APPH3100: Introduction to Quantum Mechanics

Michael Cai

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Abstract

The course starts with a recap of linear algebra and quantum mechanics, followed by an introduction to quantum optics and quantum information. Two-level systems, Bloch sphere, quantum gates, and elementary quantum algorithms will be discussed. Quantum teleportation and quantum key distribution will be introduced as applications of entanglement. The lecture content will be directly applied in experiments with entangled photons. In the following, state-of-the-art quantum algorithms will be discussed, related to cutting-edge research results in quantum computing. This includes quantum Fourier transform, quantum simulation of the Schroedinger equation, and the variational quantum eigensolver (VQE) algorithm. During the course students will do one experimental project with entangled photons and one quantum programming project. Students will be guided to implement a quantum algorithm of their choice and run it on a quantum computer (IBM, IonQ, QuEra).

Contents

Chapter 1

Quantum Systems

Lecture 1

1.1 Quantum Computing Systems

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Example. Atoms: There is a nucleaus denoted Ze with an electron denoted as e^-. Having a positively charged nucleaus and electron can be described by a hamiltonian denoted as

$$H^{at} = \frac{p^2}{2m_e} + V(r), V(r) = -\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$$

Where the hamiltonian represented the movement of the electron.

In this potential, we get discrete energy states. More precisely, we can solve the schrodinger equation denoted

$$H^{at}\phi(\vec{r}) = E_n\phi(\vec{r})$$

The eigen energies have the form

$$E_n = -\frac{1}{2}m_e c^2\frac{\alpha^2}{n^2}$$

This has discrete energy values and the smallest energy is for n=1 Where $\alpha = \frac{e^2}{4\pi\epsilon_0 hc} \approx \frac{1}{137}$

The eigenfunctions have the form of the following:

$$\phi(\vec{r}) = R_{ne}(r)Y_{em}(\theta,\phi)$$

which includes the spherical harmonics. These eigenfunctions are also orthonormal wave functions. There are also the three quantum numbers denoted as: h,l, and m which are the principal quantum number, angular momentum, and projection angular momentum.

Intuitively for the hydrogen model, we see that the energystates come close and close as a factor of $\frac{1}{n^2}$

> **Remark.** Simplification: We only use a two level system denoted as E_1, E_2 with wavfunction denoted as ψ_{100}, ψ_{210} which are going to be known as the s-orbital and the p-orbital which is a two level system.

Example. Spin $-\frac{1}{2}$: These systems include electrons, protons, and neutrons which have spins which are an intrinsic form of angular momentum. All these are spin $\frac{-1}{2}$ particles. Spin always comes with a magnetic moment. One example is a electron and it has two states which are denoted as

$$|\uparrow\rangle, |\downarrow\rangle$$

These are orthoganal to each other with angular momentums $\frac{h}{2}$and $-\frac{h}{2}$. These electrons are in a

magnetic field pointing in the z direction $B = B\hat{e_Z}$

The interaction is denoted as

$$\hat{H}_z = \vec{\mu} \cdot \vec{B} = -(-g_s \mu_B \vec{S}/h) \cdot B$$

where $\mu_B = \frac{eh}{2m_e}$ which is the Bohr magneton. $g_s = 2$ which is known as the g-factor. The spin operator can be denoted in the following way

$$\vec{S} = (S_x, S - y, S_z)^T$$

which is simply $\frac{h}{2}$ multipled with the Pauli matrices. We can rewrite this as

$$g_s \mu_B \frac{S_z}{\overline{h}} B_z = \mu_B B_z \sigma_z$$

Thus we get that

$$H_z \left|\uparrow\right\rangle = \mu B_z \left|\uparrow\right\rangle$$

and negative for the latter.

With a 0 magnetic field, the spin up and spin down are the same. When you increase the energy, they have different states denoted as $\mu_B B_Z$ and $-\mu_B B_z$. What you get here is called level splitting

Example. Photon Polarization: the electric field of a light wave in the z-direction may be in the form where the wave propagates in the z-direction. This is going to polarized in the plane of the chalk board. This can be written as

$$\overline{E}(z, y) = (E_x, E_y e^{i\theta}) e^{i(kz - \omega t)}$$

where the values are known to be the angular frequency, wavelength, and wave vector. We can rewrite this polarization vector as

$$E_x \hat{e_x} + E_y e^{i\theta} e_y$$

with $E_0 = \sqrt{E_x^2 + E_y^2}$. Thus it could have both an x and y component. If we have that $\theta = 0, E_y = 0 \Rightarrow E_x = E_0$ which is denoted as vertical linear polarization and the latter is called horizontal linear polarization if $E_y = E_0$. Each photon has its own unique polarization!

