we write

$$u = u_0 - \epsilon \qquad \text{where } \epsilon \ll 1$$

We continue with a Taylor expansion approximation of the even bound state equation. To first order, the tangent function is

$$\tan\frac{u}{2} = \tan\frac{u_0+\epsilon}{2} \approx \frac{u_0+\epsilon}{2} + \ldots$$

while the square root is

$$\sqrt{\left(\frac{u_0}{u}\right)^2 - 1} = \sqrt{\left(\frac{u_0}{u_0+\epsilon}\right)^2 - 1} = \sqrt{\left(1 - \frac{\epsilon}{u_0}\right)^{-2} - 1} \approx \sqrt{2\frac{\epsilon}{u_0}}$$

- With the approximations, the original even bound state equation becomes

$$\frac{u_0+\epsilon}{2} = \sqrt{2\frac{\epsilon}{u_0}}$$

We square both sides and take only the leading u_0^2 term from $(u_0+\epsilon)^2$ to get

$$\frac{(u_0+\epsilon)^2}{4} \approx \frac{u_0^2}{4} = 2\frac{\epsilon}{u_0} \implies \epsilon = \left(\frac{u_0}{2}\right)^3$$

Next, we solve for u in terms of u_0:

$$u = u_0 - \epsilon = u_0 - \left(\frac{u_0}{2}\right)^3$$

- We then use the equation for k to solve for E in terms of u_0:

$$k = \frac{u}{a} = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} \implies E_0 = V_0 - \frac{\hbar^2 u^2}{2ma^2} = V_0 - \frac{\hbar^2}{2ma^2}\left[u_0 - \left(\frac{u_0}{2}\right)^3\right]^2$$

Multiplying out and dropping the small terms of order u_0^6 gives

$$E_0 = V_0 - \frac{\hbar^2}{2ma^2}\left(u_0^2 - \frac{u_0^4}{4}\right)$$

We then substitute in the expression $u_0^2 = \frac{2mV_0a^2}{\hbar^2}$, which simplifies things to

$$E_0 = \frac{ma^2V_0^2}{2\hbar^2} = \frac{m\lambda^2}{2\hbar^2}$$

where the last equality uses $\lambda = aV_0$. This is the result for the bound state's energy.

- We find the corresponding wave function with the plane-wave ansatz

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < 0 \\ Be^{-\kappa x} & x > 0 \end{cases} \qquad \text{where} \qquad \kappa = \sqrt{\frac{2mE_0}{\hbar^2}} = \frac{m\lambda}{\hbar^2}$$

Because the wave function is even, $A = B$, allowing us to write $\psi = Ae^{-\kappa|x|}$. we find the coefficient A from the normalization condition

$$1 \equiv \int |\psi(x)|^2 \,\mathrm{d}x = A^2 \int_{-\infty}^{\infty} e^{-2\kappa|x|} \,\mathrm{d}x$$

Because ψ is even, we can integrate over only half the real line and double the result:

$$1 = 2A^2 \int_0^\infty e^{-2\kappa x} \,\mathrm{d}x = -\frac{A^2}{\kappa} e^{-2\kappa x}\bigg|_0^\infty = \frac{A^2}{\kappa} \implies A^2 = \kappa$$

The wave function is thus

$$\psi(x) = \sqrt{\kappa} e^{-\kappa|x|} \qquad \text{where} \qquad \kappa = \frac{m\lambda}{\hbar^2}$$

1.2.2 Bound States in a Delta Potential Take 2

Find the energies and wave functions of the bound states of a quantum particle of mass m in a delta function potential well using a plane wave ansatz and appropriate boundary conditions.

- Write the potential well in the form $V(x) = -\lambda\delta(x)$. The stationary Schrödinger equation for the potential reads

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \lambda\delta(x)\psi = E\psi$$

We find the boundary condition on the derivative ψ' by integrating the Schrödinger equation over a small region $[-\epsilon, \epsilon]$.

$$-\frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\bigg|_{-\epsilon}^{\epsilon} - \lambda\int_{-\epsilon}^{\epsilon} \delta(x)\psi(x)\,\mathrm{d}x = E\int_{-\epsilon}^{\epsilon}\psi(x)\,\mathrm{d}x$$

In the limit $\epsilon \to 0$, this becomes

$$-\frac{\hbar^2}{2m}\left[\psi'(0_+) - \psi'(0_-)\right] - \lambda\psi(0) = 0$$

where $\psi'(0_+)$ and $\psi'(0_-)$ denote ψ's derivatives from the right and left, respectively. The appropriate boundary condition $\psi'(x)$ are thus

$$\psi'(0_+) - \psi'(0_-) = -\frac{2m\lambda\psi(0)}{\hbar^2}$$

- We construct the wavefunction with a plane-wave ansatz:

$$\psi(x) = \begin{cases} Ae^{\kappa x} & x < 0 \\ Be^{-\kappa x} & x > 0 \end{cases}$$

As boundary conditions, we require that ψ is continuous and that ψ' obey the earlier condition $\psi'(0_+) - \psi'(0_-) = \frac{2m\lambda\psi(0)}{\hbar^2}$. Applying the continuity condition at $x = 0$ gives

$$Ae^{\kappa\cdot 0} = Be^{-\kappa\cdot 0} \implies A = B$$

Applying the condition on the derivatives (and using $A = B$) gives

$$-\kappa A^{-\kappa\cdot 0} - \kappa A^{\kappa\cdot 0} = -\frac{2m\lambda}{\hbar^2}\psi(0) = -\frac{2m\lambda}{\hbar^2}Ae^{\kappa\cdot 0} \implies \kappa = \frac{m\lambda}{\hbar^2}$$

The wave function is thus

$$\psi(x) = Ae^{-\kappa|x|} \qquad \text{where} \qquad \kappa = \frac{m\lambda}{\hbar^2}$$

- We can find the bound state's energy from

$$\kappa = \sqrt{\frac{2mE_0}{\hbar^2}} \implies E_0 = \frac{m\lambda^2}{2\hbar^2}$$

which matches the result from the previous problem. To find the wave function, we just need the value of A, which we find with the usual normalization condition

$$1 \equiv \int |\psi(x)|^2 \,\mathrm{d}x = A^2 \int_{-\infty}^{\infty} e^{-2\kappa|x|}\,\mathrm{d}x = 2A^2 \int_0^{\infty} e^{-2\kappa x}\,\mathrm{d}x \implies A^2 = \kappa$$

The wave function is thus

$$\psi(x) = \sqrt{\kappa}e^{-\kappa|x|} \qquad \text{where} \qquad \kappa = \frac{m\lambda}{\hbar^2},$$

in agreement with the result from the previous problem.

1.2.3 Theory: Scattering

- The basic scattering problem involves a particle with energy E and two regions of the x axis with potentials V_1 and V_3 respectively, where $E > V_1, V_3$. Both energies and potentials are positive quantities. Because $E > V_1, V_3$, the particle is free in the regions of V_1 and V_2.

  Near the origin, between regions 1 and 3, the particle encounters a small potential barrier where $V(x) > E$; the exact form of $V(x)$ is not important for our purposes. We call this region 3.

- The general ansatz solutions in regions 1 and 3 are

$$\psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x} \qquad \text{and} \qquad \psi_3 = A_3 e^{-ik_2 x} + B_3 e^{ik_2 x}$$

  The terms with A coefficients represent movement toward the potential barrier

- In region 2, we don't know $V(x)$, so we have to be more general. Because ψ_2 comes from a second-order linear differential equation (i.e. the Schrödinger equation), its general form is a linear combination of two linearly independent functions, e.g.

$$\psi_2 = Cf(x) + Dg(x)$$

  where f and g are linearly independent solutions of the Schrödinger equation in region 2.

- Because $E > V_1, V_3$, the states in regions 1 and 3 are free, meaning the particle's Hamiltonian has a continuous spectrum of energy eigenvalues. As a result, energy eigenvalues aren't particularly useful for characterizing the problem.

  Instead, for unbound situations with a potential barrier, we describe the problem in terms of transmissivity T and reflectivity R, which describe the probabilities of the scattered particle passing through and reflecting from the barrier, respectively.

Probability Current

- For scattering problems with T and R, we work in terms of probability current

$$j(x) = \frac{\hbar}{2mi}\left[\psi^*(x)\psi'(x) - \psi'^*(x)\psi(x)\right] = \frac{\hbar}{m}\operatorname{Im}\left\{\psi^*\psi'(x)\right\}$$

  where ψ^* and ψ' denotes the complex conjugate and derivative of ψ, respectively.

- Substituting in the region 1 ansatz $\psi_1 = A_1 e^{ik_1 x} + B_1 e^{-ik_1 x}$ gives the probability current in region 1:

$$\begin{aligned} j_1 &= \frac{\hbar}{m}\operatorname{Im}\left\{A_1 A_1^* ik_1 - B_1 B_1^* ik_1 + B_1^* A_1 ik_1 e^{2ik_1 x} - B_1 A_1^* ik_1 e^{-2ik_1 x}\right\} \\ &= \frac{\hbar k_1}{m}(A_1 A_1^* - B_1 B_1^*) \equiv v_1(A_1 A_1^* - B_1 B_1^*) = v_1(|A|^2 - |B|^2) \end{aligned}$$

  Noting that $\frac{\hbar k_1}{m}$ has units of velocity, we've defined the constant $v_1 \equiv \frac{\hbar k_1}{m}$.

  The procedure for j_3 in region 3 is analogous. The result is

$$j_3 = v_3(B_3 B_3^* - A_3 A_3^*) = v_3(|B|_3^3 - |A|_3^3) \qquad \text{where} \qquad v_3 \equiv \frac{\hbar k_3}{m}$$

- Next, we run into a slight problem: the plane waves in regions 1 and 3 can't be normalized. They oscillate! Instead, we normalize ψ_1 and ψ_3 per unit "probability velocity". We redefine

$$\tilde{\psi}_1 = \frac{A_1}{\sqrt{v_1}} e^{ik_1 x} + \frac{B_1}{\sqrt{v_1}} e^{-ik_1 x} \qquad \text{and} \qquad \tilde{\psi}_3 = \frac{A_3}{\sqrt{v_3}} e^{-ik_3 x} + \frac{B_3}{\sqrt{v_3}} e^{ik_3 x}$$

  The corresponding probability currents, using the normalized $\tilde{\psi}_1$ and $\tilde{\psi}_3$ are

$$\begin{aligned} \tilde{j}_1(x) &= A_1^* A_1 - B_1^* B_1 = |A_1|^2 - |B_1|^2 \\ \tilde{j}_3(x) &= B_3^* B_3 - A_3^* A_3 = |B_3|^2 - |A_3|^2 \end{aligned}$$

  As a general rule, we always normalize plane waves with the probability velocity $\frac{1}{\sqrt{v}}$ *where* $v = \frac{hk}{m}$.

- The next step in the scattering problem is formulating four boundary conditions on ψ requiring continuity and continuous differentiability at the two boundary regions between regions 1 and 2 and between regions 2 and 3.

  We end up with 4 linearly independent equations for six unknown coefficients. Our plan is to eliminate C and D and express B_1 and B_3 in terms of A_1 and A_3. The amplitudes A_1 and A_3 of the waves incident on the potential barrier thus parameterize our problem. Informally, all this means is that if we know the wavefunction of the incident particle (by specifying the incident amplitudes A_1, A_3), we can solve the scattering problem by finding the reflected amplitudes B_1, B_3. In general, it is best practice to parameterize a scattering problem with the *incident* amplitudes A_1 and A_3.

  In any case, we end up with a matrix equation

$$\begin{bmatrix} B_1 \\ B_3 \end{bmatrix} = \mathbf{S} \begin{bmatrix} A_1 \\ A_3 \end{bmatrix} \qquad \text{or more concisely} \qquad \boldsymbol{B} = \mathbf{S}\boldsymbol{A}$$

  where $\mathbf{S}$ is called the *scattering matrix*, in our case a 2×2 matrix. By convention, we parameterize a 2×2 scattering matrix in terms of the parameters r and t:

$$\mathbf{S} = \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix}$$

Probability Conservation

- Some identities:

$$T = |t|^2 \quad R = |r|^2 \qquad \text{and} \qquad \tilde{T} = \left|\tilde{t}\right|^2 \quad \tilde{R} = |\tilde{r}|^2$$

  The identities $T + R = 1$ and $\tilde{T} + \tilde{R} = 1$ imply probability conservation, i.e. the total incident and reflected probabilities sum to one.

- In general, the incident current is the sum of the two squares of the incidence amplitudes A_1 and A_3, while the reflected current is the sum of the reflected amplitudes B_1 and B_3, i.e.

$$j_{\text{in}} = |A_1|^2 + |A_3|^2 \qquad \text{and} \qquad j_{\text{ref}} = |B_1|^2 + |B_3|^2$$

  In terms of the coefficient vector $\boldsymbol{A}$, the incident probability current is

$$j_{\text{in}} = A_1 A_1^* + A_3 A_3^* = \begin{bmatrix} A_1^*, A_3^* \end{bmatrix} \begin{bmatrix} A_1 \\ A_3 \end{bmatrix} = \boldsymbol{A}^\dagger \boldsymbol{A}$$

  An analogous procedure with the reflected amplitudes gives $j_{\text{out}} = \boldsymbol{B}^\dagger \boldsymbol{B}$.

- Conservation of probability requires $j_{\text{in}} = j_{\text{ref}}$ or $\boldsymbol{A}^\dagger \boldsymbol{A} = \boldsymbol{B}^\dagger \boldsymbol{B}$. Combining the scattering matrix equation $\boldsymbol{B} = \mathbf{S}\boldsymbol{A}$ with the requirement $\boldsymbol{A}^\dagger \boldsymbol{A} = \boldsymbol{B}^\dagger \boldsymbol{B}$ implies

$$\boldsymbol{A}^\dagger \boldsymbol{A} \equiv \boldsymbol{B}^\dagger \boldsymbol{B} = (\boldsymbol{A}^\dagger \mathbf{S}^\dagger)(\mathbf{S}\boldsymbol{A}) \implies \boldsymbol{S}^\dagger \mathbf{S} = \mathbf{I}$$

  In other words, the scattering matrix $\mathbf{S}$ must be unitary to conserve probability in scattering problems

1.2.4 Scattering Off a Delta Potential

Analyze a quantum particle scattering off of a delta function potential.

- We consider a particle of energy E scattering off the potential $V(x) = \lambda\delta(x)$. We'll divide the problem into two separate cases. First, we'll assume the particle is incident on the potential barrier only from the left, so the incident amplitude vector reads $\boldsymbol{A} = (1, 0)$. In this case, the scattering matrix equation reads

$$\boldsymbol{B} = \mathbf{S}\boldsymbol{A} = \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} r \\ t \end{bmatrix}$$

- Similarly, if we assume the particle is incident only from the right, i.e. $A = (0, 1)$, the scattering equation reads

$$\boldsymbol{B} = \mathbf{S}\boldsymbol{A} = \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \tilde{t} \\ \tilde{r} \end{bmatrix}$$

- First, for $\boldsymbol{A} = (1, 0)$ and $\boldsymbol{B} = (r, t)$, the wave functions in region 1 and 3 are

$$\begin{aligned} \psi_1(x) &= \frac{A_1}{\sqrt{v}} e^{ikx} + \frac{B_1}{\sqrt{v}} e^{-ikx} = \frac{e^{ikx}}{\sqrt{v}} + \frac{r}{\sqrt{v}} e^{-ikx} \\ \psi_3 &= \frac{A_3}{\sqrt{v}} e^{-ikx} + \frac{B_3}{\sqrt{v}} e^{ikx} = 0 + \frac{t}{\sqrt{v}} e^{ikx} \end{aligned}$$

  Note that because the potential is the same on both sides of the delta function, $k_1 = k_3 \equiv k$ and $v_1 = v_3 \equiv v$.

- On to boundary conditions. Continuity between regions 1 and 3 requires

$$\psi_1(0) = \psi_3(0) \implies 1 + r = t$$

  For the the boundary conditions on the derivative ψ', we reuse the earlier differentiability condition $\psi'(0_+) - \psi'(0_-) = \frac{2m\lambda\psi(0)}{\hbar^2}$ from the previous problem involving bound states in a delta potential. Changing the sign of of λ because the delta function in a scattering problem points upward, and changing notation from $\psi'_\pm$ to $\psi'_{1,3}$the differentiability condition becomes

$$\psi_3'(0) - \psi_1'(0) = \frac{2m\lambda}{\hbar^2}\psi(0) \implies ik(t + r - 1) = \frac{2m\lambda}{\hbar^2} t$$

  Substituting in the earlier continuity requirement $t = 1 + r$ gives

$$2ikr = \frac{2m\lambda}{\hbar^2}(1 + r) \implies r = -\frac{i\alpha}{k + i\alpha} \qquad \text{where} \qquad \alpha = \frac{m\lambda}{\hbar^2}$$

  The expression for the parameter t is then

$$t = 1 + r = 1 - \frac{i\alpha}{k + i\alpha} = \frac{k}{k + i\alpha}$$

- We would then find $\tilde{r}$ and $\tilde{t}$ using an analogous procedure with the incidence vector $\boldsymbol{A} = (0, 1)$. It turns out (exercise left to the reader) that the results are the same:

$$\tilde{r} = -\frac{i\alpha}{k + i\alpha} \qquad \text{and} \qquad \tilde{t} = \frac{k}{k + i\alpha}$$

  The probability matrix can then be written

$$\mathbf{S} = \frac{1}{k + i\alpha} \begin{bmatrix} -i\alpha & k \\ k & -i\alpha \end{bmatrix} \qquad \text{where} \qquad \alpha = \frac{m\lambda}{\hbar^2}$$

On the Problem's Symmetry: A few notes on why the scattering matrix for the delta potential has only two independent parameters, i.e. why $\tilde{t} = t$ and $\tilde{r} = r$.

- Start by noting that the wave functions $\psi_{1,3}$ in regions 1 and 3 solve the stationary Schrödinger equation

$$H\psi = E\psi \qquad \text{where} \qquad H = -\frac{\hbar^2}{m}\frac{\partial^2}{\partial x^2} + V(x)$$

  We then take the Schrödinger equation's complex conjugate to get

$$H\psi^* = E\psi^*$$

  In other words, if ψ is a wave function for the energy eigenvalue E, then so is ψ^*. This holds in general for any real Hamiltonian.

- In our specific problem in regions 1 and 3, the conjugate wave function reads

$$\psi_1^* = \frac{A_1^*}{\sqrt{v}}e^{-ikx}e + \frac{B_1^*}{\sqrt{v}}e^{ikx} \qquad \text{and} \qquad \psi_3^* = \frac{A_3^*}{\sqrt{v}}e^{ikx}e + \frac{B_3^*}{\sqrt{v}}e^{ikx}$$

  Recall $k_1 = k_3 = k$ and $v_1 = v_3 = v$.

- Conjugation effectively switches the role of the incident and reflected waves: the waves with B coefficients are now incident and waves with A coefficients reflected. The equation linking the incident and reflected waves becomes

$$\begin{bmatrix} A_1^* \\ A_3^* \end{bmatrix} = \mathbf{S}\begin{bmatrix} B_1^* \\ B_3^* \end{bmatrix} \qquad \text{or more concisely} \qquad \boldsymbol{A}^* = \mathbf{S}\boldsymbol{B}^*$$

  Recall the original equation, before conjugation, was $\boldsymbol{B} = \mathbf{S}\boldsymbol{A}$ and note that the scattering matrix $\mathbf{S}$ is the same, since the potential is invariant under conjugation.

- Remember probability conservation requires that $\mathbf{S}$ be unitary, i.e. $\mathbf{S}^\dagger\mathbf{S} = \mathbf{I}$. With this in mind, multiply the original equation $\boldsymbol{B} = \mathbf{S}\boldsymbol{A}$ from the left by $\mathbf{S}^\dagger$, and then take the complex conjugate of the equation, which gives

$$\mathbf{S}^\dagger\mathbf{B} = \mathbf{A} \implies \mathbf{A}^* = \mathbf{S}^T\mathbf{B}^*$$

  Substituting the result $\mathbf{A}^* = \mathbf{S}^T\mathbf{B}^*$ into the conjugate equation $\boldsymbol{A}^* = \mathbf{S}\boldsymbol{B}^*$ gives

$$\mathbf{S}^T\mathbf{B}^* = \mathbf{S}\boldsymbol{B}^*$$

  meaning that $\mathbf{S}$ is symmetric for scattering off a delta potential. This symmetry is the reason why $t = \tilde{t}$ in the delta function scattering matrix. Formally, this is a consequence of the problem's Hamiltonian being invariant under time reversal.

- Next, why $r = \tilde{r}$. This is a consequence of the problem's reflection symmetry. Start again with the Schrödinger equation:

$$H\psi(x) = E\psi(x)$$

  The parity transformation $x \to -x$ (recall H is invariant under parity) gives:

$$H\psi(-x) = E\psi(-x)$$

The parity-transformed wave functions for regions 1 and 3 are

$$\psi_1(-x) = \frac{A_1}{\sqrt{v}} e^{-ikx} + \frac{B_1}{\sqrt{v}} e^{ikx} \qquad \text{and} \qquad \psi_3(-x) = \frac{A_3}{\sqrt{v}} e^{ikx} + \frac{B_3}{\sqrt{v}} e^{-ikx}$$

The roles of the incident and reflected waves are mixed up under parity: $\psi_1(-x)$ now refers to the region of $x > 0$ (right of the delta function), and $\psi_3(-x)$ to the region of $x < 0$. The equation linking the incident and reflected waves becomes

$$\begin{bmatrix} B_3 \\ B_1 \end{bmatrix} = \mathbf{S} \begin{bmatrix} A_3 \\ A_1 \end{bmatrix} \qquad \text{(after reflection)}$$

Recall the original equation, before parity transformation, was

$$\begin{bmatrix} B_1 \\ B_3 \end{bmatrix} = \mathbf{S} \begin{bmatrix} A_1 \\ A_3 \end{bmatrix} \qquad \text{(before reflection)}$$

- We can get the reflected equation from the original one by multiplying the original equation by the first Pauli spin matrix $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. The reflected equation is

$$\sigma_x \boldsymbol{B} = \mathbf{S} \sigma_x \boldsymbol{A} \implies \boldsymbol{B} = \sigma_x \mathbf{S} \sigma_x \boldsymbol{A}$$

Substituting the expression for $\boldsymbol{B}$ into the original equation $\boldsymbol{B} = \mathbf{S}\boldsymbol{A}$ gives

$$\sigma_x \mathbf{S} \sigma_x \boldsymbol{A} = \mathbf{S}\boldsymbol{A} \implies \mathbf{S} = \sigma_x \mathbf{S} \sigma_x$$

The relationship $\mathbf{S} = \sigma_x \mathbf{S} \sigma_x$ holds in general for any even Hamiltonian. Applied to our parameterization of $\mathbf{S}$, we have

$$\mathbf{S} = \sigma_x \mathbf{S} \sigma_x \iff \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} = \sigma_x \begin{bmatrix} r & \tilde{t} \\ t & \tilde{r} \end{bmatrix} \sigma_x = \begin{bmatrix} \tilde{r} & t \\ \tilde{t} & r \end{bmatrix}$$

The result is $r = \tilde{r}$ and $t = \tilde{t}$. This accounts for both of the symmetries in our delta function scattering matrix! So invariance under parity transformation is a powerful symmetry: it reduces the number of independent elements in the scattering matrix by two, even under in the absence of time reversal symmetry.

1.3 Third Exercise Set

1.3.1 Theory: Uncertainty Product of Observable Quantities

- We are interested in finding an expression for the uncertainty in the product $\Delta A \Delta B$ of two arbitrary observable quantities A and B. We start by assigning both A and B a corresponding Hermitian operator (Hermitian because A and B are observable). The operators are

$$A = A^\dagger \qquad \text{and} \qquad B = B^\dagger$$

- By definition, the uncertainty in A is

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 = \langle (A - \langle A \rangle) \rangle \equiv \langle \tilde{A}^2 \rangle$$

where we've defined $\tilde{A} = A - \langle A \rangle I$. Here $\langle A \rangle$ is a scalar and I is the identity operator.

- First, the definition of an operator's expectation value and some review of bra-ket notation.

$$\langle A\rangle = \int \psi^* A\psi \,\mathrm{d}x \equiv \langle\psi|\, A\,|\psi\rangle = \langle\psi|A\psi\rangle$$

Because A is Hermitian, $\langle\psi|A\psi\rangle = \langle A\psi|\psi\rangle$. This is a special case of the more general adjoint relationship $\langle A\psi|\psi\rangle = \langle\psi|A^*\psi\rangle$ with $A = A^*$ because A is Hermitian.

- The expectation value of a Hermitian operator is real. The classic proof reads

$$\langle A\rangle \equiv \langle\psi|A\psi\rangle = \langle A^*\psi|\psi\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^* \equiv \langle A\rangle^* \implies \langle A\rangle \in \mathbb{R}$$

- In general, the sum of two Hermitian operators $A = A^\dagger$ and $B = B^\dagger$ is

$$(A+B)^\dagger = A^\dagger + B^\dagger = A + B$$

So the sum of two Hermitian operators is a Hermitian operator. If we return to $\tilde{A} = A - \langle A\rangle\, I$ it follows that $\tilde{A}^\dagger = \tilde{A}$ since both A and I are Hermitian.

- We return to the product $\Delta A\Delta B$. First, we square everything, since uncertainty is expressed as $(\Delta A)^2$.

$$\begin{aligned}(\Delta A\Delta B)^2 &= \big\langle\tilde{A}^2\big\rangle\big\langle\tilde{B}^2\big\rangle = \langle\psi|\,\tilde{A}^2\,|\psi\rangle\,\langle\psi|\,\tilde{B}^2\,|\psi\rangle = \left\langle\tilde{A}\psi\middle|\tilde{A}\psi\right\rangle\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle\\ &= \left\|\tilde{A}\psi\right\|^2\left\|\tilde{B}\psi\right\|^2\end{aligned}$$

The last equality occurs in the Cauchy-Schwartz inequality:

$$\left\|\tilde{A}\psi\right\|^2\left\|\tilde{B}\psi\right\|^2 \geq \left|\left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle\right|^2 = \left|\left\langle\psi\middle|\tilde{A}\tilde{B}\psi\right\rangle\right|^2$$

- Next, some more manipulations of the last result:

$$\left|\langle\psi|\,\tilde{A}\tilde{B}\,|\psi\rangle\right|^2 = \left|\langle\psi|\,\tfrac{1}{2}\big(\tilde{A}\tilde{B} - \tilde{B}\tilde{A} + \tilde{A}\tilde{B} + \tilde{B}\tilde{A}\big)\,|\psi\rangle\right|^2$$

We introduce two quantities: the commutator and anti-commutator. They're written

$$\big[\tilde{A},\tilde{B}\big] = \tilde{A}\tilde{B} - \tilde{B}\tilde{A} \qquad \text{and} \qquad \big\{\tilde{A},\tilde{B}\big\} = \tilde{A}\tilde{B} + \tilde{B}\tilde{A}$$

Intermezzo: Some Properties of Commutators

- The anti-commutator of two Hermitian operators is a Hermitian operator

$$\begin{aligned}\big\{A,B\big\}^\dagger &= (AB+BA)^\dagger = (AB)^\dagger + (BA)^\dagger = B^\dagger A^\dagger + A^\dagger B^\dagger\\ &= AB + BA = \big\{A,B\big\}\end{aligned}$$

- The commutator of two Hermitian operators is anti-Hermitian

$$\begin{aligned}\big[A,B\big]^\dagger &= (AB-BA)^\dagger = (AB)^\dagger - (BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger\\ &= -(AB-BA) = -\big[A,B\big]\end{aligned}$$

- Finally, the expectation value of an anti-Hermitian operator $A^\dagger = -A$ is

$$\langle A\rangle = \langle\psi|A\psi\rangle = \langle A^*\psi|\psi\rangle = \langle -A\psi|\psi\rangle = -\langle A\psi|\psi\rangle = -\langle\psi|A\psi\rangle^* = -\langle A\rangle^*$$

The result implies $\langle A\rangle$ is a purely imaginary number if A is anti-Hermitian.

Back to the Uncertainty Principle

- Specifically, back to where we left off with

$$\begin{aligned}(\Delta A\Delta B)^2 &= \cdots = \left\|\tilde{A}\psi\right\|^2\left\|\tilde{B}\psi\right\|^2 \geq \left|\left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle\right|^2 = \cdots \\ &= \left|\langle\psi|\,\tfrac{1}{2}[\tilde{A},\tilde{B}] + \tfrac{1}{2}\{\tilde{A},\tilde{B}\}\,|\psi\rangle\right|^2 = \left|\left\langle\tfrac{1}{2}[\tilde{A},\tilde{B}] + \tfrac{1}{2}\{\tilde{A},\tilde{B}\}\right\rangle\right|^2 \\ &= \frac{1}{4}\left(\left|\left\langle[\tilde{A},\tilde{B}]\right\rangle\right|^2 + \left|\left\langle\{\tilde{A},\tilde{B}\}\right\rangle\right|^2\right)\end{aligned}$$

  In last parentheses we have a sum of two positive quantities, so we can drop the anti-commutator if we write

$$\frac{1}{4}\left(\left|\left\langle[\tilde{A},\tilde{B}]\right\rangle\right|^2 + \left|\left\langle\{\tilde{A},\tilde{B}\}\right\rangle\right|^2\right) \geq \frac{1}{4}\left|\left\langle[\tilde{A},\tilde{B}]\right\rangle\right|^2 = \left(\frac{1}{2}|\langle[A,B]\rangle|\right)^2$$

  The last equality uses the identity $\left[\tilde{A},\tilde{B}\right] = [A,B]$, which follows from some basic algebra and the definitions $\tilde{A} = A - \langle A\rangle I$ and $\tilde{B} = B - \langle B\rangle I$:

$$\left[\tilde{A},\tilde{B}\right] = \left[A - \langle A\rangle I, B - \langle B\rangle I\right] = \ldots = AB - BA = [A,B]$$

- Okay, so here's the entire derivation so far in one place. Note the two inequalities.

$$\begin{aligned}(\Delta A\Delta B)^2 &= \langle\tilde{A}^2\rangle\langle\tilde{B}^2\rangle = \langle\psi|\,\tilde{A}^2\,|\psi\rangle\,\langle\psi|\,\tilde{B}^2\,|\psi\rangle = \left\langle\tilde{A}\psi\middle|\tilde{A}\psi\right\rangle\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle \\ &= \left\|\tilde{A}\psi\right\|^2\left\|\tilde{B}\psi\right\|^2 \geq \left|\left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle\right|^2 = \left|\left\langle\psi\middle|\tilde{A}\tilde{B}\psi\right\rangle\right|^2 \\ &= \left|\langle\psi|\,\tfrac{1}{2}(\tilde{A}\tilde{B} - \tilde{B}\tilde{A} + \tilde{A}\tilde{B} + \tilde{B}\tilde{A})\,|\psi\rangle\right|^2 \equiv \left|\langle\psi|\,\tfrac{1}{2}[\tilde{A},\tilde{B}] + \tfrac{1}{2}\{\tilde{A},\tilde{B}\}\,|\psi\rangle\right|^2 \\ &= \left|\left\langle\tfrac{1}{2}[\tilde{A},\tilde{B}] + \tfrac{1}{2}\{\tilde{A},\tilde{B}\}\right\rangle\right|^2 = \frac{1}{4}\left(\left|\left\langle[\tilde{A},\tilde{B}]\right\rangle\right|^2 + \left|\left\langle\{\tilde{A},\tilde{B}\}\right\rangle\right|^2\right) \\ &\geq \frac{1}{4}|\langle[A,B]\rangle|^2 = \left(\frac{1}{2}|\langle[A,B]\rangle|\right)^2\end{aligned}$$

- Now we apply the result specifically to x and p, where $x = x$, $p = -i\hbar\frac{\partial}{\partial x}$ and $[x,p] = i\hbar$. The result is

$$(\Delta x\Delta p)^2 \geq \left(\tfrac{1}{2}|\langle[x,p]\rangle|\right)^2 = \left(\tfrac{1}{2}|\langle i\hbar\rangle|\right)^2 = \left(\tfrac{1}{2}|i\hbar|\right)^2 = \left(\tfrac{\hbar}{2}\right)^2 \implies \Delta x\Delta p \geq \frac{\hbar}{2}$$

1.3.2 Wave Function Minimizing the Uncertainty Product

Find all wave functions with the minimum position-momentum uncertainty product allowed by the Heisenberg uncertainty principle, i.e. find all wave functions for which $\Delta x\Delta p = \frac{\hbar}{2}$.

- To solve this problem, we need a wavefunction for which both inequalities in the above theory section are strict equalities. First, the Cauchy-Schwartz inequality is an equality for two linearly dependent vectors.

$$\left\|\tilde{A}\psi\right\|^2\left\|\tilde{B}\psi\right\|^2 = \left|\left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle\right|^2 \quad \text{if} \quad \tilde{A}\psi = \alpha\tilde{B}\psi, \qquad \alpha \in \mathbb{C}$$

  The second inequality is an equality if

$$\left\langle\{\tilde{A},\tilde{B}\}\right\rangle = 0$$

- We have two conditions:

$$\left|\tilde{A}\psi\right\rangle = \alpha\left|\tilde{B}\psi\right\rangle \qquad \text{and} \qquad \left\langle\{\tilde{A},\tilde{B}\}\right\rangle = 0$$

  We start with the second condition and perform some manipulations...

$$\begin{aligned} 0 &\equiv \left\langle\{\tilde{A},\tilde{B}\}\right\rangle = \langle\psi|\,\tilde{A}\tilde{B}+\tilde{B}\tilde{A}\,|\psi\rangle = \langle\psi|\,\tilde{A}\tilde{B}\,|\psi\rangle + \langle\psi|\,\tilde{B}\tilde{A}\,|\psi\rangle \\ &= \left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle + \left\langle\tilde{B}\psi\middle|\tilde{A}\psi\right\rangle = 0 \end{aligned}$$

  And then substitute in the Cauchy-Schwartz condition...

$$\begin{aligned} 0 &= \left\langle\tilde{A}\psi\middle|\tilde{B}\psi\right\rangle + \left\langle\tilde{B}\psi\middle|\tilde{A}\psi\right\rangle = \left\langle\alpha\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle + \left\langle\tilde{B}\psi\middle|\alpha\tilde{B}\psi\right\rangle \\ &= \alpha^*\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle + \alpha\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle = (\alpha^*+\alpha)\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle = 0 \end{aligned}$$

  Mathematically, the equality holds if either of the two product terms equal zero. But the bra-ket term is $\left\langle\tilde{B}\psi\middle|\tilde{B}\psi\right\rangle = \langle\tilde{B}^2\rangle = (\Delta B)^2$, and this term being zero would imply zero uncertainty in B, which implies infinite uncertainty in A. We reject this option as non-physical, so we're left with $(\alpha^*+\alpha) = 0$, meaning α is a purely imaginary number. To make this requirement explicit, we write $\alpha = ic$ where $c \in \mathbb{R}$. The Cauchy-Schwartz condition then reads

$$\left|\tilde{A}\psi\right\rangle = ic\left|\tilde{B}\psi\right\rangle, \qquad c \in \mathbb{R}$$

  Substituting in the definition $\tilde{A} = A - \langle A\rangle I$ gives

$$|A\psi\rangle - \langle A\rangle\,|\psi\rangle = ic\,|B\psi\rangle - ic\langle B\rangle\,|\psi\rangle$$

- Any solutions ψ to this equation will satisfy the equality

$$\Delta A \Delta B = \frac{1}{2}\big|\langle[A,B]\rangle\big|$$

  For the specific case $A \to x$ and $B \to p$ where $p \to -i\hbar\frac{\partial}{\partial x}$ and $|\psi\rangle = \psi(x)$, the equation reads

$$x\psi - \langle x\rangle\,\psi = \hbar c\frac{\partial\psi}{\partial x} - ic\,\langle p\rangle\,\psi$$

1.4 Fourth Exercise Set

1.4.1 Wave Function Minimizing the Uncertainty Product (continued)

Continued from the previous exercise set...

- *Review of last exercise set*: We started with two Hermitian operators A and B and showed

$$\Delta A \Delta B \geq \frac{1}{2}|\langle[A,B]\rangle|$$

  An equality $=$ replaces the inequality $\geq$ if

$$\left\langle\{\tilde{A},\tilde{B}\right\rangle = 0 \qquad \text{and} \qquad \tilde{A}\,|\psi\rangle = \alpha\tilde{B}\,|\psi\rangle$$

  where $\tilde{A} = A - \langle A\rangle$, $\tilde{B} = B - \langle B\rangle$ and $\alpha = ic$ where $c \in \mathbb{R}$ is real constant.

  In the concrete momentum-position case, the minimum uncertainty condition reads

$$x\psi(x) - \langle x\rangle\,\psi = \hbar c\psi'(x) - ic\,\langle p\rangle\,\psi$$

  The wave functions ψ solving this equation will minimize the product $\Delta x \Delta p$.

- Rearranging the equation for ψ' gives

$$\psi'(x) = \left(\frac{x - \langle x \rangle}{c\hbar} + \frac{i\,\langle p \rangle}{\hbar}\right)\psi(x)$$

Next, we separate variables and integrate:

$$\frac{\mathrm{d}\psi}{\psi} = \frac{x - \langle x \rangle}{c\hbar} + \frac{i\,\langle p \rangle}{\hbar} \implies \ln\psi = \frac{(x - \langle x \rangle)^2}{2c\hbar} + \frac{i\,\langle p \rangle}{\hbar}x + \lambda$$

Solving for x gives

$$\psi(x) = e^{\lambda}\exp\left(\frac{(x - \langle x \rangle)^2}{2c\hbar}\right)e^{-i\frac{\langle p \rangle}{\hbar}x}$$

- Now we just have to normalize the wavefunction:

$$\int_{-\infty}^{\infty}|\psi(x)|^2\,\mathrm{d}x \equiv 1 = \left|e^{\lambda}\right|^2\int_{-\infty}^{\infty}\exp\left(\frac{(x - \langle x \rangle)^2}{2c\hbar}\right)\mathrm{d}x$$

Note that c must be negative for the integral to converge. To make this requirement explicit, we'll write

$$1 \equiv \left|e^{\lambda}\right|^2\int_{-\infty}^{\infty}\exp\left(-\frac{(x - \langle x \rangle)^2}{2\sigma^2}\right)\mathrm{d}x$$

where we introduce σ to match the form of a Gauss bell curve, which then implies

$$\left|e^{\lambda}\right|^2 = \frac{1}{\sqrt{2\pi\sigma^2}}$$

The final result for $\psi(x)$ is

$$\psi(x) = \frac{1}{\sqrt[4]{2\pi\sigma^2}}\exp\left(\frac{(x - \langle x \rangle)^2}{4\sigma^2}\right)e^{-i\frac{\langle p \rangle}{\hbar}x}$$

These functions are called *Gaussian wave packets.* This concludes the problem: the functions minimizing the product $\Delta x \Delta p$ are Gaussian wave packets.

As a final note, the $e^{-i\frac{\langle p \rangle}{\hbar}x}$ term is a plane wave, with wavelength

$$\frac{\langle p \rangle}{\hbar}\lambda = 2\pi \implies \lambda = \frac{h}{\langle p \rangle}$$

1.4.2 Theory: Time Evolution of a Wave Function

- We find the time evolution of a wave function by solving the Schrödinger equation

$$H\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

One option is to solve the stationary Schrödinger equation

$$H\psi_n(x) = E_n\psi_n(x)$$

and expand the initial state $\psi(x,0)$ in terms of the basis functions ψ_n solving the stationary Schrödinger equation, i.e. writing $\psi(x,0)$ as

$$\psi(x,0) = \sum_n c_n\psi_n(x)$$

- We then find the time evolution by adding a time-dependent phase factor to the eigenfunction expansion

$$\psi(x,t) = \sum_n c_n \psi_n(x) e^{-i\frac{E_n}{\hbar}t}$$

In Dirac bra-ket notation, the stationary Schrödinger equation and eigenfunction expansion of the initial state read

$$H\left|n\right\rangle = E_n \left|n\right\rangle \qquad \text{and} \qquad \left|\psi, 0\right\rangle = \sum_n c_n \left|n\right\rangle$$

and the time evolution reads

$$\left|\psi, t\right\rangle = \sum_n c_n e^{-i\frac{E_n}{\hbar}t}\left|n\right\rangle$$

The time evolution depends on the potential $V(x)$ we're working in.

1.4.3 Theory: Time-Dependent Expectation Values and Operators

- Consider an operator A. A function of the operator is defined in terms of the function's Taylor series:

$$f(A) = \sum_n \frac{1}{\sqrt{N!}} f^{(n)}(A) A^N$$

- Next, consider an arbitrary observable $A = A^\dagger$. We then ask what is the expectation value $\left\langle A, t\right\rangle$ of A at time t? We can find the wave function $\left|\psi, t\right\rangle$ with

$$\left|\psi, t\right\rangle = \sum_n c_n e^{-i\frac{E_n}{\hbar}t}\left|n\right\rangle$$

We'll now show that we get the same result by acting on the initial state $\left|\psi, 0\right\rangle$ with the time evolution operator, i.e. we will prove the equality

$$\left|\psi, t\right\rangle \equiv \sum_n c_n e^{-i\frac{E_n}{\hbar}t}\left|n\right\rangle = e^{-i\frac{H}{\hbar}t}\left|\psi, 0\right\rangle$$

- To show this, we first expand $\left|\psi, 0\right\rangle$ in terms of its eigenstates and bring the operator inside the sum.

$$e^{-i\frac{H}{\hbar}t}\left|\psi, 0\right\rangle = e^{-i\frac{H}{\hbar}t}\sum_n c_n \left|n\right\rangle = \sum_n c_n e^{-i\frac{H}{\hbar}t}\left|n\right\rangle$$

We write the exponent of the Hamiltonian operator in terms of the exponential function's Taylor series:

$$e^{-i\frac{H}{\hbar}t}\left|\psi, 0\right\rangle = \sum_n c_n \left[\sum_m \frac{1}{m!}\left(-\frac{it}{\hbar}\right)^m H^m \left|n\right\rangle\right]$$

- First, we'll tackle the term $H^m\left|n\right\rangle$, recalling that $\left|n\right\rangle$ are eigenfunctions of H:

$$H^m\left|n\right\rangle = H^{m-1}\left(H\left|n\right\rangle\right) = H^{m-1}\left(E_n\left|n\right\rangle\right) = \cdots = E_n^m\left|n\right\rangle$$

This step is important—it converts the operator H to the scalar values E_n. We then have

$$e^{-i\frac{H}{\hbar}t}|\psi,0\rangle = \sum_n c_n\left[\sum_m \frac{1}{m!}\left(-\frac{it}{\hbar}\right)^m E_n^m\right]|n\rangle = \sum_n c_n e^{-i\frac{E_n}{\hbar}t}|n\rangle$$

This completes the proof that

$$|\psi,t\rangle = \sum_n c_n e^{-i\frac{E_n}{\hbar}t}|n\rangle = e^{-i\frac{H}{\hbar}t}|\psi,0\rangle$$

In other words, instead of finding a time evolution by expanding an initial state $|\psi,0\rangle$ in terms of basis functions, we can act directly on the initial state with the time evolution operator.

Time-Dependent Expectation Values

- Next, we return to the expectation value $\langle A,t\rangle$:

  $$\langle A,t\rangle \equiv \langle\psi,t|A|\psi,t\rangle$$

  We've just shown the ket term can be found with the time evolution operator

  $$|\psi,t\rangle = e^{-i\frac{H}{\hbar}t}|\psi,0\rangle$$

  We find the bra term by taking the complex conjugate of the ket term:

  $$\langle\psi,t| = \langle\psi,0|\left(e^{-i\frac{H}{\hbar}t}\right)^\dagger = \langle\psi,0|e^{i\frac{H}{\hbar}t}$$

  Note that the $|\psi,0\rangle$ ket term is reversed under complex conjugation! We then have

  $$\langle A,t\rangle = \langle\psi,0|e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}|\psi,0\rangle \equiv \langle\psi,0|A(t)|\psi,0\rangle$$

  where we've defined $A(t) = e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}$ for shorthand.

- The above result is useful: we have a new way to find a time-dependent expectation value. If we are given an initial state $|\psi,0\rangle$, we can use the time evolution operator to get

  $$\langle A,t\rangle = \langle\psi,0|e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}|\psi,0\rangle \equiv \langle\psi,0|$$

  In other words, we don't need to find the time evolution of the wave function $|\psi,t\rangle$. This is convenient, since finding $|\psi,t\rangle$ is often tedious.