Polarization is a property carried by the individual photons that constitute the light field.

$$\vec{V} = E_0 \hat{e_x}, \vec{H} = E_0 \hat{e_y}$$

The polarization state vector of a single photon can be written as a superposition of $\left|H\right\rangle + e^{-i\phi} \left|V\right\rangle$ which is a two level system

Example. Superconducting Qubits: Suppose we have a LC-circuit with a inductor and a capacitor which creates a resonance with a frequency with angular frequency $\omega_c = \frac{1}{\sqrt{2c}}$

Suppose we super cool it down such that the wire becomes superconducting and for the case where $k_b T \ll \overline{h}\omega_c$ is much smaller than the excitation frequency of the circuit, we get discrete energy states for the oscillation that correspond to a quantum harmonic oscillator. We can write the hamiltonian of the circuit in the form

$$\hat{H} = \hat{q}^2/2C + \phi^2/2C$$

which is similar to the momentum and position operator we see in a quantum harmonic oscillator. $\hat{\phi}$ is the magnetic flux operator, $\hat{q}$ is the charge operator.

This creates a quadratic potential well with energy states $E_0 = h\frac{\omega}{2}$ with spaces of $h\omega$. The energies thus can be expressed as

$$E_n = h\omega_c (n + \frac{1}{2})$$

If you want this to be a two level system, it is practically bad since you might couple to many other

states due to its equal spacings. We can replace the inductor l with a Josephson junction (quantum tunneling/nonlinear inductor) denoted as L_g . The hamiltonian of this system is not modified as

$$\hat{H} = \frac{q^2}{2C} - E_y \cos\phi$$

which is a anharmonic oscillator with energy levels that are different with spacings that get smaller and smaller as it goes up. This is useful for defining a two level system practical for control purposes where the energy levels $\omega_{21} < \omega_{10} \approx 2\pi \cdot 5GHz$ which can be controlled by microwaves. Thus we get a two level system!

Remark. Linear Algebra Review:

Definition 1.1.1. wave functions can be interpreted as vectors in a vector space V which is a hilbert space. We denote these in Dirac notation by $|\psi\rangle$. For linear combinations. For $c_i \in C$and $|\psi_i\rangle \in V$ we have that

$$|\psi\rangle = c_1 |\psi_1\rangle + \cdots + c_n |\psi_n\rangle \in V$$

A set fo vectors $|\psi\rangle$ is linearly independent if none of the vectors can be written as a linear combination of the other vectors. In additional, if such a set spans the entire vector space, it is called a basis.

Definition 1.1.2. Two level systems are described by 2 dimensional vector spaces in C^2 spanned by two basis vectors $|v_1\rangle$ $|v_2\rangle$. Any vector in that vector space can be expressed as

$$|\psi\rangle = c_1 |v_1\rangle + c_2 |v_2\rangle$$

Column vectors can be written as

$$|\psi\rangle = (c_1 c_2)^T$$

and the complex conjugate can be written as

$$|\psi\rangle = (c_1 c_2)^*$$

The scalar product is denoted as

$$\langle\beta|\alpha\rangle = (b_1^* b_2^*)(a_1 a_2)^T$$

Lecture 2

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Chapter 2

Schrodinger's Equation

2.1 Time Independent Equation

Remark. The time-independent Schrödinger equation is

$$\hat{H}\psi(x) = E\psi(x),$$

and for stationary states the probability density is time independent:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi(x,t)\right|^2 = 0.$$

For the case $V(x) = 0$, a solution is the plane wave

$$\phi(x) = e^{ikx}.$$

Since

$$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} \quad \text{with } p = \hbar k,$$

this solution represents a free particle. However, note that the plane wave is not normalizable (its probability density does not integrate to 1 over all space). To construct a physical (normalizable) state, we use a superposition of plane waves:

$$\phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \gamma(k)\, e^{ikx}\, \mathrm{d}k,$$

where $\gamma(k)$ is a weight function (analogous to a set of coefficients c_k in a discrete expansion) chosen so that $\phi(x)$ is square-integrable.

Remark. We now choose a specific form for $\gamma(k)$; for example, a Gaussian centered at k_0:

$$\gamma(k) = A\, \exp\left[-\frac{a^2(k-k_0)^2}{4}\right].$$

The Fourier transform yields

$$\phi(x) = \frac{\sqrt{2}A}{a}\, \exp\left[-\frac{x^2}{a^2}\right]\, e^{ik_0 x}.$$

Here, $e^{ik_0 x}$ represents a plane wave, while the Gaussian envelope $\exp\left(-x^2/a^2\right)$ determines the localization in position space. Note that a narrow Gaussian in momentum space (i.e. a well-defined momentum) corresponds to a wide Gaussian in position space. In this case the uncertainties satisfy

$$\Delta x\, \Delta k = \frac{1}{2}.$$

Including the time dependence (recalling that for each plane wave e^{ikx} we have

$$\phi(t) \propto e^{-i\omega t}, \quad \text{with } \omega = \frac{E}{\hbar} = \frac{\hbar k^2}{2m}),$$

we can write the full time-dependent wave function.