- Finally, some vocabulary. Finding $|A,t\rangle$ via time evolution of the wave function, i.e.

  $$\langle A,t\rangle = \langle\psi,t|A|\psi,t\rangle$$

  is called the *Schrödinger approach.* Finding $|A,t\rangle$ via time evolution of the A operator, i.e.

  $$\langle A,t\rangle = \langle\psi,0|e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}|\psi,0\rangle = \langle\psi,0|A(t)|\psi,0\rangle$$

  is called the *Heisenberg approach.*

Theory: Time Evolution of an Operator

- Next, we ask how to find the time evolution $A(t)$ of an operator A? To do this, we solve the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) = \frac{\mathrm{d}}{\mathrm{d}t}\left[e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}\right] = \left(\tfrac{i}{\hbar}H\right)e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t} + e^{i\frac{H}{\hbar}t}A\left(-i\tfrac{H}{\hbar}e^{-i\frac{H}{\hbar}t}\right)$$

This is found with the Taylor series definition of an operator A. In both terms, we have the product of the Hamiltonian H with the time evolution operator. These operators commute, so we can switch their order of multiplication and factor to get

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) = e^{i\frac{H}{\hbar}t}\left(\frac{i}{\hbar}HA - \frac{i}{\hbar}AH\right)e^{-i\frac{H}{\hbar}t} = e^{i\frac{H}{\hbar}t}\frac{i}{\hbar}[H,A]e^{-i\frac{H}{\hbar}t} \equiv \frac{i}{\hbar}[H,A](t)$$

So, we find $A(t)$ by solving the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) = \frac{i}{\hbar}[H,A](t)$$

- One more useful identity: consider two operators A and B. We're interested in the time evolution of their product AB:

$$\begin{aligned}(AB)(t) &= e^{i\frac{H}{\hbar}t}ABe^{-i\frac{H}{\hbar}t} = e^{i\frac{H}{\hbar}t}AIBe^{-i\frac{H}{\hbar}t}\\ &= e^{i\frac{H}{\hbar}t}Ae^{-i\frac{H}{\hbar}t}e^{i\frac{H}{\hbar}t}Be^{-i\frac{H}{\hbar}t} = A(t)B(t)\end{aligned}$$

1.4.4 Time Evolution of the Gaussian Wave Packet

Given a Gaussian wave function $\psi(x,0)$ and the time-independent Hamiltonian $H = \frac{p^2}{2m} + V(x)$, find the initial wavefunction's time evolution $\psi(x,t)$.

- We'll work in the potential $V(x) = 0$. Because the basis functions of a free particle are continuous, and n is traditionally used to index discrete quantities, we'll index the basis functions with k. For a particle in a constant potential, the eigenfunctions are plane waves. We have

$$\psi_k(x) = \frac{e^{ikx}}{\sqrt{2\pi}} \qquad \text{and} \qquad E_k = \frac{\hbar^2k^2}{2m}$$

Note the normalization of the plane wave with $\sqrt{2\pi}$. The factor $\frac{1}{\sqrt{2\pi}}$ is chosen so that a product of two basis functions produces a delta function:

$$\left\langle k\middle|\tilde{k}\right\rangle \equiv \int \psi_k^*(x)\psi_{\tilde{k}}(x)\,\mathrm{d}x = \frac{1}{2\pi}\int e^{i(\tilde{k}-k)x}\,\mathrm{d}x \equiv \delta(\tilde{k}-k)$$

- First, an overview: To perform the time evolution, we first expand the initial state $\psi(x,0)$ in terms of the basis functions ψ_k

$$\psi(x,0) = \int c(k)\frac{e^{ikx}}{\sqrt{2\pi}}\,\mathrm{d}k$$

Note that we use integration instead of summation because the basis functions are continuous and not discrete. The above expansion is a Fourier transform of $c(k)$ from the k to the x domain, so $c(k)$ is found with the inverse Fourier transform

$$c(k) = \int \psi(x,0)\frac{e^{-ikx}}{\sqrt{2\pi}}\,\mathrm{d}x$$

We would then find the time evolution with

$$\psi(x,t) = \int c(k) e^{-i\frac{E_k}{\hbar}t} \frac{e^{ikx}}{\sqrt{2\pi}} \, \mathrm{d}k$$

Again, integration replaces summation.

- In the end, we'll be more interested in the observables x and p than the actual wave function. For example the expectation values of x and p at time t, written

$$\langle x, t\rangle \equiv \langle \psi, t| \, x \, |\psi, t\rangle \qquad \text{and} \qquad \langle p, t\rangle \equiv \langle \psi, t| \, p \, |\psi, t\rangle$$

Likewise, we'll be interested in the uncertainties

$$\Delta x(t) = \sqrt{\langle x^2, t\rangle - \langle x, t\rangle^2} \qquad \text{and} \qquad \Delta p(t) = \sqrt{\langle p^2, t\rangle - \langle p, t\rangle^2}$$

Note: Directly performing the above eigenfunction expansion and time evolution by solving the integrals is a tedious mathematical exercise. We'll take a slight detour, and introduce some machinery that solves the problem in a more physically elegant way.

Theory: Commutator Properties

- First, a distributive property: $[AB, C] = A[B, C] + [A, C]B$.
- And second: $[\lambda A, B] = \lambda[A, B]$
- And finally: $[B, A] = -[A, B]$

Back to the Time Evolution of the Gaussian Wave Packet

- We now have the formalism we need to easily find the expectation values

$$\langle x, t\rangle \equiv \langle \psi, t| \, x \, |\psi, t\rangle \qquad \text{and} \qquad \langle p, t\rangle \equiv \langle \psi, t| \, p \, |\psi, t\rangle$$

for a Gaussian wave packet with the simple Hamiltonian $H = \frac{p^2}{2m}$. Using the Heisenberg approach, we'll first find the time evolution of the operators x and p, then find the expectation values with

$$\langle A, t\rangle = \langle \psi, 0| \, A(t) \, |\psi, 0\rangle$$

- First, the equation for the operator $x(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = \frac{i}{\hbar}[H, x](t) = \frac{i}{\hbar}\left[\frac{p^2}{2m}, x\right](t)$$

Writing $p^2 = pp$, applying basic commutator properties and recalling the result $[x, p] = i\hbar$ gives

$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = \frac{i}{2m\hbar}\left(p[p, x] + [p, x]p\right)(t) = \frac{i}{2m\hbar}\left(-pi\hbar - i\hbar p\right)(t) = \frac{p(t)}{m}$$

Second, the differential for the operator $p(t)$, noting that $[p^2, p] = 0$, is

$$\frac{\mathrm{d}}{\mathrm{d}p}(t) = \frac{i}{\hbar}\left[H, p\right](t) = \frac{i}{\hbar}\left[\frac{p^2}{2m}, p\right](t) = 0$$

The general solution is a constant: $p(t) = p_0$. We need an initial condition to find a solution specific to our problem, which we get from general expression

$$A(t)\big|_{t=0} = e^{i\frac{H}{\hbar}\cdot 0} A e^{-i\frac{H}{\hbar}\cdot 0} = A$$

In our case, $p(0) = p$, which implies $p(t) = p$. In other words, the momentum operator stays the same with time; it is always the usual

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

for all time t. Next, with $p(t)$ known, we solve the equation for $x(t)$:

$$\frac{\mathrm{d}}{\mathrm{d}x} = \frac{p(t)}{m} = \frac{p}{m} \implies x(t) = \frac{p}{m}t + x_0$$

With the initial condition $x(0) = x$, we now have the expression for the time evolution of the operator $x(t)$

$$x(t) = \frac{p}{m}t + x \to -i\frac{\hbar}{m}t\frac{\partial}{\partial x} + x$$

- With $x(t)$ and $p(t)$ known, we can find the expectation values using

$$\langle A, t\rangle = \langle \psi, 0|\, A(t)\, |\psi, 0\rangle$$

We start with momentum:

$$\langle p, t\rangle = \langle \psi, 0|\, p(t)\, |\psi, 0\rangle = \langle \psi, 0|\, p\, |\psi, 0\rangle \equiv \langle p, 0\rangle = \langle p\rangle$$

In other words, because $p(t) = p$ is constant, we can just find the initial expectation value $\langle p, 0\rangle$ using the initial wave function. This is the same $\langle p\rangle$ term in the exponent of the plane wave term in the Gaussian wave packet.

Next, the expectation value of position. Inserting $x(t)$ and splitting the bra-ket into two parts gives

$$\begin{aligned}\langle x, t\rangle &= \langle \psi, 0|\, x(t)\, |\psi, 0\rangle = \langle \psi, 0|\, \frac{p}{m}t + x\, |\psi, 0\rangle \\ &= \frac{t}{m}\langle \psi, 0|\, p\, |\psi, 0\rangle + \langle \psi, 0|\, x\, |\psi, 0\rangle = \frac{t}{m}\langle p, 0\rangle + \langle x, 0\rangle\end{aligned}$$

These are the same $\langle x\rangle$ and $\langle p\rangle$ term in the exponents of the initial the Gaussian wave packet.

- Next, we want to find the uncertainties

$$\Delta x(t) = \sqrt{\langle x^2, t\rangle - \langle x, t\rangle^2} \qquad \text{and} \qquad \Delta p(t) = \sqrt{\langle p^2, t\rangle - \langle p, t\rangle^2}$$

It remains to find the the time evolution of the operators p^2 and x^2 and then the expectation values $\langle p^2, t\rangle$ and $\langle x^2, t\rangle$. We start with the operator $p^2(t)$.

$$\langle p^2, t\rangle = \langle \psi, 0|\, p^2(t)\, |\psi, 0\rangle = \langle \psi, 0|\, \left[p(t)\right]^2 |\psi, 0\rangle = \langle \psi, 0|\, p^2\, |\psi, 0\rangle$$

In other words, $\langle p^2, t\rangle$ is the expectation value of the time-independent operator p^2.

Next, the evolution of $x(t)$. Using $x^2(t) = \big[x(t)\big]^2$, substituting in the definition of $x(t)$, and splitting up the expectation value into three terms gives

$$\begin{aligned}
\left\langle x^2, t\right\rangle &= \langle\psi, 0|\, x^2(t)\, |\psi, 0\rangle = \langle\psi, 0|\, \big[x(t)\big]^2\, |\psi, 0\rangle = \langle\psi, 0| \left(\frac{p}{m}t + x\right)^2 |\psi, 0\rangle \\
&= \langle\psi, 0| \left(\frac{p^2t^2}{m^2} + \frac{t}{m}(px + xp) + x^2\right) |\psi, 0\rangle \\
&= \frac{t^2}{m^2}\langle\psi, 0|\, p^2\, |\psi, 0\rangle + \frac{t}{m}\langle\psi, 0|\, px + xp\, |\psi, 0\rangle + \langle\psi, 0|\, x^2\, |\psi, 0\rangle
\end{aligned}$$

We've now succeeded in expressing the time-dependent expectation values of x, x^2, p and p^2 in terms of quantities that appear in the initial state, namely the exponent parameters $\langle x\rangle$ and $\langle p\rangle$.

- From the beginning of this problem, recall the initial wave function is

$$\psi(x, 0) = \frac{1}{\sqrt[4]{2\pi\sigma^2}}\exp\left(\frac{(x - \langle x\rangle)^2}{4\sigma^2}\right)e^{-i\frac{\langle p\rangle}{\hbar}x}$$

The associated probability density is

$$\rho(x, t) = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(\frac{(x - \langle x\rangle)^2}{2\sigma^2}\right)$$

The expectation values of x and p are simply

$$\langle\psi, 0|\, x\, |\psi, 0\rangle = \langle x\rangle \qquad \text{and} \qquad \langle\psi, 0|\, p\, |\psi, 0\rangle = \langle p\rangle$$

By definition, the initial uncertainty in x is

$$\Delta x(0) = \sqrt{\left\langle x^2, 0\right\rangle - \langle x, 0\rangle^2}$$

There is a shortcut: for a Gaussian wave packet, the uncertainty is simply the wave packet's standard deviation σ. We can take advantage of this relationship to easily find $\left\langle x^2, 0\right\rangle$:

$$\Delta x(0) = \sqrt{\left\langle x^2, 0\right\rangle - \langle x, 0\rangle^2} = \sigma \implies \left\langle x^2, 0\right\rangle = \sigma^2 + \langle x, 0\rangle^2$$

- Another shortcut: instead of the definition, we find the uncertainty in p using the uncertainty principle, which for a Gaussian wave packet is the equality

$$\Delta x \Delta p = \frac{\hbar}{2} \implies \Delta p(0) = \frac{\hbar}{2\Delta x(0)} = \frac{\hbar}{2\sigma}$$

With $\Delta p(0)$ in hand, we can find $\left\langle p^2, 0\right\rangle$ with

$$\Delta p(0) = \sqrt{\left\langle p^2, 0\right\rangle - \langle p, 0\rangle^2} = \frac{\hbar}{2\sigma} \implies \left\langle p^2, 0\right\rangle = \frac{\hbar^2}{4\sigma^2} + \langle p, 0\rangle^2$$

- The last piece needed to find $\left\langle x^2, t\right\rangle$ is the quantity $\langle\psi, 0|\, px + xp\, |\psi, 0\rangle$. To find this, we'll use the relationship $px = p^\dagger x^\dagger = (xp)^\dagger$. In general,

$$\left\langle A^\dagger\right\rangle = \left\langle\psi\middle|A^\dagger\psi\right\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^* = \langle A\rangle^*$$

which implies $\left\langle A + A^\dagger\right\rangle = \langle A\rangle + \langle A\rangle^* = 2\operatorname{Re}\langle A\rangle$. The expression $\langle\psi, 0|\, px + xp\, |\psi, 0\rangle$ then simplifies to

$$\langle\psi, 0|\, px + xp\, |\psi, 0\rangle = 2\operatorname{Re}\langle\psi, 0|\, xp\, |\psi, 0\rangle$$

We ran out of time at this point. The problem is completed in the next exercise set.

1.5 Fifth Exercise Set

1.5.1 Time Evolution of a Gaussian Wave Packet (continued)

- In the last exercise set, we wanted to find the uncertainties

$$\Delta x(t) = \sqrt{\langle x^2, t\rangle - \langle x, t\rangle^2} \qquad \text{and} \qquad \Delta p(t) = \sqrt{\langle p^2, t\rangle - \langle p, t\rangle^2}$$

We approached finding the time evolution of the operators $x(t)$ and $p(t)$ using the Heisenberg approach. We left off with the following operator expressions:

$$p(t) = p \qquad \text{and} \qquad x(t) = \frac{pt}{m} + x$$

For expected momentum values, we found

$$\langle p, t\rangle = \langle p, 0\rangle \qquad \text{and} \qquad \left\langle p^2, t\right\rangle = \left\langle p^2, 0\right\rangle$$

For expected position values, we found

$$\begin{aligned}\langle x, t\rangle &= \frac{t}{m}\langle p, 0\rangle + \langle x, 0\rangle \\ \left\langle x^2, t\right\rangle &= \frac{t^2}{m^2}\langle \psi, 0|\, p^2\, |\psi, 0\rangle + \frac{t}{m}\langle \psi, 0|\, px + xp\, |\psi, 0\rangle + \langle \psi, 0|\, x^2\, |\psi, 0\rangle\end{aligned}$$

We found nearly all of the initial expectation values in terms of the parameters $\langle x\rangle, \langle p\rangle$ and σ in the wave packet. The result were:

$$\begin{aligned}&\langle p, 0\rangle = \langle p\rangle \qquad \langle x, 0\rangle = \langle x\rangle \\ &\left\langle x^2, 0\right\rangle = \sigma^2 + \langle x\rangle^2 \qquad \left\langle p^2, 0\right\rangle = \left(\frac{\hbar}{2\sigma}\right)^2 + \langle p\rangle^2\end{aligned}$$

The only remaining expectation value is $\langle px + xp, 0\rangle$, which we showed to be

$$\langle xp + px, 0\rangle = 2\operatorname{Re}\left[\,\langle xp, 0\rangle\,\right]$$

We find the expectation value by definition, using the wave function:

$$\begin{aligned}\langle xp + px, 0\rangle = 2\operatorname{Re}\left[\,\langle xp, 0\rangle\,\right] &= 2\operatorname{Re}\int_{-\infty}^{\infty}\psi^*(x,0)x\left[-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right]\psi(x,0)\,\mathrm{d}x \\ &= 2\operatorname{Re}\int_{-\infty}^{\infty}\psi^*(x,0)\cdot x\cdot(-i\hbar)\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{1}{\sqrt[4]{2\pi\sigma^2}}e^{-\frac{(x-\langle x\rangle)^2}{4\sigma^2}}e^{i\frac{\langle p\rangle}{\hbar}x}\right]\mathrm{d}x \\ &= 2\int_{-\infty}^{\infty}\psi^*(x,0)x\langle p\rangle\,\psi(x,0)\,\mathrm{d}x = 2\langle p\rangle\langle x\rangle\end{aligned}$$

Note that the imaginary portion of the derivative in the middle line disappears when taking the real component.

- We now have everything we need to find the uncertainties Δx and Δp. Starting with Δp, we have:

$$\left[\Delta p(t)\right]^2 = \left\langle p^2, t\right\rangle - \langle p, t\rangle^2 = \left(\frac{\hbar}{2\sigma}\right)^2 + \langle p\rangle^2 - \langle p\rangle^2 = \left(\frac{\hbar}{2\sigma}\right)^2$$

For position, the uncertainty Δx is

$$\begin{aligned}
\left[\Delta x(t)\right]^2 &= \langle x^2, t\rangle - \langle x, t\rangle^2 = \frac{t^2}{m^2}\langle p^2, 0\rangle + \frac{t}{m}\langle px + xp, 0\rangle + \langle x^2, 0\rangle - \left(\frac{t}{m}\langle p, 0\rangle + \langle x, 0\rangle\right)^2 \\
&= \frac{t^2}{m^2}\left[\langle p\rangle^2 + \left(\frac{\hbar}{2\sigma}\right)^2\right] + \frac{t}{m}2\langle p\rangle\langle x\rangle + \sigma^2 + \langle x\rangle^2 - \frac{t^2}{m^2}\langle p\rangle^2 - 2\frac{t}{m}\langle p\rangle\langle x\rangle - \langle x\rangle^2 \\
&= \sigma^2 + \left(\frac{\hbar t}{2m\sigma}\right)^2
\end{aligned}$$

The product in the two uncertainties is

$$\Delta x(t)\Delta p(t) = \left(\frac{\hbar}{2\sigma}\right)^2\left(\sigma^2 + \left(\frac{\hbar t}{2m\sigma}\right)^2\right) = \frac{\hbar}{2}\sqrt{1 + \left(\frac{\hbar t}{2m\sigma^2}\right)^2}$$

Note that the product in uncertainties starts at the initial value $\frac{\hbar}{2}$ and increases with time. This immediately implies that the time evolution $\psi(x, t > 0)$ of the initial Gaussian wave packet $\psi(x, 0)$ is no longer a Gaussian wave packet. It couldn't be—it has an uncertainty product greater $\Delta x\Delta p > \frac{\hbar}{2}$, while Gaussian wave packets are by definition constructed to have $\Delta x\Delta p = \frac{\hbar}{2}$.

1.5.2 Theory: Quantum Harmonic Oscillator

- The Hamiltonian of a particle of mass m in a harmonic oscillator reads

$$H = \frac{p^2}{2m} + \frac{kx^2}{2} = \frac{p^2}{2m} + \frac{m\omega}{2}x^2, \qquad \omega = \sqrt{\frac{k}{m}}$$

We analyze the harmonic oscillator using the annihilation and creation operators. The annihilation operator a is

$$a = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p}{p_0}\right) \qquad \text{where} \qquad x_0 = \sqrt{\frac{\hbar}{m\omega}}, \quad p_0 = \frac{\hbar}{x_0}$$

while the creation operator, equal to the adjoint of a, is

$$a^\dagger = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - i\frac{p}{p_0}\right)$$

The annihilation and creation operators don't commute—their commutator is

$$\left[a, a^\dagger\right] = 1$$

Adding and subtracting the two operators give expressions for x and p

$$x = \frac{x_0}{\sqrt{2}}(a + a^\dagger) \qquad \text{and} \qquad p = \frac{p_0}{\sqrt{2}i}(a - a^\dagger)$$

- In terms of a and $a^\dagger$, the harmonic oscillator's Hamiltonian reads

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

The Hamiltonian's eigenstates are indexed by $n = 0, 1, 2, \ldots$ and read

$$H|n\rangle = \hbar\omega\left(n + \frac{1}{2}\right)|n\rangle, \quad n = 0, 1, 2, \ldots$$

The annihilation and creation operators act on the oscillator's eigenstates as follows:

$$a|n\rangle = \sqrt{n}\,|n-1\rangle \qquad \text{and} \qquad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

Note the operator equality $a^\dagger a|n\rangle = n|n\rangle$—in other words, acting on an eigenstate $|n\rangle$ with the operator $a^\dagger a$ reveals the state's index n.

Theory: Ehrenfest Theorem
In our case (for a harmonic oscillator), the theorem reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x, t\rangle = \frac{\langle p, t\rangle}{m} \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle p, t\rangle = \left\langle -\frac{\mathrm{d}}{\mathrm{d}x}V(x)\right\rangle = -k\langle x, t\rangle$$

1.5.3 Time Evolution of a Particle in a Harmonic Oscillator

Consider a particle in a harmonic potential with the initial eigenfunction

$$|\psi, 0\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$$

Compute the wavefunction's time evolution $|\psi, t\rangle$ the time-dependent expectation values $\langle x, t\rangle$ and $\langle p, t\rangle$ and use this to determine the validity of the Ehrenfest theorem. Finally, determine the product of uncertainties $\Delta x(t)\Delta p(t)$.

- First, we find the wavefunction's time evolution. This is relatively simple, since the initial wavefunction is a linear combination of the Hamiltonian's eigenstates. We just have to add the time-dependent phase factors $e^{-i\frac{E_n}{\hbar}t}$. Substituting in the energies for a particle in a harmonic oscillator, the result is

$$|\psi, t\rangle = \frac{1}{\sqrt{2}}e^{-i\frac{E_0}{\hbar}t}|0\rangle + \frac{1}{\sqrt{2}}e^{-i\frac{E_1}{\hbar}t}|1\rangle = \frac{1}{\sqrt{2}}e^{-i\frac{\omega}{2}t}|0\rangle + \frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}|1\rangle$$

- Next, working with x in terms of the annihilation and creation operators, we find the expectation value $\langle x\rangle$ as

$$\langle x\rangle = \frac{x_0}{\sqrt{2}}\left\langle a + a^\dagger\right\rangle = \frac{x_0}{\sqrt{2}}\left(\langle a\rangle + \langle a\rangle^*\right) = \sqrt{2}x_0 \operatorname{Re}\langle a\rangle$$

  Following similar lines for $\langle p\rangle$, we have

$$\langle p\rangle = \frac{p_0}{\sqrt{2}i}\left\langle a - a^\dagger\right\rangle = \frac{p_0}{\sqrt{2}i}\left(\langle a\rangle - \langle a\rangle^*\right) = \sqrt{2}p_0 \operatorname{Im}\langle a\rangle$$

  These two results are useful: they show that by finding the expectation value $\langle a\rangle$ we also determine the values of $\langle x\rangle$ and $\langle p\rangle$. Naturally, the next step is to find $\langle a\rangle$ (we'll find the time-dependent form)

$$\langle a, t\rangle = \langle\psi, t|\,a\,|\psi, t\rangle = \langle\psi, t|\left(\frac{1}{\sqrt{2}}e^{-i\frac{\omega}{2}t}a|0\rangle + \frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}a|1\rangle\right)$$

The annihilation operator eliminates the ground state, i.e. $a|0\rangle = 0$ and turns the first state into the ground state, i.e. $a|1\rangle = |0\rangle$. The expression for $\langle a,t\rangle$ becomes

$$\begin{aligned}\langle a,t\rangle &= \langle\psi,t|\,\frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}\,|0\rangle = \left(\frac{1}{\sqrt{2}}e^{i\frac{\omega}{2}t}\,\langle 0| + \frac{1}{\sqrt{2}}e^{i\frac{3\omega}{2}t}\,\langle 1|\right)\frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}\,|0\rangle\\ &= \frac{1}{2}e^{-i\omega t}\end{aligned}$$

where the last equality makes use of the eigenstates' orthogonality. With $\langle a,t\rangle$ known, we can now find the expectation values of position and momentum These are

$$\langle x,t\rangle = \sqrt{2}x_0\,\mathrm{Re}\,\langle a,t\rangle = \frac{x_0}{\sqrt{2}}\cos\omega t \qquad \text{and} \qquad \langle p,t\rangle = \sqrt{2}p_0\,\mathrm{Im}\,\langle a,t\rangle = -\frac{p_0}{\sqrt{2}}\sin\omega t$$

- Next, we confirm the validity of the Ehrenfest theorem.

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x,t\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{x_0}{\sqrt{2}}\cos\omega t\right) = -\frac{\omega x_0}{\sqrt{2}}\sin\omega \stackrel{?}{=} \frac{\langle p,t\rangle}{m} = -\frac{p_0}{\sqrt{2}}\sin\omega t$$

Comparing the equalities, canceling like terms and inserting the definition of p_0 and ω, we have

$$\omega x_0 \stackrel{?}{=} \frac{p_0}{m} = \frac{\hbar}{x_0 m} \implies \omega \stackrel{?}{=} \frac{h}{m x_0^2} = \frac{\hbar}{m}\frac{m\omega}{\hbar} = \omega$$

which satisfies the first part of the Ehrenfest theorem. To confirm the second part of the theorem, we compute

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(-\frac{p_0}{\sqrt{2}}\sin\omega t\right) = -\frac{p_0\omega}{\sqrt{2}}\cos\omega t \stackrel{?}{=} -k\,\langle x,t\rangle$$

The equality reduces to

$$p_0\omega \stackrel{?}{=} kx_0 \implies \frac{\hbar}{x_0}\omega = m\omega^2 x_0 \implies x_0^2 \stackrel{?}{=} \frac{\hbar}{m\omega}$$

The last equality leads to $\omega = \omega$, already shown above when confirming the first part of the Ehrenfest theorem.

- Finally, we compute the product $\Delta x(t)\Delta p(t)$. By definition,

$$\Delta x(t) = \sqrt{\langle x^2,t\rangle - \langle x,t\rangle^2} \qquad \text{and} \qquad \Delta p(t) = \sqrt{\langle p^2,t\rangle - \langle p,t\rangle^2}$$

First, we express $\langle x\rangle$ in terms of the annihilation operator a:

$$\begin{aligned}\left\langle x^2\right\rangle &= \left\langle\left[\frac{x_0}{\sqrt{2}}(a+a^\dagger)\right]^2\right\rangle = \frac{x_0^2}{2}\left\langle a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}\right\rangle\\ &= \frac{x_0^2}{2}\left\langle a^2 + 2a^\dagger a + a^{\dagger 2} + 1\right\rangle\end{aligned}$$

Where the last equality uses the identity $\left[a,a^\dagger\right] = 1 \implies aa^\dagger = 1 + a^\dagger a$. Continuing on, we have

$$\left\langle x^2\right\rangle = \frac{x_0^2}{2}\left(2\left\langle a^\dagger a\right\rangle + \left\langle a^2\right\rangle + \left\langle a^{\dagger 2}\right\rangle + 1\right) = x_0^2\left(\mathrm{Re}\left\langle a^2\right\rangle + \left\langle a^\dagger a\right\rangle + \tfrac{1}{2}\right)$$

Next, we express $\langle p^2 \rangle$ in terms of a with a similar procedure:

$$\begin{aligned}
\left\langle p^2 \right\rangle &= \left(\frac{p_0}{\sqrt{2}i}\right)^2 \left\langle (a-a^\dagger)^2 \right\rangle = -\frac{p_0}{2}\left\langle a^2 - aa^\dagger - a^\dagger a + a^{\dagger 2}\right\rangle \\
&= -\frac{p_0}{2}\left\langle a^2 - 2a^\dagger a - 1 + a^{\dagger 2}\right\rangle = p_0^2\left(-\operatorname{Re}\left\langle a^2\right\rangle + \left\langle a^\dagger a\right\rangle + \tfrac{1}{2}\right)
\end{aligned}$$

- Next, we find the expectation value $\langle a^2, t\rangle$:

$$\left\langle a^2, t\right\rangle = \langle \psi, t| \left(\frac{1}{\sqrt{2}}e^{-i\frac{\omega}{2}t}a^2\,|0\rangle + \frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}a^2\,|1\rangle\right)$$

Brief intermezzo to note that

$$a^2\,|0\rangle = a\,(a\,|0\rangle) = a\cdot 0 = 0 \qquad \text{and} \qquad a^2\,|1\rangle = a\,(a\,|1\rangle) = a\,|0\rangle = 0$$

With these identities in hand, we have

$$\left\langle a^2, t\right\rangle = \langle \psi, t|\cdot 0 = 0$$

- One more expectation value to go: $\langle a^\dagger a, t\rangle$

$$\begin{aligned}
\left\langle a^\dagger a, t\right\rangle &= \langle \psi, t| \left(\frac{1}{\sqrt{2}}e^{-i\frac{\omega}{2}t}a^\dagger a\,|0\rangle + \frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}a^\dagger a\,|1\rangle\right) = \langle \psi, t|\,\frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}\,|1\rangle \\
&= \left(\frac{1}{\sqrt{2}}e^{i\frac{\omega}{2}t}\,\langle 0| + \frac{1}{\sqrt{2}}e^{i\frac{3\omega}{2}t}\,\langle 1|\right)\frac{1}{\sqrt{2}}e^{-i\frac{3\omega}{2}t}\,|1\rangle = \frac{1}{2}
\end{aligned}$$

The derivation uses the identity $a^\dagger a\,|n\rangle = n\,|n\rangle$ and the eigenstates' orthogonality.

- We now have everything we need to find the product of uncertainties in x and p. Putting the pieces together, we have

$$\begin{aligned}
\left\langle x^2, t\right\rangle &= x_0^2\left(\operatorname{Re}\left\langle a^2\right\rangle + \left\langle a^\dagger a\right\rangle + \tfrac{1}{2}\right) = x_0^2\left(0 + \tfrac{1}{2} + \tfrac{1}{2}\right) = x_0^2 \\
\left\langle p^2, t\right\rangle &= p_0^2\left(-\operatorname{Re}\left\langle a^2\right\rangle + \left\langle a^\dagger a\right\rangle + \tfrac{1}{2}\right) = p_0^2\left(0 + \left\langle a^\dagger a\right\rangle + \tfrac{1}{2}\right) = p_0^2 \\
\langle x, t\rangle &= \sqrt{2}x_0\operatorname{Re}\langle a, t\rangle = \frac{x_0}{\sqrt{2}}\cos\omega t \\
\langle p, t\rangle &= \sqrt{2}p_0\operatorname{Im}\langle a, t\rangle = -\frac{p_0}{\sqrt{2}}\sin\omega t
\end{aligned}$$

The uncertainties $\Delta x(t)$ and Δp are then

$$\begin{aligned}
\left[\Delta x(t)\right]^2 &= \left\langle x^2, t\right\rangle - \langle x\rangle^2 = x_0^2 - \frac{x_0^2}{2}\cos^2\omega t = x_0^2\left(1 - \frac{\cos^2\omega t}{2}\right) \\
\left[\Delta p(t)\right]^2 &= \left\langle p^2, t\right\rangle - \langle p\rangle^2 = p_0^2 - \frac{p_0^2}{2}\sin^2\omega t = p_0^2\left(1 - \frac{\sin^2\omega t}{2}\right)
\end{aligned}$$

The product in uncertainties is

$$\begin{aligned}
\Delta x(t)\Delta p(t) &= x_0 p_0\sqrt{\left(1 - \frac{\cos^2\omega t}{2}\right)\left(1 - \frac{\sin^2\omega t}{2}\right)} \\
&= \hbar\sqrt{\frac{1}{2} + \frac{1}{4}\sin^2\omega t\cos^2\omega t} = \hbar\sqrt{\frac{1}{2} + \frac{1}{16}\sin^2 2\omega t}
\end{aligned}$$

In other words, the product of uncertainties oscillates in time between a minimum value of $\frac{\hbar}{\sqrt{2}}$ to a maximum value of $\frac{3\hbar}{4}$.

Take Two, Using the Heisenberg Approach

- We start with an expression for $\langle x, t\rangle$, using the Heisenberg approach

$$\langle x, t\rangle = \sqrt{2}x_0 \operatorname{Re} \langle \psi, 0|\, a(t) \,|\psi, 0\rangle$$

We start with the equation for the operator $a(t)$:

$$\dot{a}(t) = \frac{i}{\hbar}[H, a](t)$$

Making use of $\left[a, a^\dagger\right] = 1$ and $\left[a^\dagger, a\right] = -1$, the commutator $[H, a]$ is

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

and the equation for $a(t)$ reads

$$\begin{aligned}
&\dot{a}(t) = -i\omega a(t) \implies \frac{\mathrm{d}a}{a} = -i\omega\,\mathrm{d}t \implies \ln a(t) = -i\omega t + C\\
&a(t) = De^{-i\omega t}
\end{aligned}$$

We find the constant D with the initial condition $a(0) = a$, giving the final solution

$$a(t) = ae^{-i\omega t}$$

Inserting $a(t)$ into the expression $\langle x, t\rangle = \sqrt{2}x_0 \operatorname{Re} \langle \psi, 0|\, a(t) \,|\psi, 0\rangle$ gives

$$\langle x, t\rangle = \sqrt{2}x_0 \operatorname{Re} \langle \psi, 0|\, ae^{-i\omega t} \,|\psi, 0\rangle = \sqrt{2}x_0 \operatorname{Re}\left[e^{-i\omega t} \langle \psi, 0|\, a \,|\psi, 0\rangle\right]$$

This general result holds for any initial state $|\psi, 0\rangle$ of a particle in a harmonic potential. For our specific initial state, the expression reads

$$\langle \psi, 0|\, a \,|\psi, 0\rangle = \langle \psi, 0| \left(\frac{1}{\sqrt{2}}a\,|0\rangle + \frac{1}{\sqrt{2}}a\,|1\rangle\right)|\psi, 0\rangle = \langle \psi, 0| \frac{1}{\sqrt{2}}\,|0\rangle = \frac{1}{2}$$

The result for $\langle x, t\rangle$ then reads

$$\begin{aligned}
\langle x, t\rangle &= \sqrt{2}x_0 \operatorname{Re}\left[e^{-i\omega t} \langle \psi, 0|\, a \,|\psi, 0\rangle\right] = \sqrt{2}x_0 \operatorname{Re}\left[\frac{1}{2}e^{-i\omega t}\right]\\
&= \frac{x_0}{\sqrt{2}}\cos\omega t
\end{aligned}$$

which matches the result from the earlier Schrödinger approach.

1.6 Sixth Exercise Set

1.6.1 Theory: Coherent States of the Quantum Harmonic Oscillator

- The annihilation operator's eigenstates are called *coherent states* of the quantum harmonic oscillator's Hamiltonian. Coherent states $|\psi\rangle$ of a QHO satisfy the eigenvalue equation

$$a\,|\psi\rangle = \lambda\,|\psi\rangle\,, \qquad \lambda \in \mathbb{C}$$

Recall that a is not Hermitian, so the eigenvalue λ is in general complex. By convention, we make the potentially complex nature of λ explicit by writing

$$a\,|z\rangle = z\,|z\rangle$$

Where $|z\rangle$ is just a new notation for the coherent eigenstate and z is the corresponding eigenvalue.

- The next step is to find the coherent states' time evolution $|z, t\rangle$. One way to do this is to expand the coherent state in the QHO eigenstate basis $|n\rangle$ in the form

$$|z\rangle = \sum_n c_n |n\rangle$$

Inserting this expression for $|z\rangle$ in to the eigenvalue equation $a|z\rangle = z|z\rangle$ gives

$$a|z\rangle = z|z\rangle \implies \sum_n c_n a|n\rangle = \sum_n c_n z|n\rangle$$

Substituting in the annihilation operator's action $a|n\rangle = \sqrt{n}|n-1\rangle$ on the QHO eigenstates $|n\rangle$ leads to

$$\sum_{n=1}^{\infty} c_n \sqrt{n}|n-1\rangle = \sum_{n=0}^{\infty} c_n z|n\rangle$$

Note that n starts at 1 in the left sum because the annihilation operator eliminates the ground state $|0\rangle$. Keeping in mind the orthogonality of the eigenstates with different n, the above equality only holds if the coefficients of each $|n\rangle$ term in the left and right sums are equal, i.e.

$$c_{n+1}\sqrt{n+1} = c_n z \implies c_{n+1} = \frac{z}{\sqrt{n+1}} c_n$$

This is a recursive relation between the coefficients c_n of the eigenstate expansion of the coherent states. We can recognize the general form from the pattern in the first few terms:

$$\begin{aligned}
n = 0 &\implies c_1 = c_0 z \\
n = 1 &\implies c_2 = c_1 \frac{z}{\sqrt{2}} = c_0 \frac{z^2}{\sqrt{1\cdot 2}} \\
&\vdots \\
c_n &= \frac{z^n}{\sqrt{n!}} c_0
\end{aligned}$$

As long as we know c_0, we can find all c_n with the above expression. Returning to the expansion of the coherent $|z\rangle$, we have

$$|z\rangle = \sum_n c_n |n\rangle = c_0 \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle$$

- We find c_0 by requiring the coherent states are normalized:

$$1 \equiv \langle z|z\rangle = \left(c_0^* \sum_n \frac{{z^*}^n}{\sqrt{n!}} \langle n|\right)\left(c_0 \sum_m \frac{z^m}{\sqrt{m!}} |m\rangle\right)$$

We only have to evaluate one sum, since orthogonality of the QHO eigenstates means $\langle n|m\rangle = \delta_{nm}$. We then have

$$1 \equiv \langle z|z\rangle = |c_0|^2 \sum_n \frac{{z^*}^n z^n}{n!} = |c_0|^2 \sum_n \frac{|z|^{2n}}{n!} = |c_0|^2 e^{|z|^2} \equiv 1$$

Solving the last equality for c_0 gives $c_0 = e^{-\frac{|z|^2}{2}}$. We now have everything we need for the eigenfunction expansion of the coherent states. Putting the pieces together gives

$$|z\rangle = \sum_n c_n |n\rangle = c_0 \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle = e^{-\frac{|z|^2}{2}} \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle$$

- We now consider another way to write the coherent states $|z\rangle$ using creation operator's action on the QHO eigenstates:

$$
\begin{aligned}
a^\dagger |0\rangle &= |1\rangle \implies |1\rangle = a^\dagger |0\rangle \\
a^{\dagger|1\rangle} &= \sqrt{2}\,|2\rangle \implies |2\rangle = \frac{a^\dagger |1\rangle}{\sqrt{2}} = \frac{\left(a^\dagger\right)^2}{\sqrt{1\cdot 2}}\,|0\rangle \\
&\;\vdots \\
|n\rangle &= \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}\,|0\rangle
\end{aligned}
$$

Substituting in the expression for the QHO eigenstate $|n\rangle$ into the expansion of the coherent states $|z\rangle$ gives

$$
|z\rangle = \sum_n c_n |n\rangle = \sum_n \frac{z^n c_0}{\sqrt{n!}} \frac{\left(a^\dagger\right)^n}{\sqrt{n!}}\,|0\rangle = e^{-\frac{|z|^2}{2}} \sum_n \frac{z^n \left(a^\dagger\right)^n}{n!}\,|0\rangle = e^{-\frac{|z|^2}{2}} e^{z a^\dagger}\,|0\rangle
$$

In other words, the coherent states $|z\rangle$ and ground state $|0\rangle$ are related by the exponential operator $e^{za^\dagger}$ via

$$
|z\rangle = e^{-\frac{|z|^2}{2}} e^{z a^\dagger}\,|0\rangle
$$

- Next, we will find the time evolution $|z,t\rangle$ of the coherent states. This is

$$
|z,t\rangle = e^{-i\frac{E_n}{\hbar}t}\,|z\rangle = e^{-\frac{|z|^2}{2}} \sum_n \frac{z^n}{\sqrt{n!}} \left(e^{-i\omega(n+\frac{1}{2})t}\right)|n\rangle
$$

where we have substituted in the QHO's energy eigenvalues $E_n = \hbar\omega\big(n+\frac{1}{2}\big)$. Some rearranging of $|z,t\rangle$ leads to

$$
|z,t\rangle = e^{-i\frac{\omega}{2}t} e^{-\frac{|z|^2}{2}} \sum_n \frac{z^n e^{-i\omega n t}}{\sqrt{n!}}\,|n\rangle = e^{-i\frac{\omega}{2}t} e^{-\frac{|z|^2}{2}} \sum_n \frac{(z e^{-i\omega t})^n}{\sqrt{n!}}\,|n\rangle
$$

Next, a slight trick. Using $\left|ze^{-i\omega t}\right| = |z|\left|e^{-i\omega t}\right| = |z|$, we re-write the coefficient $e^{-\frac{|z|^2}{2}}$ to get

$$
|z,t\rangle = e^{-i\frac{\omega}{2}t} e^{-\frac{\left|ze^{-i\omega t}\right|^2}{2}} \sum_n \frac{(z e^{-i\omega t})^n}{\sqrt{n!}}\,|n\rangle
$$

Except for the factor $e^{-i\frac{\omega}{2}t}$, this expression has the same form as the earlier result

$$
|z\rangle = e^{-\frac{|z|^2}{2}} \sum_n \frac{z^n}{\sqrt{n!}}\,|n\rangle
$$

with z replaced by $ze^{-i\omega t}$. We use this relationship to write

$$
|z,t\rangle = e^{-i\frac{\omega}{2}t}\left|ze^{-i\omega t}\right\rangle
$$

- Finally, an approach to finding the time evolution $|z,t\rangle$ in the Heisenberg picture. We write $|z,t\rangle$ in terms of the time evolution operator and use the earlier relationship between $|z\rangle$ and $|0\rangle$ via the creation operator $a^\dagger$ to get

$$
|z,t\rangle = e^{-i\frac{H}{\hbar}t}\,|z\rangle = e^{-i\frac{H}{\hbar}t}\left(e^{-\frac{|z|^2}{2}} e^{za^\dagger}\,|0\rangle\right) = e^{-\frac{|z|^2}{2}} e^{-i\frac{H}{\hbar}t} e^{za^\dagger} e^{i\frac{H}{\hbar}t} e^{-i\frac{H}{\hbar}t}\,|0\rangle
$$

The three terms $e^{-i\frac{H}{\hbar}t}e^{za^\dagger}e^{i\frac{H}{\hbar}t}$, with the exponent written as a Taylor series, are

$$\begin{aligned}
e^{-i\frac{H}{\hbar}t}e^{za^\dagger}e^{i\frac{H}{\hbar}t} &= e^{-i\frac{H}{\hbar}t}\left(\sum_n \frac{(za^\dagger)^n}{n!}\right)e^{i\frac{H}{\hbar}t} = \sum_n \frac{z^n}{n!}e^{-i\frac{H}{\hbar}t}(a^\dagger)^n e^{i\frac{H}{\hbar}t} \\
&= \sum_n \frac{z^n}{n!}\left[e^{-i\frac{H}{\hbar}t}a^\dagger e^{i\frac{H}{\hbar}t}e^{-i\frac{H}{\hbar}t}a^\dagger e^{i\frac{H}{\hbar}t}\cdots e^{-i\frac{H}{\hbar}t}a^\dagger e^{i\frac{H}{\hbar}t}\right] \\
&= \sum_n \frac{z^n}{n!}\left(e^{-i\frac{H}{\hbar}t}a^\dagger e^{i\frac{H}{\hbar}t}\right)^n
\end{aligned}$$

Recall that in the Heisenberg approach the time evolution of an operator $\mathcal{O}$ reads $\mathcal{O}(t) = e^{i\frac{H}{\hbar}t}\mathcal{O}e^{-i\frac{H}{\hbar}t}$. Applied to our above expression (note the reversed roles of the time evolution operators), we see

$$e^{-i\frac{H}{\hbar}t}e^{za^\dagger}e^{i\frac{H}{\hbar}t} = \sum_n \frac{z^n}{n!}\left(a^\dagger(-t)\right)^n = e^{za^\dagger(-t)}$$

The initial expression for $|z,t\rangle$ in the Heisenberg picture then simplifies to

$$|z,t\rangle = e^{-\frac{|z|^2}{2}}e^{za^\dagger(-t)}e^{-i\frac{H}{\hbar}t}|0\rangle = e^{-\frac{|z|^2}{2}}e^{za^\dagger(-t)}e^{-i\frac{\omega}{2}t}|0\rangle$$

- Next, we find an expression for $a^\dagger(-t)$. In the Heisenberg approach, this is

$$a^\dagger(-t) = e^{-i\frac{H}{\hbar}t}a^\dagger e^{i\frac{H}{\hbar}t} = \left[e^{-i\frac{H}{\hbar}t}ae^{i\frac{H}{\hbar}t}\right]^\dagger = \left[a(-t)\right]^\dagger$$

Using the relationship $a(t) = ae^{-i\omega t}$ from the previous exercise set, we finally have

$$a^\dagger(-t) = \left[a(-t)\right]^\dagger = \left[ae^{i\omega t}\right]^\dagger = a^\dagger e^{-i\omega t}$$

Substituting the expression for $a^\dagger(-t)$ into the time evolution $|z,t\rangle$ to get

$$|z,t\rangle = e^{-\frac{|z|^2}{2}}e^{ze^{-i\omega t}a^\dagger}e^{-i\frac{\omega}{2}t}|0\rangle = e^{-i\frac{\omega}{2}t}e^{-\frac{\left|ze^{-i\omega t}\right|^2}{2}}e^{ze^{-i\omega t}a^\dagger}|0\rangle$$

Recall that, like before in the Schrödinger approach, the equality $|z|^2 = \left|ze^{-i\omega t}\right|^2$ allows us to introduce the phase factor $e^{-i\omega t}$ into the exponent of $e^{-\frac{|z|^2}{2}}$. Note the similarity between this last result for $|z,t\rangle$ to the initial expression

$$|z,t\rangle = e^{-i\frac{H}{\hbar}t}e^{-\frac{|z|^2}{2}}e^{za^\dagger}|0\rangle$$

Aside from the factor $e^{-i\frac{\omega}{2}t}$, the expressions are the same, just with z shifted to $ze^{-i\omega t}$. This allows us to write

$$|z,t\rangle = e^{-i\frac{\omega}{2}t}e^{-\frac{\left|ze^{-i\omega t}\right|^2}{2}}e^{ze^{-i\omega t}a^\dagger}|0\rangle = e^{-i\frac{\omega}{2}t}\left|ze^{-i\omega t}\right\rangle$$

in agreement with the earlier result using the Schrödinger approach.