Remark. Suppose we wish to prepare a particle in a wave packet with a momentum distribution sharply peaked around k_0. In momentum space, this means

$$\frac{1}{a} \ll k_0.$$

We then Taylor expand the dispersion relation $\omega(k)$ about k_0:

$$\omega(k) \approx \omega(k_0) + \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} (k - k_0).$$

Writing $k = k_0 + \delta$, the wave function becomes

$$\phi(x,t) = \frac{1}{\sqrt{2\pi}}\, e^{ik_0 x}\, e^{-i\omega(k_0)t} \int_{-\infty}^{\infty} \gamma(k_0+\delta)\, e^{i\delta\left(x - \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} t\right)}\, \mathrm{d}\delta.$$

This shows that there are two relevant velocities:

- The **phase velocity**:
$$v_{pw} = \frac{\omega(k_0)}{k_0} = \frac{\hbar k_0}{2m} = \frac{p}{2m},$$
which is the velocity associated with the phase of the carrier wave.
- The **group velocity**:
$$v_g = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} = \frac{\hbar k_0}{m} = \frac{p}{m},$$
which is the velocity at which the envelope (and thus the particle) propagates.

Thus, although the carrier wave has a phase velocity of $p/(2m)$, the actual particle travels at the group (or classical) velocity p/m. In addition, if the momentum spread is not extremely narrow, the wave packet will spread over time.

Remark. Now consider a situation with a potential $V(x)$ such that at some point the energy E of the particle equals the potential, meaning the kinetic energy is zero there. These are the classical turning points where $E = V(x)$. However, the quantum mechanical wave function can "leak" (tunnel) beyond these classical turning points.

For example, consider a step potential defined by

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

We label region 1 (where $x < a$) and region 2 (where $x \geq a$). Suppose that in region 1 $E > 0$ so that the solution is oscillatory:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi,$$

with the solution

$$\psi_1(x) = e^{ikx}, \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}.$$

In region 2 the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V_0\,\psi = E\psi.$$

Rearranging, we have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = (E - V_0)\psi.$$

If $E < V_0$, then $E - V_0$ is negative; defining

$$\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}},$$

the differential equation becomes

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \kappa^2\psi,$$

with general solution

$$\psi_2(x) = A\,e^{-\kappa x} + B\,e^{\kappa x}.$$

For a physically acceptable solution (one that does not blow up as $x \to \infty$), we choose the decaying exponential (set $B = 0$). Notice that while the wave function $\psi(x)$ remains continuous across the boundary at $x = a$, its derivative may be discontinuous because the potential is discontinuous there.

Lecture 3

2.2 Infinite Square Well

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Remark. We will solve for a case called the infinite square well. We can write the potential to be

$$V(x) = \begin{cases} \infty, & \text{if } x < 0; \\ \infty, & \text{if } x > a; \\ 0, & \text{otherwise.} \end{cases}$$

$$E\psi = \frac{-\hbar^2}{2m}\left[\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\right]$$

The solutions we have here are going to be

$$A_0 = e^{\pm ikx}, k = \sqrt{\frac{2mE}{\hbar^2}}$$

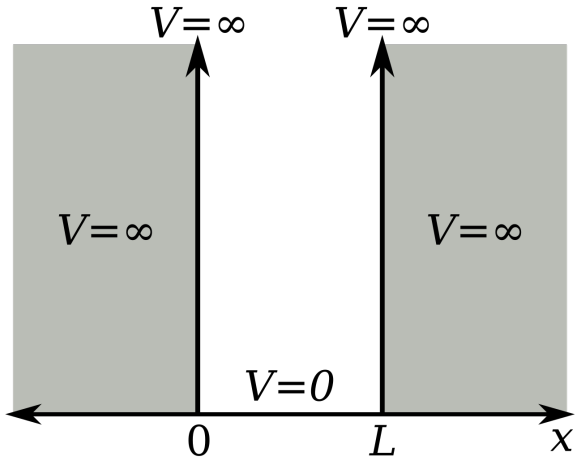

Figure 2.1

Recall that we have the equation

$$\psi = Ae^{\alpha x}$$

$$-\left[A\alpha^2 e^{\alpha x}\right]\frac{\hbar^2}{2m} = Ex$$

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

$$\alpha^2 = \frac{2mE}{\hbar^2} \rightarrow \alpha = \pm i\sqrt{\frac{2mE}{\hbar^2}}$$

Remark. Second Order Differential Equation:

$$\psi = A\sin(kx) + B\cos(kx)$$

Note that $\sin(kx) = \frac{e^{ikx}-e^{-ikx}}{2}$ and $\cos(kx)$ to have a positive term. We notice that immediately that the $\cos(kx)$ term cannot be in the solution since the potential is $V(0) = 0$.

$$\psi = A\sin(kx)$$

with an additional constraint that

$$\psi(x = a) = 0$$

$$A\sin(ka) = 0$$

$$ka = n\pi, k = \frac{n\pi}{a}$$

There are only quantized values of k which means that the energy is also quantized where

$$E = \frac{\hbar^2 k^2}{2m}$$

$$E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2$$

Thus quantized energy states come from boundary conditions which lead to quantized energies. For free particles, energy is continuous but as we put boundary conditions, energy is discretized.