- Next, we want to get a better sense for the behavior of the wave function $|z,t\rangle$. From the last exercise set, we know the following expressions for any state of quantum harmonic oscillator:

$$\langle x\rangle = \sqrt{2}x_0\,\mathrm{Re}\,\langle a\rangle \qquad \langle p\rangle = \sqrt{2}p_0\,\mathrm{Im}\,\langle a\rangle$$
$$\left\langle x^2\right\rangle = x_0^2\left(\left\langle a^\dagger a\right\rangle + \mathrm{Re}\left\langle a^2\right\rangle \tfrac{1}{2}\right) \qquad \left\langle p^2\right\rangle = p_0^2\left(\left\langle a^\dagger a\right\rangle - \mathrm{Re}\left\langle a^2\right\rangle \tfrac{1}{2}\right)$$

Next, using the eigenvalue equation $a\,|z\rangle = z\,|z\rangle$ for coherent states, we have

$$\langle z|\,(a^\dagger)^n a^m\,|z\rangle = \langle a^n z|a^m z\rangle = \langle z^n z|z^m z\rangle = {z^*}^n z^m$$

We will use this expression to evaluate the expectation values of x and p above. Note the difference between z as an eigenvalue and $|z\rangle$ as a coherent state.

- Next, using the just-derived identity $\langle z|\,(a^\dagger)^n a^m\,|z\rangle = {z^*}^n z^m$, the expectation value $\langle a\rangle$ is

$$\langle a\rangle = \langle 1\cdot a\rangle = \left\langle (a^*)^0 a\right\rangle = {z^*}^0 z^1 = 1\cdot z^1 = z$$

Using $\langle a\rangle = z$, the expectation values of x and p are

$$\langle x\rangle = \sqrt{2}x_0 \operatorname{Re} z \qquad \text{and} \qquad \langle p\rangle = \sqrt{2}p_0 \operatorname{Im} z$$

To find $\left\langle x^2\right\rangle$ and $\left\langle p^2\right\rangle$, we first have to find $\left\langle a^\dagger a\right\rangle$ and $\left\langle a^2\right\rangle$. These are

$$\left\langle a^\dagger a\right\rangle = |z|^2 \qquad \text{and} \qquad \left\langle a^2\right\rangle = z^2$$

$\left\langle x^2\right\rangle$ and $\left\langle p^2\right\rangle$ are then

$$\left\langle x^2\right\rangle = x_0^2\left(|z|^2 + \operatorname{Re} z^2 + \tfrac{1}{2}\right) \qquad \text{and} \qquad \left\langle p^2\right\rangle = p_0^2\left(|z|^2 - \operatorname{Re} z^2 + \tfrac{1}{2}\right)$$

- Next, using the general complex number identity $\operatorname{Re} z^2 = \frac{z^2 + {z^*}^2}{2}$, we write

$$|z|^2 + \operatorname{Re} z^2 = |z|^2 + \frac{z^2 + {z^*}^2}{2} = \frac{1}{2}\big(z + z^*\big)^2 = \frac{1}{2}(2\operatorname{Re} z)^2 = 2\operatorname{Re}^2 z$$

which, substituted into $\left\langle x^2\right\rangle$, gives

$$\left\langle x^2\right\rangle = x_0^2\left(|z|^2 + \operatorname{Re} z^2 + \tfrac{1}{2}\right) = x_0^2\left(2\operatorname{Re}^2 z + \tfrac{1}{2}\right)$$

a similar procedure for $\left\langle p^2\right\rangle$ gives

$$\left\langle p^2\right\rangle = p_0^2\left[-\tfrac{1}{2}\big(z - z^*\big) + \tfrac{1}{2}\right] = p_0^2\left(2\operatorname{Im}^2 z + \tfrac{1}{2}\right)$$

- Next, the uncertainties Δx and Δp are

$$\begin{aligned}
\big(\Delta x\big)^2 &= \left\langle x^2\right\rangle - \langle x\rangle^2 = x_0^2\left(2\operatorname{Re}^2 z + \tfrac{1}{2}\right) - \left(\sqrt{2}x_0\operatorname{Re} z\right)^2 = \frac{x_0^2}{2}\\
\big(\Delta p\big)^2 &= \left\langle p^2\right\rangle - \langle p\rangle^2 = p_0^2\left(\tfrac{1}{2} + 2\operatorname{Im}^2 z\right) - \left(\sqrt{2}p_0\operatorname{Im} z\right)^2 = \frac{p_0^2}{2}
\end{aligned}$$

The product of uncertainties, recalling the definition $p_0 = \frac{\hbar}{x_0}$, is

$$\Delta x\Delta p = \sqrt{\frac{x_0^2}{2}\frac{p_0^2}{2}} = \frac{x_0 p_0}{2} = \frac{\hbar}{2}$$

Note that the product of uncertainties takes the minimum possible value $\frac{\hbar}{2}$, meaning a coherent state $|z\rangle$ of the QHO must be a Gaussian wave packet.

- Recall the general form of a Gaussian wave packet is

$$\psi(x) = \frac{1}{\sqrt[4]{2\pi\sigma^2}} \exp\left(-\frac{(x - \langle x \rangle)^2}{4\sigma^2}\right) e^{i\frac{\langle p \rangle}{\hbar}x}$$

For the coherent state $|z\rangle$, substituting in the values of $\langle x \rangle$, $\langle p \rangle$ and $\sigma^2 \equiv \langle x^2 \rangle$, the Gaussian wave packet reads

$$\psi_z(x) = \frac{1}{\sqrt[4]{\pi x_0^2}} \exp\left[-\frac{\left(x - \sqrt{2}x_0 \operatorname{Re} z\right)^2}{2x_0^2}\right] e^{i\frac{\sqrt{2}p_0 \operatorname{Im} z}{\hbar}x}$$

- Finally, we will examine two more properties of the coherent states of a QHO: the expectation values of the Hamiltonian H. First, recall the Hamiltonian can be written in terms of a and $a^\dagger$ as

$$H = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right)$$

We evaluate this with the help of the earlier identity $\langle z| (a^\dagger)^n a^m |z\rangle = z^{*^n} z^m$. Applied to $a^\dagger a$, we have

$$\langle H \rangle = \frac{\hbar\omega}{2} + \hbar\omega\langle a^\dagger a\rangle = \frac{\hbar\omega}{2} + \hbar\omega z^* z = \frac{\hbar\omega}{2} + \hbar\omega|z|^2$$

For the expectation value $\langle H^2 \rangle$ we first write H in terms of a and $a^\dagger$:

$$H^2 = \hbar^2\omega^2\left(a^\dagger a a^\dagger a + a^\dagger a + \tfrac{1}{4}\right)$$

To simplify $a^\dagger a a^\dagger a$ we use the commutator identity

$$\left[a^\dagger, a\right] = -1 \implies aa^\dagger = 1 + a^\dagger a$$

Substituting $aa^\dagger = 1 + a^\dagger a$ into H^2 and an intermediate step of algebra gives

$$H^2 = \hbar^2\omega^2\left(a^{\dagger^2} a^2 + 2a^\dagger a + \tfrac{1}{4}\right)$$

We again use the earlier identity $\langle z| (a^\dagger)^n a^m |z\rangle = z^{*^n} z^m$ to get

$$\langle H^2 \rangle = \hbar^2\omega^2\left(z^{*^2} z^2 + 2z^* z + \tfrac{1}{4}\right) = \hbar^2\omega^2\left(|z|^4 + 2|z|^2 + \tfrac{1}{4}\right)$$

energy uncertainty is

$$\begin{aligned}(\Delta H)^2 &= \langle H^2 \rangle - \langle H \rangle^2 = \hbar^2\omega^2\left(|z|^4 + 2|z|^2 + \tfrac{1}{4}\right) - \left(\frac{\hbar\omega}{2} + \hbar\omega|z|^2\right)^2 \\ &= \hbar^2\omega^2|z|^2 \implies \Delta H = \hbar\omega|z|\end{aligned}$$

- Next, note the ratio

$$\frac{\Delta H}{\langle H \rangle} = \frac{\hbar\omega|z|}{\hbar\omega\left(|z|^2 + \frac{1}{2}\right)} \approx \frac{1}{|z|}, \quad |z| \gg 1 \quad \implies \quad \lim_{|z|\to\infty} \frac{\Delta H}{\langle H \rangle} = 0$$

In other words, the relative uncertainty in energy $\frac{\Delta H}{\langle H \rangle}$ approaches zero for large $|z|$.

We want a better understanding of what $|z| \gg 1$ means. To do this, we first examine the earlier expressions for a QHO coherent state:

$$\langle x \rangle = \sqrt{2} x_0 \operatorname{Re} z \qquad \text{and} \qquad \langle x, t \rangle = \sqrt{2} x_0 \operatorname{Re} \left\{ z e^{-i\omega t} \right\}$$

If we write the complex number z in the polar form $z = |z| e^{i\delta}$, $\langle x, t \rangle$ becomes

$$\langle x, t \rangle = \sqrt{2} x_0 \operatorname{Re} \left\{ z e^{i\delta - i\omega t} \right\} = \sqrt{2} x_0 |z| \cos(\omega t - \delta)$$

In other words, large $|z|$ means a large amplitude of oscillation in the time-dependent expectation value $\langle x, t \rangle$.

1.6.2 Harmonic Oscillator in an Electric Field

Consider a particle of mass m and charge q at the equilibrium position x_0 of a spring with spring constant k constrained to oscillate along the x axis. At time $t = 0$, we turn on an external electric field $\mathcal{E}$ in the positive x direction. Solve for the particle's motion using quantum mechanics.

- First, we find the classical solution with Newton's law to get a feel for the solution. Newton's law reads:

  $$m\ddot{x} = -kx + q\mathcal{E}$$

  Turning the field exerts a force on the particle in the x direction, moving the equilibrium position to $\tilde{x}_0 = x_0 + x_1 > x_0$. The particle starts at the far left amplitude x_0 and oscillates about the new equilibrium position $\tilde{x}_0$ with amplitude x_1.

  Placing the origin at $x_0 \equiv 0$, the initial conditions are $x(0) = 0$ and $\dot{x}(0) = 0$. The solution is

  $$x(t) = x_1(1 - \cos \omega t) \qquad \text{where} \qquad \omega = \sqrt{\frac{k}{m}}, \quad x_1 = \frac{q\mathcal{E}}{k}$$

- Next, the quantum mechanical picture. The particle's Hamiltonian is

  $$H(t) = \begin{cases} \frac{p^2}{2m} + \frac{1}{2}kx^2 & t < 0 \\ \frac{p^2}{2m} + \frac{1}{2}kx^2 - q\mathcal{E}x & t > 0 \end{cases}$$

  Note that turning on the field adds the potential energy term $-q\mathcal{E}x$ to the initial Hamiltonian.

  Notation: all quantities for $t > 0$, after the field is turned on, will be written with a tilde.

- In the classical picture, the particle takes the initial position $x(0) = 0$. This doesn't carry over in quantum mechanics—specifying an exact position violates the uncertainty principle. Instead, we place the particle in the harmonic oscillator's ground state: $|\psi, 0\rangle = |0\rangle$ where $H|0\rangle = \frac{1}{2}\hbar\omega|0\rangle$. Our goal will be to find the time-dependent wave function $|\psi, t\rangle$ and then compute the position expectation value $\langle x, t \rangle$.

- Let's begin! First, we expand the electric field Hamiltonian to a perfect square

  $$\tilde{H} = \frac{p^2}{2m} + \frac{k}{2}\left(x - \frac{e\mathcal{E}}{k}\right)^2 - \frac{1}{2}k\left(\frac{q\mathcal{E}}{k}\right)^2 = \frac{p^2}{2m} + \frac{k}{2}(x - x_1)^2 - \frac{1}{2}kx_1^2$$

Where we have substituted in the amplitude $x_1 = \frac{q\mathcal{E}}{k}$ from the classical solution. Next, we denote the post-field potential

$$\tilde{V}(x) = \frac{k}{2}(x - x_1)^2 - \frac{1}{2}kx_1^2$$

Note that while the pre-field potential $V(x) = \frac{1}{2}kx^2$ has its minimum at $(0,0)$, the post-field potential $\tilde{V}(x)$'s minimum is shifted to $\left(x_1, -\frac{1}{2}kx_1^2\right)$. With this shift of the equilibrium position in mind, we introduce new coordinates

$$\tilde{x} = x - x_1 \qquad \text{and} \qquad \tilde{p} = -i\hbar\frac{\mathrm{d}}{\mathrm{d}\tilde{x}} = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x} = p$$

The Hamiltonian $\tilde{H}$ then reads

$$\tilde{H} = \frac{\tilde{p}^2}{2m} + \frac{1}{2}k\tilde{x}^2 - \frac{1}{2}kx_1^2$$

- The Hamiltonian's shifted annihilation operator is

$$\tilde{a} = \frac{1}{\sqrt{2}}\left(\frac{\tilde{x}}{x_0} + i\frac{\tilde{p}}{p_0}\right)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $p_0 = \frac{\hbar}{x_0}$. The difference between $\tilde{a}$ and the unshifted a is

$$\tilde{a} - a = -\frac{x_1}{\sqrt{2}x_0} \implies \tilde{a} = a - \frac{x_1}{\sqrt{2}x_0}$$

- Recall the annihilation operator actions on the quantum harmonic oscillator's eigenstates as $a\left|n\right\rangle = \sqrt{n}\left|n-1\right\rangle$ and $a\left|0\right\rangle = 0$. In our case, the shifted annihilation operator $\tilde{a}$ acts on our problem's initial state $\left|\psi,0\right\rangle = \left|0\right\rangle$ as

$$\tilde{a}\left|\psi,0\right\rangle = \left(a - \frac{x_1}{\sqrt{2}x_0}\right)\left|0\right\rangle = 0 - \frac{x_1}{\sqrt{2}x_0}\left|0\right\rangle \implies \tilde{a}\left|\psi,0\right\rangle = -\frac{x_1}{\sqrt{2}x_0}\left|\psi,0\right\rangle$$

In other words, our initial state $\left|\psi,0\right\rangle$ is an eigenstate of the shifted annihilation operator $\tilde{a}$ with the eigenvalue $-\frac{x_1}{\sqrt{2}x_0}$. This means the initial state is a coherent state of the annihilation operator $\tilde{a}$, so we can use the results from the theory section on coherent states.

- From the theory section, an coherent state $\left|\psi,0\right\rangle$ satisfying $a\left|\psi,0\right\rangle = z\left|\psi,0\right\rangle$ with eigenvalue z evolves in time as

$$\left|\psi,t\right\rangle = e^{-\frac{\omega}{2}t}\left|ze^{-i\omega t}\right\rangle$$

where the eigenvalue z changes with time as $z(t) = ze^{-i\omega t}$. Meanwhile, the position expectation value is

$$\langle x\rangle = \sqrt{2}x_0 \operatorname{Re} z$$

In our case, the time-dependent expectation value of the shifted position $\tilde{x}$ is thus

$$\langle\tilde{x},t\rangle = \sqrt{2}x_0 \operatorname{Re} z(t) = \sqrt{2}x_0 \operatorname{Re}\left\{-\frac{x_1}{\sqrt{2}x_0}e^{-i\omega t}\right\} = -x_1\cos\omega t$$

The unshifted position is $x = x_1 + \tilde{x}$, which implies

$$\langle x,t\rangle = x_1 - x_1\cos\omega t = x_1(1 - \cos\omega t)$$

in agreement with the classical result $x(t) = x_1(1 - \cos\omega t)$.

1.7 Seventh Exercise Set

1.7.1 Theory: Two-Dimensional Harmonic Oscillator

- We generalize the harmonic oscillator to two dimensions by introducing the vector operators

$$\boldsymbol{r} = (x, y) \qquad \text{and} \qquad \boldsymbol{p} = (p_x, p_y) = \left(-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}\right) = -i\hbar\boldsymbol{\nabla}$$

We write the oscillator's Hamiltonian as

$$H = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 = \frac{p_x^2}{2m} + \frac{1}{2}k_x x^2 + \frac{p_y^2}{2m} + \frac{1}{2}k_y y^2 \equiv H_x + H_y$$

In other words, we can write the two-dimensional Hamiltonian as the sum of two one-dimensional Hamiltonians corresponding to motion in the x and y directions.

- We want to solve the stationary Schrödinger equation

$$H\psi(x, y) = E\psi(x, y)$$

The equation can be solved with separation of variables because the two-dimensional Hamiltonian can be decomposed into the sum of one-dimensional x and y Hamiltonians. We make this separation explicit by defining

$$H_x\psi_{n_x} = E_{n_x}\psi_{n_x}(x) \qquad \text{where} \qquad E_{n_x} = \hbar\omega_x\big(n_x + \tfrac{1}{2}\big), \quad \omega_x = \sqrt{\frac{k_x}{m}}$$

$$H_y\psi_{n_y} = E_{n_y}\psi_{n_y}(y) \qquad \text{where} \qquad E_{n_y} = \hbar\omega_y\big(n_y + \tfrac{1}{2}\big), \quad \omega_y = \sqrt{\frac{k_y}{m}}$$

for $n_x, n_y = 0, 1, 2, \ldots$ and then writing

$$H\psi(x, y) = E\psi(x, y) \to H\psi_{n_x}(x)\psi_{n_y}(y) = (E_{n_x} + E_{n_y})\psi_{n_x}(x)\psi_{n_y}(y)$$

- In terms of the annihilation and creation operators, the Hamiltonian reads

$$H = H_x + H_y = \hbar\omega_x\big(a_x^\dagger a_x + \tfrac{1}{2}\big) + \hbar\omega_y\big(a_y^\dagger a_y + \tfrac{1}{2}\big)$$

where the annihilation and creation operators are defined as

$$a_x = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p_x}{p_{0_x}}\right) \qquad \text{where} \qquad x_0 = \sqrt{\frac{\hbar}{m\omega_x}}, \quad p_{0_x} = \frac{\hbar}{x_0}$$

$$a_y = \frac{1}{\sqrt{2}}\left(\frac{y}{y_0} + i\frac{p_y}{p_{0_y}}\right) \qquad \text{where} \qquad y_0 = \sqrt{\frac{\hbar}{m\omega_y}}, \quad p_{0_y} = \frac{\hbar}{y_0}$$

With the annihilation and creation operators defined, we write

$$H_x\left|n_x\right\rangle = \hbar\omega_x\big(n_x + \tfrac{1}{2}\big)\left|n_x\right\rangle \qquad \text{and} \qquad H_y\left|n_y\right\rangle = \hbar\omega_y\big(n_y + \tfrac{1}{2}\big)\left|n_y\right\rangle$$

And for the two-dimensional Hamiltonian we write separation of variables as

$$H\left|n_x\right\rangle\left|n_y\right\rangle = \big[\hbar\omega_x\big(n_x + \tfrac{1}{2}\big) + \hbar\omega_y\big(n_y + \tfrac{1}{2}\big)\big]\left|n_x\right\rangle\left|n_y\right\rangle$$

A slightly shorter notation for the same expression reads

$$H\left|n_x n_y\right\rangle = \big[\hbar\omega_x\big(n_x + \tfrac{1}{2}\big) + \hbar\omega_y\big(n_y + \tfrac{1}{2}\big)\big]\left|n_x n_y\right\rangle$$

A Few Special Cases

- Consider the degenerate case with $k_x > 0$ and $k_y = 0$. In this case the y Hamiltonian has only a kinetic term:

$$H_x = \frac{p_x^2}{2m} + \frac{1}{2}k_x x^2 \qquad \text{and} \qquad H_y = \frac{p_y^2}{2m}$$

  In this case the y Hamiltonian's eigenfunctions are simply plane waves:

$$H_y e^{i\kappa_y y} = \frac{\hbar^2 \kappa_y^2}{2m} e^{i\kappa_y y} \qquad \text{or} \qquad H_y \left|\kappa_y\right\rangle = \frac{\hbar^2\kappa_y^2}{2m}\left|\kappa_y\right\rangle$$

  We would then solve the eigenvalue equation

$$H\left|n_x\kappa_y\right\rangle = \left[\hbar\omega_2\big(n_x + \tfrac{1}{2}\big) + \frac{\hbar^2\kappa_y^2}{2m}\right]\left|n_x\kappa_y\right\rangle$$

- Next, if both spring constants are zero with $k_x = k_y = 0$ (i.e. a free particle in two dimensions) we have the purely kinetic Hamiltonian $H = \frac{\boldsymbol{p}^2}{2m}$. Both the x and y eigenfunctions are plane waves

$$H_x e^{i\kappa_x x} = \frac{\hbar^2\kappa_x^2}{2m} e^{i\kappa_x x} \qquad \text{and} \qquad H_y e^{i\kappa_y y} = \frac{\hbar^2\kappa_y^2}{2m} e^{i\kappa_y y}$$

  and we solve the equation

$$H\left|\kappa_x\kappa_y\right\rangle = \left[\frac{\hbar^2\kappa_x^2}{2m} + \frac{\hbar^2\kappa_y^2}{2m}\right]\left|\kappa_x\kappa_y\right\rangle \qquad \text{or} \qquad H\left|\boldsymbol{\kappa}\right\rangle = \frac{\hbar^2\boldsymbol{\kappa}^2}{2m} = \left|\boldsymbol{\kappa}\right\rangle$$

  where $\boldsymbol{\kappa} = (\kappa_x, \kappa_y)$.

- Finally, we consider the case $k_x = k_y \equiv k > 0$ when both spring constants are equal. The potential then reads

$$V(\boldsymbol{r}) = \frac{1}{2}k(x^2 + y^2) = \frac{1}{2}kr^2$$

  Note that the potential depends only on the distance r from the origin; such an oscillator is called *isotropic*.

  Because $k_x = k_y \equiv k$ we have $\omega_x = \omega_y \equiv \omega = \sqrt{\frac{k}{m}}$. The stationary Schrödinger then reads

$$H\left|n_x n_y\right\rangle = \hbar\omega(n_x + n_y + 1)\left|n_x n_y\right\rangle$$

  The system's lowest possible energy occurs for $n_x = n_y = 0$, where the stationary Schrödinger equation reads $H\left|00\right\rangle = \hbar\omega\left|00\right\rangle$. This is the ground state, and the energy $E_{00} = \hbar\omega$ is called the zero-point energy.

  The first two excited states are

$$H\left|10\right\rangle = \hbar\omega\left|10\right\rangle \qquad \text{and} \qquad H\left|01\right\rangle = \hbar\omega\left|01\right\rangle$$

  Note that the first excited states is doubly degenerate—two linearly independent eigenfunctions $\left|10\right\rangle$ and $\left|01\right\rangle$ have the same energy. In general, the nth excited state of a 2D isotropic harmonic oscillator has degeneracy $n + 1$.

Theory: The z Component of Angular Momentum

- Eigenstates $|\psi\rangle$ of the z component of angular momentum operator L_z satisfy

$$L_z |\psi\rangle = \lambda |\psi\rangle$$

The operator L_z can be written

$$L_z = xp_y - yp_x = -\hbar \frac{\partial}{\partial \phi}$$

where ϕ is the azimuthal angle in the spherical coordinate system. Using the definition $L_z = -\hbar \frac{\partial}{\partial \phi}$ in spherical coordinates, the eigenvalue equation in coordinate notation reads

$$-i\hbar\psi'(\phi) = \lambda\psi(\phi)$$

Separating variables and integrating the equation gives

$$\ln \psi = \frac{i\lambda}{\hbar}\phi + C \implies \psi(\phi) = \tilde{C} e^{i\frac{\lambda}{\hbar}\phi}$$

To satisfy periodicity over a full rotation of 2π, we require $\psi(\phi + 2\pi) = \psi(\phi)$, which implies the quantization

$$\frac{\lambda}{\hbar} = m; \qquad m \in \mathbb{Z} \implies \psi(\phi) = \tilde{C} e^{im\phi}$$

We find the integration constant $\tilde{C}$ with the normalization condition

$$1 \equiv \int_0^{2\pi} \psi^*(\phi)\psi(\phi)\,\mathrm{d}\phi = 2\pi \left|\tilde{C}\right|^2 \implies \tilde{C} = \frac{1}{\sqrt{2\pi}}$$

The eigenfunctions of the angular momentum operator L_z are thus

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \qquad m \in \mathbb{Z}$$

In Dirac notation, the eigenfunctions are written simply $|m\rangle$, where the reference to the angular momentum operator is usually clear from context.

Using the relationship $\lambda = hm$, the eigenvalue equation in Dirac notation reads

$$L_z |\psi\rangle = m\hbar |\psi\rangle$$

1.7.2 Two-Dimensional Isotropic Harmonic Oscillator

Consider a two-dimensional isotropic harmonic oscillator. Within the subspace of energy eigenstates with energy $E = 2\hbar\omega$, find those states that are also eigenstates of the z-component of angular momentum L_z.

- The energy $E = 2\hbar\omega$ corresponds to the isotropic oscillator's first two excited states $|10\rangle$ and $|01\rangle$. These states have degeneracy two, meaning the subspace is spanned by two linearly independent states. The subspace is formed of all normalized linear combinations of $|01\rangle$ and $|10\rangle$, i.e. all $|\psi\rangle$ for which

$$|\psi\rangle = \alpha |10\rangle + \beta |01\rangle, \qquad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1$$

The Hamiltonian acts on $|\psi\rangle$ as

$$
\begin{aligned}
H|\psi\rangle &= \alpha H|10\rangle + \beta H|01\rangle = \alpha 2\hbar\omega|10\rangle + \beta 2\hbar\omega|01\rangle \\
&= 2\hbar\omega\big(\alpha|10\rangle + \beta|01\rangle\big) = 2\hbar\omega|\psi\rangle
\end{aligned}
$$

Evidently, ψ is an eigenfunction of H with energy eigenvalue $2\hbar\omega$. We are interested in ψ that are also eigenfunctions of L_z, which must satisfy the eigenvalue equation

$$
L_z|\psi\rangle = m\hbar|\psi\rangle
$$

- It is possible to find functions that are simultaneously eigenfunctions of two operators if the two operators commute. Applied to our problem, if we show that H and L_z commute, we can be sure there exist functions that are eigenfunctions of both H and L_z. In other words, we want to show our problem is solvable by proving $\big[H, L_z\big] = 0$. We will first write the Hamiltonian in polar coordinates:

$$
H = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}kr^2 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}kr^2 = -\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right] + \frac{1}{2}kr^2
$$

Using the definition of L_z in polar coordinates, the commutator reads

$$
\begin{aligned}
\big[H, L_z\big] &= \left[-\frac{\hbar^2}{2m}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right] + \frac{1}{2}kr^2, -i\hbar\frac{\partial}{\partial\phi}\right] \\
&= \left[-\frac{\hbar^2}{2mr^2}\frac{\partial^2}{\partial\phi^2}, -i\hbar\frac{\partial}{\partial\phi}\right] = 0
\end{aligned}
$$

The entire proof rests on the commutativity of second derivatives, i.e.

$$
\frac{\partial^2}{\partial\phi\partial r} = \frac{\partial^2}{\partial r\partial\phi} \qquad \text{and} \qquad \frac{\partial^2}{\partial\phi^2}\frac{\partial}{\partial\phi} = \frac{\partial}{\partial\phi}\frac{\partial^2}{\partial\phi^2}
$$

The derivatives with respect to ϕ then cancel the r-dependent terms in the Hamiltonian. All we did here is show that eigenfunctions solving our problem exist in the first place by showing H and L_z commute.

- To actually solve the problem, we will take both a heuristic and a formal approach. We start with a heuristic approach. From the introductory theory section, the eigenfunctions solving $H|10\rangle = 2\hbar\omega|10\rangle$ and $H|01\rangle = 2\hbar\omega|01\rangle$ can be written in the separated form

$$
\psi_{10}(x, y) = \psi_1(x)\psi_0(y) \qquad \text{and} \qquad \psi_{01}(x, y) = \psi_0(x)\psi_1(y)
$$

Next, recall the annihilation operator action on the ground state produces

$$
a|0\rangle = 0|0\rangle
$$

In other words, $|0\rangle$ is an eigenstate of the annihilation operator (i.e. a coherent state) with eigenvalue $z = 0$. From the previous exercise set, we know that the eigenfunctions of coherent states are Gaussian wave packets. If $z = 0$, then $\langle x\rangle = 0$ and $\langle p\rangle = 0$, and the wavefunction would read

$$
\psi_0(x) = \frac{1}{\sqrt[4]{\pi x_0^2}} e^{-\frac{x^2}{2x_0^2}}
$$

- We can get an expression for the first excited state $|1\rangle$ with the creation operator $a^\dagger |0\rangle = |1\rangle$. In the coordinate representation of the operator, this reads

$$\begin{aligned}\psi_1(x) = a^\dagger \psi_0(x) &= \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - i\frac{p}{p_0}\right)\psi_0(x) = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - \frac{\hbar}{p_0}\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x) \\ &= \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - x_0\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x)\end{aligned}$$

Applied to the Gaussian wave packet $\psi_0(x)$, we have

$$\begin{aligned}\psi_1(x) &= \frac{1}{\sqrt{2}}\frac{x}{x_0}\psi_0(x) - \frac{x_0}{\sqrt{2}}\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{1}{\sqrt[4]{\pi x_0^2}}e^{-\frac{x^2}{2x_0^2}}\right] = \frac{1}{\sqrt{2}}\frac{x}{x_0}\psi_0(x) + \frac{x_0}{\sqrt{2}}\frac{x}{x_0^2}\psi_0(x) \\ &= \frac{\sqrt{2}}{x_0}x\psi_0(x)\end{aligned}$$

We can then write the states ψ_{10} and ψ_{01} as

$$\begin{aligned}\psi_{10}(x,y) = \psi_1(x)\psi_0(y) &= \frac{\sqrt{2}}{x_0}x\psi_0(x)\psi_0(y) = \frac{\sqrt{2}}{x_0}\frac{x}{\sqrt{\pi x_0^2}}e^{-\frac{x^2}{2x_0^2}}e^{-\frac{y^2}{2x_0^2}} \\ &= \frac{\sqrt{2}}{x_0}\frac{x}{\sqrt{\pi x_0^2}}e^{-\frac{r^2}{2x_0^2}} = \frac{\sqrt{2}r\cos\phi}{x_0\sqrt{\pi x_0^2}}e^{-\frac{r^2}{2x_0^2}}\end{aligned}$$

and, analogously,

$$\psi_{01}(x,y) = \psi_0(x)\psi_1(y) = \frac{\sqrt{2}r\sin\phi}{x_0\sqrt{\pi x_0^2}}e^{-\frac{r^2}{2x_0^2}}$$

We ran out of time at this point; the problem is continued in the eight exercise set.

1.8 Eight Exercise Set

1.8.1 Two-Dimensional Isotropic Harmonic Oscillator (continued)

We left off in the previous exercise set having found the harmonic oscillator's states $\psi_{10}(x,y)$ and $\psi_{01}(x,y)$; these were

$$\psi_{10}(x,y) = \frac{\sqrt{2}r\cos\phi}{x_0\sqrt{\pi x_0^2}}e^{-\frac{r^2}{2x_0^2}} \qquad \text{and} \qquad \psi_{01}(x,y) = \frac{\sqrt{2}r\sin\phi}{x_0\sqrt{\pi x_0^2}}e^{-\frac{r^2}{2x_0^2}}$$

These are the two linearly independent states spanning the isotropic harmonic oscillator's subspace of eigenstates with energy $E = 2\hbar\omega$. Our next step is to find the linear combinations of ψ_{10} and ψ_{01} that are also eigenstates of the operator L_z.

- Recall that the eigenfunctions of L_z are

$$\psi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \qquad m \in \mathbb{Z}$$

Recall also the identities $\cos\phi + i\sin\phi = e^{i\phi}$ and $\cos\phi - i\sin\phi = e^{-i\phi}$.

- Comparing these identities to the definitions of ψ_{10}, ψ_{01} and $\psi_m(\phi)$, we can construct the L_z eigenstate with $m = 1$ via

$$|m=1\rangle = \frac{1}{\sqrt{2}}\big(\,|10\rangle + i\,|01\rangle\,\big)$$

where the $\frac{1}{\sqrt{2}}$ term ensures the state is normalized. To confirm the state $|m=1\rangle$ is normalized, note that

$$\begin{aligned}\langle m=1|m=1\rangle &= \frac{1}{2}\big(\,\langle 10| - i\,\langle 01|\,\big)\big(\,|10\rangle + i\,|01\rangle\,\big)\\ &= \frac{1}{2}\big(\,\langle 10|10\rangle - i\,\langle 01|10\rangle + i\,\langle 10|01\rangle + \langle 01|01\rangle\,\big)\\ &= \frac{1}{2}\big(1 - i + i + 1\big) = 1\end{aligned}$$

Finally, we construct the state with $m = -1$ with

$$|m=-1\rangle = \frac{1}{\sqrt{2}}\big(\,|10\rangle - i\,|01\rangle\,\big)$$

Formal Approach

- Consider an eigenstate $|\psi\rangle$ that is both an eigenstate of H with $E = 2\hbar\omega$ and an eigenstate of L_z. This state must satisfy

$$|\psi\rangle = \alpha\,|10\rangle + \beta\,|01\rangle \qquad \text{and} \qquad L_z\,|\psi\rangle = \lambda\,|\psi\rangle\,.$$

First, we write the 2D Hamiltonian H in terms of the creation and annihilation operators:

$$H = \hbar\omega_x\big(a_x^\dagger a_x + \tfrac{1}{2}\big) + \hbar\omega_y\big(a_y^\dagger a_y + \tfrac{1}{2}\big) \equiv H_x + H_y$$

- For the isotropic oscillator with $\omega_x = \omega_y$, this simplifies to

$$H = \hbar\omega\big(a_x^\dagger a_x + a_y^\dagger a_y + 1\big)$$

More so, both the constants x_0, y_0 and p_{0_x}, p_{0_y} are equal for the x and y annihilation and creation operators; we have

$$a_x = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p_x}{p_0}\right) \qquad \text{and} \qquad a_y = \frac{1}{\sqrt{2}}\left(\frac{y}{x_0} + i\frac{p_y}{p_0}\right)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $p_0 = \frac{\hbar}{x_0}$.

- The angular momentum operator is $L_z = xp_y - yp_x$; in terms of the annihilation and creation operators this becomes

$$\begin{aligned}L_z &= \frac{x_0}{\sqrt{2}}\big(a_x + a_x^\dagger\big)\cdot\frac{p_0}{\sqrt{2}i}\big(a_y - a_y^\dagger\big) - \frac{x_0}{\sqrt{2}}\big(a_y + a_y^\dagger\big)\cdot\frac{p_0}{\sqrt{2}i}\big(a_x - a_x^\dagger\big)\\ &= \frac{x_0p_0}{2i}\Big[\big(a_x + a_x^\dagger\big)\big(a_y - a_y^\dagger\big) - \big(a_y + a_y^\dagger\big)\big(a_x - a_x^\dagger\big)\Big]\end{aligned}$$

Applying $x_0p_0 = \hbar$ and multiplying out the terms in parentheses and combining like terms (recall $\big[a_x, a_y\big] = \big[a_x^\dagger, a_y^\dagger\big] = \big[a_x^\dagger, a_y\big] = 0$) simplifies the expression for L_z to

$$L_z = \frac{\hbar}{2i}\big(2a_x^\dagger a_y - 2a_y^\dagger a_x\big) = \frac{\hbar}{i}\big(a_x^\dagger a_y - a_y^\dagger a_x\big)$$

- Next, using the just-derived expression for L_z in terms of $a_{x,y}$ and $a_{x,y}^\dagger$, we investigate the action of L_z on our desired state $|\psi\rangle$; we have

$$L_z |\psi\rangle = \alpha L_z |10\rangle + \beta L_z |01\rangle = \frac{\hbar}{i}\alpha\big(a_x^\dagger a_y - a_x a_y^\dagger\big) |10\rangle + \frac{\hbar}{i}\beta\big(a_x^\dagger a_y - a_x a_y^\dagger\big) |01\rangle$$

Using the identities $a|0\rangle = 0$ and $a|1\rangle = |0\rangle$, we see that $a_x^\dagger a_y |10\rangle = 0$—the a_y operator acts on the zero y component of $|10\rangle$ to produce zero. Analogously, $a_x a_y^\dagger |01\rangle = 0$, where a_x acts on the zero x component of $|01\rangle$ to produce zero. We're left with

$$L_z |\psi\rangle = -\frac{\hbar}{i}\alpha a_x |1\rangle a_y^\dagger |0\rangle + \frac{\hbar}{i}\beta a_x^\dagger |0\rangle a_y |1\rangle$$

Remember a_x and a_y act only on their respective components of $|01\rangle$ and $|10\rangle$, which can be factored into $|0\rangle|1\rangle$ and $|1\rangle|0\rangle$. Finally, using the identities $a^\dagger|0\rangle = |1\rangle$ and $a^\dagger|1\rangle = \sqrt{2}\,|2\rangle$, $L_z|\psi\rangle$ simplifies further to

$$L_z |\psi\rangle = -\frac{\hbar}{i}\alpha |0\rangle|1\rangle + \frac{\hbar}{i}\beta |1\rangle|0\rangle = \frac{\hbar}{i}\big(-\alpha|01\rangle + \beta|10\rangle\big)$$

- To be an eigenstate of L_z, $|\psi\rangle$ must satisfy the eigenvalue equation $L_z|\psi\rangle = \lambda|\psi\rangle$. Using our just-derived expression for $L_z|\psi\rangle$, the eigenvalue equation reads

$$L_z|\psi\rangle = \lambda|\psi\rangle \implies \frac{\hbar}{i}\big(-\alpha|01\rangle + \beta|10\rangle\big) \equiv \lambda\big(\alpha|10\rangle + \beta|01\rangle\big)$$

Multiplying (scalar product on the Hilbert space) the equation from the left by $\langle 10|$ and applying the orthonormality of $|00\rangle$ and $|10\rangle$ leaves

$$\frac{\hbar}{i}\beta = \lambda\alpha,$$

while multiplying the equation from the left by $\langle 01|$ produces

$$-\frac{\hbar}{i}\alpha = \lambda\beta$$

In matrix form, these two equations form a simple eigenvalue problem:

$$\begin{bmatrix} 0 & \frac{\hbar}{i} \\ -\frac{\hbar}{i} & 0 \end{bmatrix}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = \lambda\begin{bmatrix}\alpha \\ \beta\end{bmatrix}$$

We solve the problem by finding the zeros of the characteristic polynomial:

$$\det\begin{bmatrix} -\lambda & \frac{\hbar}{i} \\ -\frac{\hbar}{i} & -\lambda \end{bmatrix} \equiv 0 \implies \lambda^2 - \hbar^2 = 0 \implies \lambda = \pm\hbar$$

Recall L_z's eigenvalues are $\lambda = m\hbar$, so we have $\lambda = \hbar m = \pm\hbar \implies m = \pm 1$ (we had found the same solutions $m = \pm 1$ in the earlier heuristic approach).

- Substituting the $m = 1 \implies \lambda = \hbar$ solution into the matrix equation gives

$$\begin{bmatrix} -\hbar & \frac{\hbar}{i} \\ -\frac{\hbar}{i} & -\hbar \end{bmatrix}\begin{bmatrix}\alpha \\ \beta\end{bmatrix} = 0 \implies \beta = i\alpha$$

Substituting the $m = 1$ result $\beta = i\alpha$ into the general linear combination $|\psi\rangle = \alpha\,|10\rangle + \beta\,|01\rangle$ produces

$$|m = 1\rangle = \alpha\,|10\rangle + (i\alpha)\,|01\rangle = \alpha\big(\,|10\rangle + i\,|01\rangle\,\big)$$

The normalization condition requires $\alpha = \frac{1}{\sqrt{2}}$, which gives

$$|m = 1\rangle = \frac{1}{\sqrt{2}}\big(\,|10\rangle + i\,|01\rangle\,\big)$$

which agrees with the $m = 1$ solution in the heuristic approach.

- Substituting the $m = -1 \implies \lambda = -\hbar$ solution into the matrix equation gives

$$\begin{bmatrix} +\hbar & \frac{\hbar}{i} \\ -\frac{\hbar}{i} & +\hbar \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0 \implies \beta = -i\alpha$$

Analogously to the $m = 1$ case, substituting the $m = -1$ result $\beta = -i\alpha$ into the general linear combination $|\psi\rangle = \alpha\,|10\rangle + \beta\,|01\rangle$ produces

$$|m = -1\rangle = \alpha\,|10\rangle + (-i\alpha)\,|01\rangle = \alpha\big(\,|10\rangle - i\,|01\rangle\,\big)$$

The normalization condition requires $\alpha = \frac{1}{\sqrt{2}}$, which gives

$$|m = -1\rangle = \frac{1}{\sqrt{2}}\big(\,|10\rangle - i\,|01\rangle\,\big)$$

which agrees with the $m = -1$ solution in the heuristic approach.

- The final solution for the eigenstates of H with energy $2\hbar\omega$ that are also eigenstates of L_z is thus

$$\begin{aligned} |m = 1\rangle &= \frac{1}{\sqrt{2}}\big(\,|10\rangle + i\,|01\rangle\,\big) \\ |m = -1\rangle &= \frac{1}{\sqrt{2}}\big(\,|10\rangle - i\,|01\rangle\,\big) \end{aligned}$$

Why This Result is Useful

- Next, we ask why we would be interested in finding states that are simultaneously eigenstates of two operators (e.g. both H and L_z). As an example, consider a 2D isotropic harmonic oscillator in an external magnetic field $\boldsymbol{B}$. Its Hamiltonian is

$$H = H_0 - \boldsymbol{\mu} \cdot \boldsymbol{B}$$

where H_0 is the Hamiltonian of a 2D isotropic harmonic oscillator without a magnetic field and $\boldsymbol{\mu}$ is the particle's magnetic moment. The magnetic moment is proportional to the angular momentum, i.e. $\boldsymbol{\mu} = \gamma\boldsymbol{L}$, where γ is a constant proportionality factor.