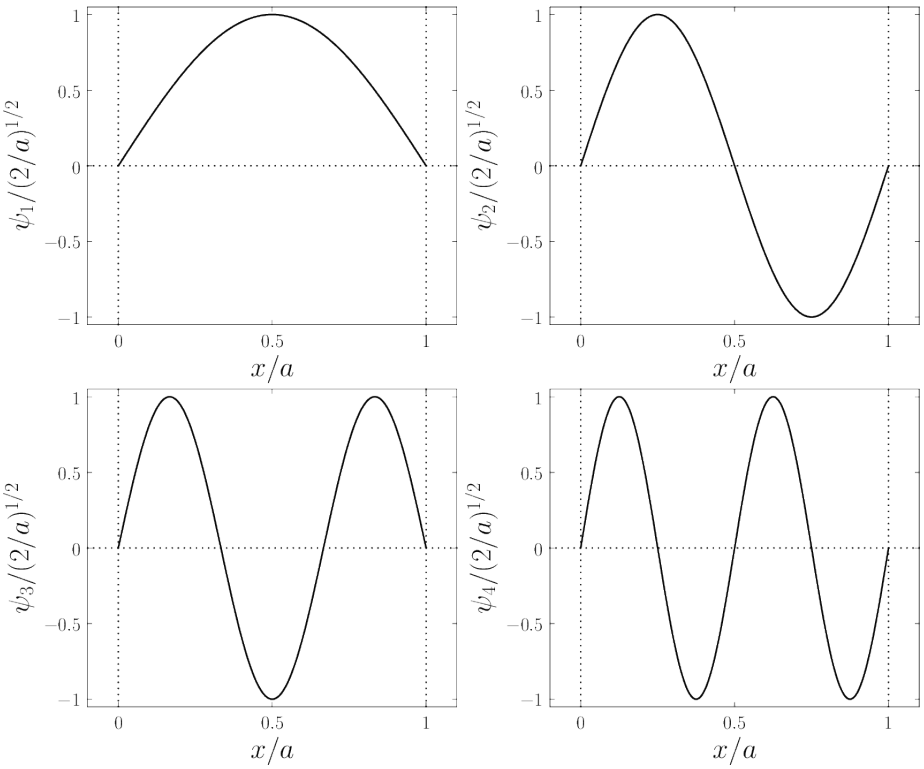

Figure 2.2

These are the solutions for $n = 1, 2, 3, 4$ where we see an additional oscillation for each term.

Example. For a given example, suppose we had a potential with 6 zeroes for our ψ , then our energy can be approximated to be

$$E \approx \frac{\hbar^2 \pi^2}{2ma^2} \times 5^2$$

Figure 2.3

Remark. Notice that we have been carrying a value A, we most normalize to calculate expectation

values. We normalize through the L2 norm which is given by

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

One nice thing about the infinite square welll is that it is finite. thus we have

$$\int_0^a A_n^2 \sin^2(\pi \frac{n}{a} x) \, \mathrm{d}x = 1$$

We can redefine the argument and rescale giving a unitless integral.

$$y = \pi \frac{n}{a} x, \mathrm{d}y = \pi \frac{n}{a} \mathrm{d}x,$$

where y is a unitless term.

$$A_n^2 \frac{a}{n\pi} \int_0^{n\pi} \sin^2(y) \, \mathrm{d}y = 1$$

$$A_n^2 \frac{a}{n\pi} \left[\frac{1}{2}(y - \sin(y)\cos(y)) \right] \Big|_0^{n\pi} = 1$$

$$A_n^2 \frac{a}{n\pi} \frac{1}{2} n\pi = 1$$

$$A_n^2 = \frac{2}{a}$$

$$A_n = \sqrt{\frac{2}{a}}$$

Thus, all normalized wave functions look like the following:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\pi \frac{nx}{a}\right)$$

Notice that the time dependence is simply a separation of variables where

$$\Psi(x,t) = \psi_n(x)\phi_n(t)$$

where

$$\phi_n(t) = e^{-iE_n \frac{t}{\hbar}}$$

Any expectation value we look at will be invariant with time. Notice that

$$e^{-i\frac{E_n}{\hbar}t} = \cos\left(\frac{E_n}{\hbar}t\right) - i\sin\left(\frac{E_n}{\hbar}t\right)$$

Remark. Superposition:

$$\psi(x,t) = \frac{1}{\sqrt{2}} \sqrt{\frac{2}{a}} \left[\sin\left(\pi \frac{x}{a}\right) + \sin\left(2\pi \frac{x}{a}\right) \right]$$

This is the solution at $t = 0$ where it is the superposition of the $n = 1$ and $n = 2$ solution. Suppose that we did not have the $\frac{1}{\sqrt{2}}$ part, we would need to normalize.

$$\psi = C\sqrt{\frac{2}{a}} \left[\psi_1 + \psi_2\right]$$

which is an equally waited superposition. We can normalize now with

$$\int_0^a |\psi|^2 \, \mathrm{d}x = |C|^2 \frac{2}{a} \int_0^a \left[|\psi_1|^2 + |\psi_2|^2 + \psi_1^* \psi_2 + \psi_1 \psi_2^* \right] \, \mathrm{d}x$$

The only contribution will come from the absolute value terms. Coming back we can write

$$\psi_n(x,t) = \frac{1}{\sqrt{a}}\left[\psi_1(x)e^{-\frac{iE_1}{\hbar}t} + \psi_2(x)e^{-\frac{iE_2}{\hbar}t}\right]$$

We will pick up when we have two stationary states in a infinite square well. We will end up getting some in phase and out of phase which will lead to varying time dependent argument presented here.

Lecture 4

2.3 Infintie Potential Square Well

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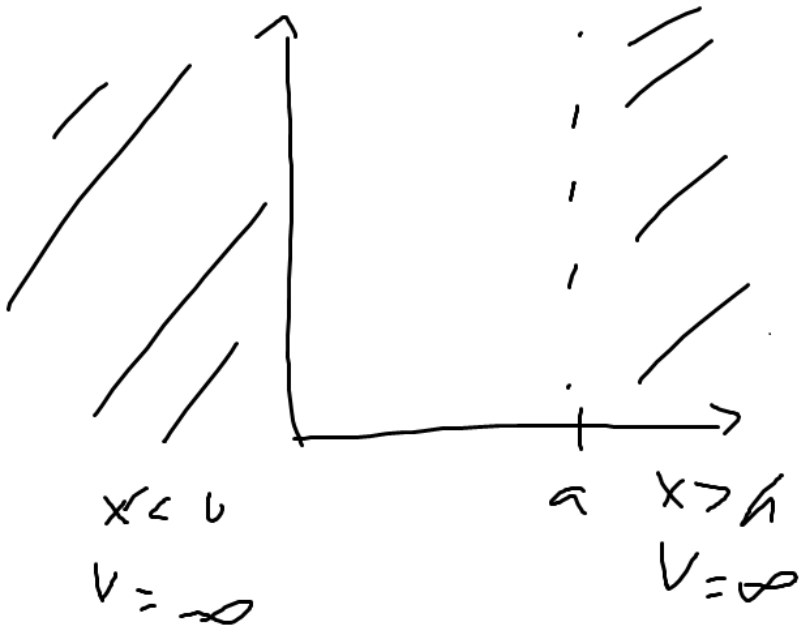

Figure 2.4

Remark. Classically what we would see is a particle going back and forth in the square well. If we take a snapshot in time, there would be an equal probability being anywhere (not really but roughly speaking). In the classic case, we recall that the energy states of the first energy level was

$$\psi = \sin\left(\pi\frac{x}{a}\right)$$

as shown in Figure 1.2 and the probability would be

$$|\psi_1|^2 = \alpha^2 \sin^2(\pi\frac{x}{a})$$

The next solution we have is where $n = 2$, $\psi = \alpha\sin\left(2\pi\frac{x}{a}\right)$ and we can observe where the function

goes to 0.

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(n\pi \frac{x}{a}\right), A = \sqrt{\frac{2}{a}}$$

$$1 = A^2 \int_0^a \mathrm{d}x |\psi_n(x)|^2$$

where we can determine the normalization factor from here.

Remark. The superposition we want to consider now is

$$\psi(x,0) = \frac{1}{\sqrt{2}} \left[\psi_1 + \psi_2\right]$$

Now we are determing the expectation value of the energy $\langle E \rangle$

$$\int_0^x \psi^* \hat{H} \psi \, \mathrm{d}x$$

note that applying the Hamiltonian operator is applied on the real operator as when operating on the first complex factor gives a different result. We see that

$$\psi_n^* = \psi_n \Rightarrow \psi = \psi^*$$

Thus we can write that

$$\langle E \rangle = \int_0^a \hat{H} \psi \psi \, \mathrm{d}x$$

We now basically have the answer where

$$\langle \hat{H} \rangle = \int_0^a (\hat{H}\psi)\psi \, \mathrm{d}x$$

$$= \frac{1}{2} \int_0^a \left[\hat{H}(\psi_1 + \psi_2)\right] (\psi_1 + \psi_2) \, \mathrm{d}x$$

$$= \frac{1}{2} \int_0^a \left[E_1\psi_1 + E_2\psi_2\right] (\psi_1 + \psi_2) \, \mathrm{d}x$$

$$= \frac{1}{2} \int_0^a \left[E_1\psi_1^2 + E_1\psi_1\psi_2 + E_2\psi_1\psi_2 + E_2\psi_2^2\right] \, \mathrm{d}x$$