- Assume the magnetic field points in the z direction (i.e. $\boldsymbol{B} = B\hat{\boldsymbol{z}}$) in which case the Hamiltonian simplifies to

$$H = H_0 - \gamma B L_z$$

In this case, the states that are simultaneously eigenstates of both H_0 and L_z will also be eigenstates of the Hamiltonian $H = H_0 - \gamma B L_z$, which is useful for analyzing particles in a external magnetic field.

For example, using our earlier solutions $|m = \pm 1\rangle$, we have the eigenvalue equation

$$\begin{aligned} H\,|m = \pm 1\rangle &= H_0\,|m = \pm 1\rangle - \gamma B L_z\,|m = \pm 1\rangle \\ &= 2\hbar\omega\,|m = \pm 1\rangle - \gamma B(\pm 1 \cdot \hbar)\,|m = \pm 1\rangle \\ &= (2\hbar\omega \pm \gamma B\hbar)\,|m = \pm 1\rangle \end{aligned}$$

In other words, $|m = \pm 1\rangle$ are indeed eigenstates of H, with eigenvalues $(2\hbar\omega \pm \gamma B\hbar)$.

1.8.2 Larmor Precession

Analyze the motion of a quantum-mechanical particle with magnetic moment $\boldsymbol{\mu}$ and angular momentum quantum number $l = 1$ in an external magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$, where $\boldsymbol{\mu}$ forms an initial angle θ with $\boldsymbol{B}$ at $t = 0$.

- We consider a particle in an external magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ whose magnetic moment $\boldsymbol{\mu}$ makes an initial angle θ with the magnetic field. The particle's Hamiltonian is

  $$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\gamma \boldsymbol{L} \cdot \boldsymbol{B} = -\gamma B L_z$$

  Recall the values of angular momentum are quantized. In general, a quantum particle with angular momentum quantum number $l = 1$ exists in a $2l+1$ dimensional Hilbert space with basis $|lm\rangle$, where $m \in \{-l, -l+1, \ldots, l-1, l\}$. In our case $l = 1$, meaning $m \in \{-1, 0, 1\}$.

- In Cartesian coordinates, the angular momentum operator is $\boldsymbol{L} = (L_x, L_y, L_z)$. The operator L^2 acts on the state $|lm\rangle$ as $L^2\,|lm\rangle = h^2 l(l+1)\,|lm\rangle$. The operator L_z acts on $|lm\rangle$ as $L_z\,|lm\rangle = \hbar m\,|lm\rangle$. In other words, the basis $|lm\rangle$ is the basis of states that are eigenstates of the operator L^2 with eigenvalue $h^2 l(l+1)$ and eigenstates of the operator L_z with eigenvalue $\hbar m$.

  In the coordinate wave function representation, the states $|lm\rangle$ are the spherical harmonics

  $$|lm\rangle = Y_{lm}(\phi, \theta)$$

  The ϕ component of Y_{lm} is proportional to $\frac{e^{iml}}{\sqrt{2\pi}}$.

- We return to the Hamiltonian of a particle with a magnetic moment in an external magnetic field: $H = -\gamma B L_z$. For a particle with $l = 1$ (and thus magnitude of angular momentum $L^2 = \hbar^2 l(l+1) = 2\hbar^2$), the Hamiltonian's eigenstates $|\psi\rangle$ occurs in a $2l+1 = 3$ dimensional Hilbert space. In the $|lm\rangle$ basis, the general expression for $|\psi\rangle$ is thus the linear combination

  $$|\psi\rangle = a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle$$

  where $l = 1$ and $m = 1, 0, -1$.

- At $t = 0$, the particle's magnetic moment forms a polar angle θ with the magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$. Our first step will be finding an appropriate expression for this initial condition in the language of quantum mechanics.

Finding the Initial State

- In general, if some state $|\psi\rangle$ is an eigenstate of the operator $\boldsymbol{L}\cdot\hat{\boldsymbol{e}}$, (i.e. the projection of angular momentum $\boldsymbol{L}$ in the direction $\hat{\boldsymbol{e}}$), and the operator acts on ψ as
$$\boldsymbol{L}\cdot\hat{\boldsymbol{e}}\,|\psi\rangle = \hbar l\,|\psi\rangle\,,$$
then we say the state $|\psi\rangle$'s angular momentum points in the direction $\hat{\boldsymbol{e}}$.

  Back to the initial condition. We write $\boldsymbol{L}\cdot\hat{\boldsymbol{e}}\,|\psi,0\rangle = \hbar\,|\psi,0\rangle$ where $\hat{\boldsymbol{e}}$ points in the initial direction of the magnetic moment $\boldsymbol{\mu}$. If we assume the magnitude moment initially lies in the x,z plane with $\phi = 0$, the unit vector $\hat{\boldsymbol{e}}$, in spherical coordinates, reads
$$\hat{\boldsymbol{e}} = (\sin\theta, 0, \cos\theta)$$
To summarize, the quantum mechanical way of saying the particle's magnetic moment forms an initial angle θ with the magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ is
$$\boldsymbol{L}\cdot\hat{\boldsymbol{e}}\,|\psi,0\rangle = \hbar\,|\psi,0\rangle$$
where $|\psi,0\rangle$ is the particle's initial wave function and $\hat{\boldsymbol{e}} = (\sin\theta, 0, \cos\theta)$.

- To find $|\psi,0\rangle$, we need to find the constants a,b,c in the linear combination $|\psi\rangle = a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle$. Inserting $\hat{\boldsymbol{e}}$ into the condition $\boldsymbol{L}\cdot\hat{\boldsymbol{e}}\,|\psi,0\rangle = \hbar\,|\psi,0\rangle$ gives
$$(L_x\sin\theta + L_z\cos\theta)\,|\psi,0\rangle = \hbar\,|\psi,0\rangle$$
Substituting in the linear combination $|\psi\rangle = a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle$ and rearranging gives
$$(L_x\sin\theta + L_z\cos\theta - h)\big(a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle\big) = 0$$

Theoretical Interlude: Action of $L_{x,y}$ on $|ml\rangle$

- Recall the eigenvalue equation $L_z\,|lm\rangle = \hbar m\,|lm\rangle$ for the operator L_z. We now ask how L_x and L_y act on the states $|lm\rangle$. To do this, we introduce the new operators
$$L_+ \equiv L_x + iL_y \qquad \text{and} \qquad L_- \equiv L_+^\dagger = L_x - iL_y$$
In terms of L_+ and L_-, L_x and L_y read
$$L_x = \frac{L_+ + L_-}{2} \qquad \text{and} \qquad L_y = \frac{L_+ - L_-}{2i}$$
The plan is to find out how L_+ and L_- act on $|lm\rangle$, and then reconstruct the action of L_x and L_y on $|lm\rangle$ using the relationship between $L_{+,-}$ and $L_{x,y}$.

- Without proof (or e.g. see the lecture notes), L_+ acts on $|lm\rangle$ as
$$L_+\,|lm\rangle = \hbar\sqrt{l(l+1) - m(m+1)}\,|l,m+1\rangle$$
$$L_-\,|lm\rangle = \hbar\sqrt{l(l+1) - m(m-1)}\,|l,m-1\rangle$$

- In our case (working with a particle with $l = 1$ and thus $m \in \{-1,0,1\}$), we have $L_+\,|11\rangle = 0$ (nominally this would create a state with $m = 2$, outside the range of allowed m). In general, $L_+\,|l,m=l\rangle = 0$, since m cannot increase beyond l.

  Next, $L_+\,|10\rangle = \sqrt{2}\hbar\,|11\rangle$ and $L_+\,|1-1\rangle = \sqrt{2}\hbar\,|10\rangle$.

  Meanwhile, L_- produces $L_-\,|11\rangle = \sqrt{2}\hbar\,|10\rangle$, $L_-\,|10\rangle = \sqrt{2}\hbar\,|1-1\rangle$ and $L_-\,|1-1\rangle = 0$, since m cannot decrease below $l = 01$. In general, $L_+\,|l,m=-l\rangle = 0$, since m cannot decrease below $-l$.

Back to Finding the Initial State

- We left off with

$$(L_x \sin\theta + L_z \cos\theta - h)\big(a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle\,\big) = 0$$

Writing $L_{x,y}$ in terms of $L_{+,-}$ and substituting the just-derived action of $L_{+,-}$ on $|11\rangle\,, |10\rangle$ and $|1-1\rangle$ gives

$$\begin{aligned}
0 &= \left(\frac{L_+ + L_-}{2}\sin\theta + L_z\cos\theta - h\right)\big(a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle\,\big)\\
&= a\left(\frac{\sqrt{2}\hbar}{2}\,|10\rangle\sin\theta + \hbar\cos\theta\,|11\rangle - h\,|11\rangle\right)\\
&\quad + b\left(\frac{\sqrt{2}\hbar}{2}\,|11\rangle\sin\theta + \frac{\sqrt{2}\hbar}{2}\sin\theta\,|1-1\rangle - \hbar\,|10\rangle\right)\\
&\quad + c\left(\frac{\sqrt{2}\hbar}{2}\,|10\rangle\sin\theta - \hbar\cos\theta\,|1-1\rangle - \hbar\,|1-1\rangle\right)
\end{aligned}$$

Notice that this equation now involves only scalar values; all operators are gone.

- Next, we find the constants a, b and c. First, divide through by $\hbar$, which cancels out from each equation. Next, multiplying the above equations by $\langle 11|$ and applying orthonormality of the states $|11\rangle$, $|10\rangle$, $|1-1\rangle$, we have

$$a\cos\theta - a + \frac{b}{\sqrt{2}}\sin\theta = 0$$

Next, multiplying the equation by $|10\rangle$ gives

$$\frac{a}{\sqrt{2}}\sin\theta - b + \frac{c}{\sqrt{2}}\sin\theta = 0$$

Finally, multiplying the equation by $|1-1\rangle$ gives

$$\frac{b}{\sqrt{2}}\sin\theta - c\cos\theta - c = 0$$

- We've found a system of three equations for the three unknowns a, b and c. Recall from e.g. introductory linear algebra that because the system of equations is homogeneous (the right side of each equation is zero), the system has a solution only up to a free parameter.

Solving the first equation for a in terms of b gives

$$a(\cos\theta - 1) + \frac{b}{\sqrt{2}}\sin\theta = 0 \implies a = \frac{b\sin\theta}{\sqrt{2}(1-\cos\theta)}$$

From the third equation, we get c in terms of b:

$$\frac{b}{\sqrt{2}}\sin\theta - c(1+\cos\theta) = 0 \implies c = \frac{b\sin\theta}{\sqrt{2}(1+\cos\theta)}$$

- The solution is easier to find with $\sin\theta$ and $\cos\theta$ written in terms of double angle identities, which produce

$$a = \frac{b}{\sqrt{2}}\cot\frac{\theta}{2} \qquad \text{and} \qquad c = \frac{b}{\sqrt{2}}\tan\frac{\theta}{2}$$

- With a and c known in terms of the free parameter b, the initial condition on $|\psi, 0\rangle$ reads

$$|\psi, 0\rangle = b\left(\frac{1}{\sqrt{2}}\cot\frac{\theta}{2}|11\rangle + |10\rangle + \frac{1}{\sqrt{2}}\tan\frac{\theta}{2}|1-1\rangle\right)$$

We find b from the normalization condition, which, with the help of some trigonometric identities, reads

$$\langle\psi, 0|\psi, 0\rangle \equiv 1 = |b|^2\left(\frac{1}{2}\cot^2\frac{\theta}{2} + 1 + \frac{1}{2}\tan^2\frac{\theta}{2}\right) = |b|^2\left(\frac{\cos^4\frac{\theta}{2} + 2\cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2} + \sin^4\frac{\theta}{2}}{2\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}}\right)$$

$$= |b|^2\frac{\left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\right)^2}{2\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} = \frac{|b|^2}{2\sin^2\frac{\theta}{2}\cos^2\frac{\theta}{2}} \equiv 1$$

Because of the $|b|^2$, b is mathematically determined only up to a constant phase factor $e^{i\phi}$ of magnitude 1; if we make the simple choice $e^{i\phi} = 1$, the normalization condition gives

$$b = \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}$$

- Substituting $b = \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}$ into the expression for $|\psi, 0\rangle$ gives the desired result

$$|\psi, 0\rangle = \cos^2\frac{\theta}{2}|11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|10\rangle + \sin^2\frac{\theta}{2}|1-1\rangle$$

To summarize: precisely this state $|\psi, 0\rangle$ satisfies the initial condition that a particle's magnitude moment $\boldsymbol{\mu}$ makes an angle θ with an external magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$.

Time Evolution of the Initial State

- With the initial state $|\psi, 0\rangle$ known, the next step is to find the time-dependent wave function $|\psi, t\rangle$ for a particle with magnetic moment $\boldsymbol{\mu}$ in an external magnetic field. We'll find the time evolution in the Schrödinger picture using the particle's Hamiltonian $H = -\gamma B L_z$.

- We'll first solve the stationary Schrödinger equation $H|\psi\rangle = E|\psi\rangle$ for the basis functions $|11\rangle$, $|10\rangle$ and $|1-1\rangle$; this gives

$$\begin{aligned}
H|11\rangle &= -\gamma B L_z|11\rangle = -\gamma B(1\cdot\hbar)|11\rangle = -\gamma B\hbar|11\rangle \\
H|10\rangle &= -\gamma B L_z|10\rangle = -\gamma B(0\cdot\hbar)|10\rangle = 0|10\rangle \\
H|1-1\rangle &= -\gamma B L_z|1-1\rangle = -\gamma B(-1\cdot\hbar)|1-1\rangle = \gamma B\hbar|1-1\rangle
\end{aligned}$$

- Using the energy eigenvalues $E_{11} = -\gamma B\hbar$, $E_{10} = 0$ and $E_{1-1} = \gamma B\hbar$, the time-evolved wave function $|\psi, t\rangle$ is then

$$\begin{aligned}
|\psi, t\rangle &= \cos^2\frac{\theta}{2}e^{-\frac{i(-\gamma B\hbar)}{\hbar}t}|11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}e^{-\frac{i\cdot 0}{\hbar}t}|10\rangle + \sin^2\frac{\theta}{2}e^{-\frac{i\gamma B\hbar}{\hbar}t}|1-1\rangle \\
&= \cos^2\frac{\theta}{2}e^{i\gamma Bt}|11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|10\rangle + \sin^2\frac{\theta}{2}e^{-\gamma Bt}|1-1\rangle \\
&= \cos^2\frac{\theta}{2}e^{i\omega_L t}|11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|10\rangle + \sin^2\frac{\theta}{2}e^{-\omega_L t}|1-1\rangle
\end{aligned}$$

where in the last line we've defined the *Larmor frequency* $\omega_L \equiv \gamma B$. The time evolution is relatively simple to find because the initial state $|\psi, 0\rangle$ was already written in the basis $|11\rangle$, $|10\rangle$, $|1-1\rangle$.

- Next, using the wave function $|\psi, t\rangle$, we will find the expectation value $\langle \boldsymbol{\mu}, t\rangle$ of the particle's magnetic moment at time t, which is related to angular momentum $\boldsymbol{L}$ via

$$\langle \boldsymbol{\mu}, t\rangle = \gamma \langle L, t\rangle = \gamma \begin{bmatrix} \langle L_x, t\rangle \\ \langle L_y, t\rangle \\ \langle L_z, t\rangle \end{bmatrix}$$

We'll start by finding L_z, using the general definition of an expectation value:

$$\begin{aligned} \langle L_z, t\rangle = \langle \psi, t| L_z |\psi, t\rangle = &\left(\cos^2 \frac{\theta}{2} e^{-i\omega_L t} \langle 11| + \sqrt{2} \sin\frac{\theta}{2}\cos\frac{\theta}{2} \langle 10| + \sin^2\frac{\theta}{2} e^{\omega_L t} \langle 1-1|\right) \\ &\cdot L_z \left(\cos^2\frac{\theta}{2} e^{i\omega_L t}\hbar |11\rangle + 0 - \sin^2\frac{\theta}{2} e^{-\omega_L t}\hbar |1-1\rangle\right) \end{aligned}$$

where the operator L_z acts on the basis states $|11\rangle$, $|10\rangle$ and $|1-1\rangle$ to produce the eigenvalues $\hbar, 0$ and $-\hbar$. Multiplying out the terms and applying the orthonormality of the basis states, followed by some trigonometric identities, leads to the considerably simpler expression

$$\begin{aligned} \langle L_z, t\rangle &= \hbar \cos^4\frac{\theta}{2} - \hbar \sin^4\frac{\theta}{2} = \hbar \left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\right)\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) \\ &= \hbar \cdot (1) \cdot (\cos\theta) = \hbar \cos\theta \end{aligned}$$

In other words, the z component of angular momentum L_z is constant!

We ran out of time at this point and continued in the ninth exercise set

1.9 Ninth Exercise Set

1.9.1 Larmor Precession (continued)

Analyze the motion of a quantum-mechanical particle with magnetic moment μ and angular momentum quantum number $l = 1$ in an external magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$, where μ forms an initial angle θ with $\boldsymbol{B}$ at $t = 0$.

- In the last exercise set we found the particle's time-dependent wave function

$$|\psi, t\rangle = \cos^2\frac{\theta}{2} e^{i\omega_L t} |11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2} |10\rangle + \sin^2\frac{\theta}{2} e^{-\omega_L t} |1-1\rangle$$

where $\omega_L \equiv \gamma B$ is the Larmor frequency. We left off with using $|\psi, t\rangle$ to find the expectation value $\langle L_z, t\rangle$, which turned out to be the constant quantity $|L_z, t\rangle = \hbar \cos\theta$. Next, we will use $|\psi, t\rangle$ to find L_x and L_y, which we will use to find the particle's magnetic moment via $|\boldsymbol{\mu}, t\rangle = \gamma\big(\langle L_x, t\rangle, \langle L_y, t\rangle, \langle L_z, t\rangle\big)$.

- It will be easiest to find $\langle L_x, t\rangle$ and $\langle L_y, t\rangle$ indirectly, in terms of the operators L_+ and L_-; recall these are related by

$$\begin{aligned} L_+ &= L_x + iL_y \qquad &\text{and}\qquad L_- &= L_x - iL_y \\ L_x &= \frac{L_+ + L_-}{2} \qquad &\text{and}\qquad L_y &= \frac{L_+ - iL_-}{2i} \end{aligned}$$

It follows that $\langle L_x, t\rangle$ and $\langle L_y, t\rangle$ can be found via

$$\langle L_x, t\rangle = \frac{1}{2}\big(\langle L_+, t\rangle + \langle L_-, t\rangle\big) \qquad \text{and} \qquad \langle L_y, t\rangle = \frac{1}{2i}\big(\langle L_+, t\rangle - \langle L_-, t\rangle\big)$$

In fact, $\langle L_-, t\rangle = \langle L_+, t\rangle^*$ is the complex conjugate of $\langle L_+, t\rangle$, so we only need to find $\langle L_+, t\rangle$, from which we can find $\langle L_-, t\rangle$ using the general identity $\langle \mathcal{O}^\dagger\rangle = \langle \mathcal{O}\rangle^*$. We then have

$$\begin{aligned}
\langle L_x, t\rangle &= \frac{1}{2}\big(\langle L_+, t\rangle + \langle L_+, t\rangle^*\big) = \operatorname{Re}\langle L_+, t\rangle \\
\langle L_y, t\rangle &= \frac{1}{2i}\big(\langle L_+, t\rangle - \langle L_+, t\rangle^*\big) = \operatorname{Im}\langle L_+, t\rangle
\end{aligned}$$

- We now find $\langle L_+, t\rangle$ using the definition of the expectation value (we'll use the identities $L_+ |1,-1\rangle = \sqrt{2}\hbar |10\rangle$, $L_+ |10\rangle = \sqrt{2}\hbar |11\rangle$, and $L_+ |11\rangle = 0$). The expectation value $\langle L_+, t\rangle$ is then:

$$\begin{aligned}
\langle L_+, t\rangle &= \langle \psi, t| L_+ |\psi, t\rangle = \langle \psi, t| \left(2\hbar \sin\frac{\theta}{2}\cos\frac{\theta}{2}|11\rangle + \sqrt{2}\hbar \sin^2\frac{\theta}{2} e^{-i\omega_L t}|10\rangle\right) \\
&= \left(\cos^2\frac{\theta}{2} e^{-i\omega_L t}\right)\cdot\left(2\hbar\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right) + \left(\sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right)\left(\sqrt{2}\hbar\sin^2\frac{\theta}{2}e^{-i\omega_L t}\right) \\
&= 2\hbar\cos\frac{\theta}{2}\sin\frac{\theta}{2}\left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\right)e^{-i\omega_L t} = \hbar\sin\theta e^{-i\omega_L t}
\end{aligned}$$

  The angular momentum components $\langle L_x, t\rangle$ and $\langle L_y, t\rangle$ are then

$$\begin{aligned}
\langle L_x, t\rangle &= \operatorname{Re}\langle L_+, t\rangle = \hbar\sin\theta\cos(\omega_L t) \\
\langle L_y, t\rangle &= \operatorname{Im}\langle L_+, t\rangle = \hbar\sin\theta\sin(\omega_L t)
\end{aligned}$$

  In one place, the components of angular momentum are

$$\langle L_x, t\rangle = \hbar\sin\theta\cos(\omega_L t) \qquad \langle L_y, t\rangle = \hbar\sin\theta\sin(\omega_L t) \qquad \langle L_z, t\rangle = \hbar\cos\theta$$

  In other words, analogously to the classical picture, the expectation values $\langle L_x, t\rangle$ and $\langle L_y, t\rangle$ precess around the direction of the external magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ with the Larmor frequency $\omega_L = \gamma B$.

- Recall that an physical measurement (observation) generally disturbs quantum mechanical systems. With this issue in mind, we'll find what happens with an observation of L_z at the time t.

Theoretical Interlude: Observations in Quantum Mechanics

- We make an observation of a physical quantity in quantum mechanics as follows. First, expand the relevant system's wave function in the basis consisting of the eigenfunctions of the operator corresponding to the quantity being measured (e.g. to measure a system's L_z, expand the system wave function in the L_z basis $|lm\rangle$.)

- The possible outcomes of the observation are the discrete eigenvalues of the operator corresponding to the quantity being measured.

  When the wavefunction is a linear combination of multiple eigenstates, each of the states' corresponding eigenvalues is a possible outcome, and the probability of each eigenvalue being the outcome is the squared absolute value of the corresponding eigenstate's coefficient.