$$= \frac{1}{2} (E_1 + E_2) \int_0^a \psi_1\psi_2(E_1 + E_2) \, \mathrm{d}x$$

Now we wish to consider the generic case

$$\int_0^a \psi_m \psi_n \, \mathrm{d}x$$

$$= \int_0^a \frac{2}{a} \sin\left(m\pi \frac{x}{a}\right) \sin\left(n\pi \frac{x}{a}\right) \mathrm{d}x$$

$$= \frac{2}{a} \int_0^a \left[\cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)\right] \, \mathrm{d}x$$

$$= \frac{2}{a} \left[\frac{a}{(m-n)\pi} \sin\left(\frac{m-n}{a}\pi x\right) - \frac{a}{(m+n)\pi} \sin\left(\frac{m+n}{a}\pi x\right)\right]\Bigg|_0^a$$

$$= 0, m \neq n$$

To summarize, we have shown that

$$\int_0^a \psi_n \psi_m \, \mathrm{d}x = \begin{cases} 1, & \text{if } m = n; \\ 0, & \text{if } m \neq n; \end{cases} = \delta_{mn}$$

therefore the cross terms must go away and will be just the average value.

Remark. Time Dependence:

$$\psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(n\pi \frac{x}{a}\right) e^{-i\frac{E_n}{\hbar}t}$$

What does our superposition look like:

$$\psi = \frac{1}{\sqrt{2}} \left[\psi_1 + \psi_2\right] = \frac{1}{\sqrt{2}} \left[\psi_1 e^{-i\frac{E_1}{\hbar}t} + \psi_2 e^{-i\frac{E_2}{\hbar}t}\right]$$

$$\langle \hat{H} \rangle = \frac{1}{2} \int_0^a (\hat{H}\psi^*)\psi \, \mathrm{d}x$$

Note that we can no longer ignore the complex conjugate term and compute the quantity

$$\begin{aligned} \langle \hat{H} \rangle &= \frac{1}{2} \int_0^a \left[\hat{H}\left(\psi_1 e^{\frac{iE_1}{\hbar}t} + \psi_2 e^{\frac{iE_2}{\hbar}t}\right)\right]\left(\psi_1 e^{-\frac{iE_1}{\hbar}t} + \psi_2 e^{-\frac{iE_2}{\hbar}t}\right) \mathrm{d}x \\ &= \frac{1}{2} \int_0^a \left[E_1\psi_1 e^{i\omega_1 t} + E_2\psi_2 e^{i\omega_2 t}\right]\left[\psi_1 e^{-i\omega_1 t} + \psi_2 e^{-i\omega_2 t}\right] \mathrm{d}x \\ &= \frac{1}{2} \int_0^a \left[E_1\psi_1^2 + E_2\psi_2^2 + E_1\psi_1\psi_2 e^{i(\omega_1-\omega_2)t} + E_2\psi_1\psi_2 e^{-i(\omega_1-\omega_2)t}\right] \mathrm{d}x \\ &= \frac{1}{2}(E_1 + E_2) + \frac{1}{2} \int_0^a E_1\psi_1\psi_2 e^{i(\omega_1-\omega_2)t} + E_2\psi_1\psi_2 e^{-i(\omega_1-\omega_2)t} \, \mathrm{d}x \\ &= \frac{1}{2}(E_1 + E_2) \end{aligned}$$

Remark. When we think about vector spaces we usually think of our own Euclidean space with three basis vectors that can create any vector in the subspace where

$$\vec{r} = a\hat{x} + b\hat{y} + c\hat{z}$$

or written as

$$\sum_{i=1}^{3} \alpha_i \hat{x}_i$$

In principle, the superposition state is the sum of two basis functions. Thus, we can write down the wave function in two different ways:

$$\psi = \sum_{n=1}^{\infty} c_n \psi_n$$

now this is our vector spanned by our basis vectors ψ_n

$$\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{a}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Now we realize that quantum mechanics is just linear algebra where r

$$\hat{H}_{\infty\times\infty}\vec{\psi} = \vec{E}$$

Note that all must happen is that we satisfy the boundary conditions and end up with a DFT.

Lecture 5

1. Infinite Square Well — Stationary States

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Consider a 1D infinite square well of width a, running from $x = 0$ to $x = a$, with

$$V(x) \;=\; \begin{cases} 0, & 0 < x < a, \\ \infty, & \text{otherwise.} \end{cases}$$

The stationary-state wavefunctions are

$$\psi_n(x) \;=\; \sqrt{\frac{2}{a}}\,\sin\!\Big(\frac{n\pi x}{a}\Big), \quad n = 1, 2, 3, \ldots$$

and the corresponding energies are

$$E_n \;=\; \frac{\hbar^2\pi^2}{2ma^2}\,n^2.$$

These eigenstates form an *orthonormal* basis in the sense that

$$\int_0^a \psi_m^*(x)\,\psi_n(x)\,dx \;=\; \delta_{m,n}.$$

Any wavefunction $\psi(x)$ satisfying the boundary conditions can be expanded as

$$\psi(x) \;=\; \sum_{n=1}^{\infty} c_n\,\psi_n(x).$$

2. Complex Vector Space and Inner Products

Finite-Dimensional Analogy. We can think of a general complex vector $\vec{r} \in \mathbb{C}^N$ as

$$\vec{r} \;=\; \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix},$$

with an inner product

$$\vec{r}^{\,\dagger}\,\vec{r} \;=\; \sum_{i=1}^{N} c_i^*\,c_i \;=\; \|\vec{r}\|^2.$$

The *outer product* $\vec{r}\,\vec{r}^{\,\dagger}$ is a matrix (an operator) formed by taking all pairwise products of components.

Ket and Bra Notation (Dirac). In quantum mechanics, we write a vector as a *ket*:

$$|\alpha\rangle \;=\; \sum_i a_i\,|u_i\rangle\,,$$

where $\{|u_i\rangle\}$ is a basis of the Hilbert space and $a_i \in \mathbb{C}$ are coefficients. The *bra* $\langle\alpha|$ is the Hermitian-conjugate (row-vector) version:

$$\langle\alpha| \;=\; \big(|\alpha\rangle\big)^{\dagger} \;=\; \sum_i a_i^*\,\langle u_i|\,.$$

The inner product $\langle\beta|\alpha\rangle$ is a scalar, generally complex:

$$\langle\beta|\alpha\rangle \;=\; \sum_{ij} b_i^*\, a_j\; \langle u_i|u_j\rangle \;=\; \sum_i b_i^*\, a_i \quad (\text{if } |u_i\rangle \text{ are orthonormal}).$$

For orthonormal $\{|u_i\rangle\}$, we have $\langle u_i|u_j\rangle = \delta_{ij}$, and the completeness relation

$$\sum_i |u_i\rangle\,\langle u_i| \;=\; \mathbf{1}.$$

3. Operators

Operators $\hat{O}$, $\hat{H}$, $\hat{p}$, etc. act on kets to produce new kets:

$$\hat{O}\;|\alpha\rangle \;=\; |\beta\rangle\,.$$

The bra version is obtained by taking the Hermitian conjugate:

$$\langle\alpha|\;\hat{O}^\dagger \;=\; \langle\beta|\,.$$

For a Hermitian operator (an observable) $\hat{O} = \hat{O}^\dagger$.

Examples. - $\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$, the energy-eigenvalue equation. - Linearity: $\hat{O}(|\alpha\rangle + |\beta\rangle) = \hat{O}\,|\alpha\rangle + \hat{O}\,|\beta\rangle$.

Noncommuting Operators. The commutator of two operators $\hat{O}_1, \hat{O}_2$ is

$$[\hat{O}_1, \hat{O}_2] \;=\; \hat{O}_1\,\hat{O}_2 \;-\; \hat{O}_2\,\hat{O}_1.$$

For position and momentum in 1D, we have $\left[\hat{p}, \hat{x}\right] = -i\hbar$, so $\hat{p}\,\hat{x} \neq \hat{x}\,\hat{p}$. In general, if two operators *do* commute, they can be *simultaneously diagonalized*. If they *do not* commute, measuring one observable disturbs the other.

4. Outer Products as Projectors

The outer product $|\alpha\rangle\,\langle\alpha|$ is itself an operator. For instance, acting on a state $|\beta\rangle$ gives

$$(|\alpha\rangle\,\langle\alpha|)\;|\beta\rangle \;=\; |\alpha\rangle\;\big(\langle\alpha|\beta\rangle\big),$$

which is a vector parallel to $|\alpha\rangle$ (scaled by the inner product). If $|\alpha\rangle$ is normalized, $|\alpha\rangle\,\langle\alpha|$ *projects* any vector onto the direction of $|\alpha\rangle$.

Completeness (Resolution of the Identity). If $\{|u_i\rangle\}$ is an orthonormal basis, then

$$\sum_i |u_i\rangle\,\langle u_i| \;=\; \mathbf{1},$$

where $\mathbf{1}$ is the identity operator. This is a powerful tool for expanding or inserting identities in quantum-mechanical derivations.

Lecture 6

2.4 Algebra Notation

Feb 12 01:10

Recall that the definition of a bra and ket vector where the ket vector is a column vector that is N dimensional and the bra vector is the dual space of the ket vector. We define the inner product as

$$\langle a|a\rangle = \sum_i a_i^* a_j\,\langle u_j|u_j\rangle$$

$$= \sum_i |a_i|^2$$

We can the normalized vector of $|a\rangle$ to be

$$\frac{|a\rangle}{\sqrt{\langle a|a\rangle}} \Rightarrow \langle a|a\rangle_{norm} = \frac{\langle a|a\rangle}{\langle a|a\rangle}$$

In the context of quantum mechanics we can have two states that we define as

$$|\psi\rangle = A \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

which represent the two states

$$\Rightarrow \langle\psi|\psi\rangle = 1 \Rightarrow A = \frac{1}{\sqrt{\alpha_1^2 + \alpha_2^2}}$$

Recall the square well and how the normalization is present here. Thus our state is

$$|\psi\rangle = \frac{1}{\sqrt{\alpha_1^2 + \alpha_2^2}} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

We write the probability of measuring such as $\sqrt{P_1}$ and $\sqrt{P_2}$. With this notation we can determine what the expectation values are.