Eigenstate	Outcome	Probability
$\|11\rangle$	$\hbar$	$\left\|\cos^2\frac{\theta}{2}e^{-i\omega_L t}\right\| = \cos^4\frac{\theta}{2}$
$\|10\rangle$	0	$2\cos^2\frac{\theta}{2}\sin^2\frac{\theta}{2}$
$\|1-1\rangle$	$-\hbar$	$\left\|\sin^2\frac{\theta}{2}e^{-i\omega_L t}\right\| = \sin^4\frac{\theta}{2}$

Table 1: Ingredients to consider in a measurement of an $l = 1$ Larmor-precessing particle's angular momentum L_z.

- Finally, immediately after an observation yielding a given eigenvalue, the system's wavefunction assumes ("collapses into") the eigenfunction corresponding to the measured eigenvalue.

Back to the Observation of L_z

- Our particle's wave function $|\psi, t\rangle$ is already expanded in L_z basis $|lm\rangle$; recall the wave function is

$$|\psi, t\rangle = \cos^2\frac{\theta}{2}e^{i\omega_L t}|11\rangle + \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|10\rangle + \sin^2\frac{\theta}{2}e^{-\omega_L t}|1-1\rangle$$

- Next, we consider the possible outcome of the observation of L_z. Our wavefunction is a combination of three states $|11\rangle$, $|10\rangle$ and $|1-1\rangle$; the corresponding L_z eigenvalues of these states are $\hbar$, 0 and $-\hbar$, and the corresponding probabilities are the squared absolute values of the corresponding eigenstate's coefficients. Table 1 summarizes the eigenstates, possible outcomes, and corresponding probabilities.

- Because of wavefunction collapse to the measured eigenvalue's corresponding eigenfunction, any measurement of L_z would cause the particle's eigenfunction to stop precessing at a polar angle θ about the magnetic field $\boldsymbol{B} = B\hat{\boldsymbol{z}}$ in agreement with classical Larmor precession.

  For example, measuring $L_z = \hbar$ would cause the particle to assume the eigenfunction $|11\rangle$, which directly points in the direction of the magnetic field and $\hat{\boldsymbol{z}}$ axis.

  The lesson here is that even though the classical and quantum-mechanical results for a particle with magnetic moment μ in an external magnetic field both display Larmor precession about the $\hat{\boldsymbol{B}}$ direction, any observation of the quantum-mechanical observation of the system breaks this agreement because of wave function collapse.

1.9.2 Rashba Coupling

Consider a particle in the two-dimensional x, y plane with spin angular momentum $S = \frac{1}{2}$ and Hamiltonian

$$H = \frac{p^2}{2m} + \lambda(p_x S_y - p_y S_x)$$

where $\boldsymbol{p} = (p_x, p_y)$ and $\boldsymbol{S} = (S_x, S_y, S_z)$ are the momentum and spin operators and λ is a constant. (The term $\lambda(p_x S_y - p_y S_x)$ is called the Rashba coupling term*). Find the Hamiltonian H's eigenfunctions and eigenvalues.*

- The Hamiltonian H acts on states in the Hilbert space $\mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_s$ where $\mathcal{H}_p$ is the momentum Hilbert space and $\mathcal{H}_s$ is the spin Hilbert space. Analogously, the states in $\mathcal{H}$ are $|\psi\rangle = |\psi_p\rangle \otimes |\psi_s\rangle$.

- Now, since we're working with states with spin $S = \frac{1}{2}$, the spin wavefunction is the linear combination
$$|\psi_s\rangle = \alpha \left|\frac{1}{2}\frac{1}{2}\right\rangle + \beta \left|\frac{1}{2} - \frac{1}{2}\right\rangle$$
where $|sm_s\rangle$ is the basis of the spin operator S^2. s is the spin quantum number and m_s is the quantum number corresponding to the projection of spin on the z axis. The spin operator S^2 acts on these basis states to produce
$$S^2 \left|\frac{1}{2}\frac{1}{2}\right\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right)\left|\frac{1}{2}\frac{1}{2}\right\rangle = \hbar^2 \frac{3}{4}\left|\frac{1}{2}\frac{1}{2}\right\rangle$$
$$S^2 \left|\frac{1}{2} - \frac{1}{2}\right\rangle = \hbar^2 \frac{1}{2}\left(\frac{1}{2}+1\right)\left|\frac{1}{2} - \frac{1}{2}\right\rangle = \hbar^2 \frac{3}{4}\left|\frac{1}{2} - \frac{1}{2}\right\rangle$$
Meanwhile, the operator S_z acts on the basis states to produce
$$S_z \left|\frac{1}{2}\frac{1}{2}\right\rangle = \frac{\hbar}{2}\left|\frac{1}{2}\frac{1}{2}\right\rangle \qquad \text{and} \qquad S_z \left|\frac{1}{2} - \frac{1}{2}\right\rangle = -\frac{\hbar}{2}\left|\frac{1}{2} - \frac{1}{2}\right\rangle$$
When working with particles with spin $S = \frac{1}{2}$, we usually denote the states $\left|\frac{1}{2}\frac{1}{2}\right\rangle$ and $\left|\frac{1}{2} - \frac{1}{2}\right\rangle$ with $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively. In this notation, the spin wave function is
$$|\psi_s\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$$
In our case, the spin Hilbert space $\mathcal{H}_s$ is two-dimensional, since it consists of all linear combinations of the two linearly independent states $|\uparrow\rangle$ and $|\downarrow\rangle$.

- Next, on to the momentum states $|\psi_p\rangle$, which correspond to the kinetic energy operator. The eigenstates of the kinetic energy operator are plane waves of the form $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$. Because the wave vectors $\boldsymbol{k}$ are continuously distributed and $\boldsymbol{k}$ generates a unique set of eigenvalues, the position space $\mathcal{H}_p$ is infinitely dimensional.

- To find the Hamiltonian's eigenfunctions and eigenvalues, we need to solve the stationary Schrödinger equation
$$H|\psi\rangle = E|\psi\rangle$$
First, to make the rest of the problem easier, we will show that H commutes with the operators p_x and p_y. First, we have
$$[H, p_x] = \left[\frac{p_x^2 + p_y^2}{2m} + \lambda(p_x S_y - p_y S_x), p_x\right]$$
The operators p_x^2 and p_x commute, as do p_y^2 and p_x, which takes care of the first term. Next, we consider the Rashba coupling term $(p_x S_y - p_y S_x)$. Because the $S_{y,x}$ operators act on the spin Hilbert space $\mathcal{H}_s$ and p_x acts on the independent momentum Hilbert space $\mathcal{H}_p$, and because p_x commutes with both p_x and p_y, the operator p_x also commutes with the Rashba term $(p_x S_y - p_y S_x)$. It follows that
$$[H, p_x] = 0$$
We can show $[H, p_y] = 0$ with an analogous procedure.

- Next, we will make use of the commutators $[H, p_x] = 0$ and $[H, p_y] = 0$. Recall that if two operators commute, it is possible to find eigenfunctions that are simultaneously eigenfunctions of both operators (see e.g. the 2D harmonic oscillator problem 1.7.2). In our case, because $\boldsymbol{p} = (p_x, p_y)$ and H commute, it is possible to find such functions that are simultaneously eigenfunctions of both operators.

  In other words, instead of finding H's eigenfunctions, we can search for $\boldsymbol{p}$'s eigenfunctions instead.

- $\boldsymbol{p}$'s eigenfunctions correspond to the momentum states $|\psi_p\rangle$. We want to solve the eigenvalue equation

$$\boldsymbol{p}\,|\psi_p\rangle = a\,|\psi_1\rangle \qquad \text{where} \boldsymbol{p} = -i\hbar\nabla$$

  Recall the momentum eigenfunctions are plane waves of the form $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, for which the eigenvalue equation, in the coordinate wavefunction representation, reads

$$\boldsymbol{p}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = -i\hbar(i\boldsymbol{k})e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \hbar\boldsymbol{k}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

  In Dirac notation, the equation reads

$$\boldsymbol{p}\,|\boldsymbol{k}\rangle = \hbar\boldsymbol{k}\,|\boldsymbol{k}\rangle$$

  where the state $|\boldsymbol{k}\rangle$ corresponds to the wavefunction $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$.

- Returning the stationary Schrödinger equation and using $|\psi_p\rangle = |\boldsymbol{k}\rangle$ we have

$$H\,|\psi\rangle = H\big(\,|\psi_p\rangle \otimes |\psi_s\rangle\,\big) = H\big(\,|\boldsymbol{k}\rangle \otimes |\psi_s\rangle\,\big) = E\big(\,|\boldsymbol{k}\rangle \otimes |\psi_s\rangle\,\big)$$

  Again, the replacement of $|\psi_p\rangle$ with $\boldsymbol{k}$ in the Schrödinger equation is possible only because H and $\boldsymbol{p}$ commute. We have thus reduced our problem to finding spin wavefunctions $|\psi_s\rangle$.

  Notation: I practice, we drop the tensor product symbol $\otimes$; in this convention the above stationary Schrödinger reads

$$H\big(\,|\boldsymbol{k}\rangle\,|\psi_s\rangle\,\big) = E\big(\,|\boldsymbol{k}\rangle\,|\psi_s\rangle\,\big)$$

- Next, substituting the Hamiltonian H into the equation $H\big(\,|\boldsymbol{k}\rangle\,|\psi_s\rangle\,\big) = E\big(\,|\boldsymbol{k}\rangle\,|\psi_s\rangle\,\big)$ and noting that each operator in the Hamiltonian acts either only on the momentum function $|\boldsymbol{k}\rangle$ or only on the spin function $|\psi_s\rangle$, we have

$$\begin{aligned}
H\big(\,|\boldsymbol{k}\rangle\,|\psi_s\rangle\,\big) &= \left[\frac{p^2}{2m} + \lambda(p_x S_y - p_y S_x)\right]\big(\,|\boldsymbol{k}\rangle \otimes |\psi_s\rangle\,\big) \\
&= \left(\frac{p^2}{2m}\,|\boldsymbol{k}\rangle\right)|\psi_s\rangle + \lambda\big(p_x\,|\boldsymbol{k}\rangle\,S_y\,|\psi_s\rangle - p_y\,|\boldsymbol{k}\rangle\,S_x\,|\psi_s\rangle\,\big) \\
&= \frac{\hbar^2 k^2}{2m}\,|\boldsymbol{k}\rangle\,|\psi_s\rangle + \lambda\hbar k_x\,|\boldsymbol{k}\rangle\,S_y\,|\psi_s\rangle - \lambda\hbar k_y\,|\boldsymbol{k}\rangle\,S_x\,|\psi_s\rangle \\
&= E\,|\boldsymbol{k}\rangle\,|\psi_s\rangle
\end{aligned}$$

  Next, to eliminate $|\boldsymbol{k}\rangle$ we multiply the equation from the left by $\langle\boldsymbol{k}|$ to get

$$\frac{\hbar^2 k^2}{2m}\,|\psi_s\rangle + \lambda\hbar(k_x S_y - k_y S_x)\,|\psi_s\rangle = E\,|\psi_s\rangle$$

  We're now left with an equation containing only the spin wavefunction $|\psi_s\rangle$.

Theoretical Interlude

- Recall that for a particle with spin $S = \frac{1}{2}$, the function $|\psi_s\rangle$ is an element of the two-dimensional spin Hilbert space $\mathcal{H}_s$ and can thus be written as the linear combination

$$|\psi_s\rangle = \alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle$$

- Just like it is more convenient to the orbital angular momentum components L_x and L_y in terms of the operators L_+ and L_-, it is best to analyze S_x and S_y in terms of the analogously defined operators S_+ and S_-, which read

$$S_+ = S_x + iS_y \qquad \text{and} \qquad S_- = S_x - iS_y$$
$$S_x = \frac{S_+ + S_-}{2} \qquad \text{and} \qquad S_y = \frac{S_+ iS_-}{2i}$$

The operators S_+ and S_- act on the spin basis states $|sm\rangle$ to produce

$$S_+\,|sm\rangle = \hbar\sqrt{s(s+1) - m(m+1)}\,|s, m+1\rangle$$
$$S_-\,|sm\rangle = \hbar\sqrt{s(s+1) - m(m-1)}\,|s, m-1\rangle$$

Back to Our Problem

- First, some useful intermediate results: $S_+\,|\uparrow\rangle = S_+\left|\frac{1}{2}\frac{1}{2}\right\rangle = 0$ (m cannot increase beyond $s = \frac{1}{2}$), $S_+\,|\downarrow\rangle = S_+\left|\frac{1}{2} - \frac{1}{2}\right\rangle = \hbar\,|\uparrow\rangle$, $S_-\,|\uparrow\rangle = S_-\left|\frac{1}{2}\frac{1}{2}\right\rangle = \hbar\,|\downarrow\rangle$ and $S_-\,|\downarrow\rangle = S_-\left|\frac{1}{2} - \frac{1}{2}\right\rangle = 0$ (m cannot increase below $-s = -\frac{1}{2}$).

- In terms of S_+ and S_- and using the above intermediate results, S_x and S_y act on $|\psi_s\rangle$ to produces

$$S_x\,|\psi_s\rangle = \frac{S_+ + S_-}{2}\big(\alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle\big) = \frac{\hbar}{2}\big(\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big)$$
$$S_y\,|\psi_s\rangle = \frac{S_+ - S_-}{2i}\big(\alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle\big) = \frac{\hbar}{2i}\big(-\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big)$$

- We can now evaluate the earlier equation

$$\frac{\hbar^2k^2}{2m}\,|\psi_s\rangle + \lambda\hbar(k_xS_y - k_yS_x)\,|\psi_s\rangle = E\,|\psi_s\rangle$$

Using the just-derived action of S_x and S_y act on $|\psi_s\rangle$, we have

$$\frac{\hbar^2k^2}{2m}\big(\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big) + \frac{\lambda k_x\hbar^2}{2i}\big(-\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big) - \frac{\lambda k_y\hbar^2}{2}\big(\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big) = E\big(\alpha\,|\downarrow\rangle + \beta\,|\uparrow\rangle\big)$$

Note that this equation contains only scalar values and the two linearly independent states $|\downarrow\rangle$ and $|\uparrow\rangle$—all operators are gone from the equation.

- Multiplying the equation from the left by $\langle\uparrow|$ and applying the orthonormality of $|\downarrow\rangle$ and $|\uparrow\rangle$ produces

$$\frac{\hbar^2k^2}{2m}\alpha + \frac{\lambda\hbar^2k_x}{2i}\beta - \frac{\lambda\hbar^2k_y}{2}\beta = E\alpha$$

while multiplying the equation from the left by $\langle\downarrow|$ produces

$$\frac{\hbar^2k^2}{2m}\beta - \frac{\lambda\hbar^2k_x}{2i}\beta - \frac{\lambda\hbar^2k_y}{2}\alpha = E\beta$$

We have a system of two equations for the two unknown coefficients α and β; in matrix form this system reads

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} & \frac{\lambda\hbar^2}{2i}(k_x - ik_y) \\ -\frac{\lambda\hbar^2}{2i}(k_x + ik_y) & \frac{\hbar^2 k^2}{2m} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

which is an (2×2) eigenvalue problem.

- Before tackling the eigenvalue problem, we'll write the 2D wave vector $\boldsymbol{k} = (k_x, k_y)$ in polar coordinates:

$$k_x + ik_y = ke^{i\phi} \qquad \text{and} \qquad k_x - ik_y = ke^{-i\phi}$$

With $\boldsymbol{k}$ written in polar coordinates, the eigenvalue equation reads

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} & \frac{\lambda\hbar^2}{2i}ke^{-i\phi} \\ -\frac{\lambda\hbar^2}{2i}ke^{i\phi} & \frac{\hbar^2 k^2}{2m} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

We find the energy eigenvalues from the zeros of the characteristic polynomial:

$$p(E) = \det \begin{bmatrix} \frac{\hbar^2 k^2}{2m} - E & \frac{\lambda\hbar^2}{2i}ke^{-i\phi} \\ -\frac{\lambda\hbar^2}{2i}ke^{i\phi} & \frac{\hbar^2 k^2}{2m} - E \end{bmatrix} = \left(\frac{\hbar^2 k^2}{2m} - E\right)^2 - \left(\frac{\lambda\hbar^2 k^2}{2}\right)^2 \equiv 0$$

The two solutions are

$$E_{+,-} = \frac{\hbar^2 k^2}{2m} \pm \frac{\lambda\hbar^2 k}{2}$$

Note that $\lambda = 0$, corresponding to zero coupling, recovers the free-particle energy $E = \frac{\hbar^2 k^2}{2m}$. In this case we have energy degeneracy 2 for each $\boldsymbol{k}$, since both energy eigenvalues $E_{+,-}$ are equal for a given value of k.

For $\lambda \neq 0$, in the presence of Rashba coupling, the degeneracy is broken, since both energy eigenvalues $E_{\pm}$ are different; shifted up or down from the free particle energy by the quantity $\frac{\lambda\hbar^2 k}{2}$.

- Next, we consider the corresponding eigenstates. In the degenerate case $\lambda = 0$, we have

$$H\left|\boldsymbol{k}\right\rangle\big(\alpha\left|\uparrow\right\rangle + \beta\left|\downarrow\right\rangle\big) = \frac{\hbar^2 k^2}{2m}\big(\alpha\left|\uparrow\right\rangle + \beta\left|\downarrow\right\rangle\big)$$

for each α and β. In other words, when $\lambda = 0$, any linear combination $\left|\psi_s\right\rangle = \big(\alpha\left|\uparrow\right\rangle + \beta\left|\downarrow\right\rangle\big)$ is an eigenstate of the Hamiltonian with the same energy eigenvalue $\frac{\hbar^2 k^2}{2m}$.

- When $\lambda \neq 0$, only two unique linear combination of $\left|\uparrow\right\rangle$ and $\left|\downarrow\right\rangle$ will be eigenstates of the Hamiltonian; we find these states by finding the eigenvectors of the earlier eigenvalue problem

$$\begin{bmatrix} \frac{\hbar^2 k^2}{2m} - E & \frac{\lambda\hbar^2}{2i}ke^{-i\phi} \\ -\frac{\lambda\hbar^2}{2i}ke^{i\phi} & \frac{\hbar^2 k^2}{2m} - E \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0$$

Substituting in the two energy eigenvalues $E_{\pm} = \frac{\hbar^2 k^2}{2m} \pm \frac{\lambda\hbar^2 k}{2}$ gives

$$\begin{bmatrix} \mp\frac{\lambda\hbar^2 k}{2} & \frac{\lambda\hbar^2}{2i}ke^{-i\phi} \\ \frac{\lambda\hbar^2}{2i}ke^{i\phi} & \mp\frac{\lambda\hbar^2 k}{2} \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = 0$$

Multiplying the matrices leads to the equation

$$\mp\frac{\lambda\hbar^2 k}{2}\alpha + \frac{\lambda\hbar^2 k}{2i}e^{-i\phi}\beta = 0 \implies \beta = \pm\alpha i e^{i\phi}$$

The two eigenvectors are thus

$$\begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \alpha\begin{bmatrix}1\\ \pm ie^{i\phi}\end{bmatrix} \qquad \text{or, when normalized,} \qquad \begin{bmatrix}\alpha\\ \beta\end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\ \pm ie^{i\phi}\end{bmatrix}$$

The corresponding eigenfunctions for the eigenvalues $E_\pm$ are thus

$$|\psi_+\rangle = |\boldsymbol{k}\rangle\,\frac{|{\uparrow}\rangle + ie^{i\phi}\,|{\downarrow}\rangle}{\sqrt{2}} \qquad \text{and} \qquad |\psi_-\rangle = |\boldsymbol{k}\rangle\,\frac{|{\uparrow}\rangle - ie^{i\phi}\,|{\downarrow}\rangle}{\sqrt{2}}$$

Next, we will analyze the just-derived wavefunctions.

Theoretical Interlude

- If the projection $\boldsymbol{S}\cdot\hat{\boldsymbol{e}}$ of a particle's spin $\boldsymbol{S}$ in the direction $\hat{\boldsymbol{e}}$ acts on the spin particle's wavefunction $|\psi_s\rangle$ to produce $\boldsymbol{S}\cdot\hat{\boldsymbol{e}}\,|\psi_s\rangle = \frac{\hbar}{2}\,|\psi_s\rangle$, then we say the particle's spin points in the direction $\hat{\boldsymbol{e}}$.

- If we write $\hat{\boldsymbol{e}}$ in spherical coordinates as

$$\hat{\boldsymbol{e}} = \big(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta\big),$$

then the equation $\boldsymbol{S}\cdot\hat{\boldsymbol{e}}\,|\psi_s\rangle = \frac{\hbar}{2}\,|\psi_s\rangle$ has the solution

$$|\psi_s\rangle = \cos\frac{\theta}{2}\,|{\uparrow}\rangle + \sin\frac{\theta}{2}e^{i\varphi}\,|{\downarrow}\rangle$$

In other words, if we know a particle's spin wavefunction $|\psi_s\rangle$ and can deduce the values of φ and θ by comparing the particle's wavefunction to the above equation, we can determine the spatial orientation $\hat{\boldsymbol{e}} = \big(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta\big)$ of the particle's spin.

Back to Our Problem

- In our case, the particle has the spin wavefunctions

$$\left|\psi_{s_\pm}\right\rangle = \frac{1}{\sqrt{2}}\,|{\uparrow}\rangle \pm \frac{1}{\sqrt{2}}ie^{i\phi}\,|{\downarrow}\rangle = \frac{1}{\sqrt{2}}\,|{\uparrow}\rangle + \frac{1}{\sqrt{2}}e^{i(\phi\pm\frac{\pi}{2})}\,|{\downarrow}\rangle$$

By comparing $\left|\psi_{s_\pm}\right\rangle$ to the above general expression for a spin wave function

$$|\psi_s\rangle = \cos\frac{\theta}{2}\,|{\uparrow}\rangle + \sin\frac{\theta}{2}e^{i\varphi}\,|{\downarrow}\rangle$$

we see that our particle has polar angle $\theta = \frac{\pi}{2}$ and azimuthal angle $\varphi = \phi\pm\frac{\pi}{2}$, where ϕ is the angle in the phase term $e^{i\phi}$ (ϕ was the azimuthal angle in the polar-coordinate representation of the wave vector $\boldsymbol{k} = (k, \phi)$).

In both cases, the particle's spin is perpendicular to the direction of the wave vector $|k\rangle$.