2.5 Expectation Values

Suppose we have some operator $\hat{O}$, then the expectation value corresponds to

$$\frac{\langle\psi|\,\hat{O}\,|\psi\rangle}{\langle\psi|\psi\rangle}$$

Assuming that the wave function is already normalized, we can compute the numerator

$$\langle\psi|\left[\hat{O}\,|\psi\rangle\right]$$

$$\hat{O}\,|\psi\rangle = \sum_i \alpha_i'\,|u_i\rangle$$

$$\langle\psi|\psi'\rangle = \sum_{i,j} \alpha_j^* \alpha_i' \langle u_j|u_i\rangle$$

$$= \sum_j \alpha_j^* \alpha_j' = \langle\hat{O}\rangle$$

This property that the operator on the wavefunction spits out a new wavefunction can be represented as a matrix of dim $N \times N$

$$\left(\quad\right)_{N\times N} \left(\right) = \left(\right)$$

One question to ask is how can we find the variance of our expectation value (probability)?

$$\sigma_{\hat{O}}^2 = \langle\left(\hat{O} - \langle\hat{O}\rangle\right)^2\rangle$$

$$\langle\psi|\left(\hat{O} - \langle\hat{O}\rangle\right)^2|\psi\rangle$$

Expanding out this quantity we can write this as

$$\langle\psi|\left(\hat{O} - \langle\hat{O}\rangle\right)\left(\hat{O} - \langle\hat{O}\rangle\right)|\psi\rangle = 0$$

Expanding the LHS2 we have

$$\hat{O}\,|\psi\rangle - \langle\hat{O}\rangle\,|\psi\rangle$$

the LHS1 is going to be the dual of LHS2. Therefore we can write this as

$$\left\langle \left(\hat{O} - \langle \hat{O} \rangle\right) \psi \right|$$

This implies that LHS2 must go to 0 where we need to find a vector such that it satisfied

$$\hat{O} \left|\psi\right\rangle = \langle \hat{O} \rangle \left|\psi\right\rangle$$

Therefore the eigenvalue of the eigenstate is going to be the expectation value of the operator. This is also the case for

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

Example.

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Another example is

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

$$\det\left(\hat{\sigma}_y - \lambda I\right) = 0$$

$$|1\rangle = \begin{pmatrix} 1 \\ i \end{pmatrix}, |-1\rangle = \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

Definition 2.5.1. We have some vector and their poperties

$$|\psi\rangle = \left(\right)$$

$$\langle\psi| = \left(|\psi\rangle^T\right)^* = |\psi\rangle^\dagger$$

$$\left[\hat{O}\left|\psi\right\rangle\right]^\dagger = [|\psi'\rangle]^\dagger$$

$$\Rightarrow \langle\psi| \hat{O}^\dagger = \langle\psi'|$$

Let us try to compute the following

$$\left\langle \psi \middle| \hat{O}\psi \right\rangle = \alpha$$

$$\left\langle \hat{O}\psi \middle| \psi \right\rangle = \langle\psi| \hat{O}^\dagger \left|\psi\right\rangle = \alpha^*$$

For Hermitian operators we have the property that

$$\hat{O} = \hat{O}^\dagger$$

2.6 Commutators

Suppose we had an operator

$$\hat{O} \left|\psi_N\right\rangle = \alpha_N \left|\psi_N\right\rangle$$

On what condition can we find a second operator that satisfies the following:

$$\hat{Q} \left|\psi_N\right\rangle = \beta_N \left|\psi_N\right\rangle$$

where different operators have the same eigenvector. We can compute the quantity

$$\hat{Q}\hat{O} \left|\psi_N\right\rangle = \beta_N \alpha_N \left|\psi_N\right\rangle$$

$$\hat{O}\hat{Q}\left|\psi_N\right\rangle = \alpha_N\beta_N\left|\psi_N\right\rangle$$

Therefore we must have that

$$\hat{Q}\hat{O} - \hat{O}\hat{Q} = 0$$
$$\left[\hat{Q},\hat{O}\right] = 0$$

where these two operators are simultaneously diagonalizable. Hello

Lecture 7

2.7 Infinite Square Well

Feb 19 01:10

Consider the wave function

$$\left|\psi_n\right\rangle = \sqrt{\frac{2}{a}}\sin\left(n\pi\frac{x}{a}\right)$$

where $\langle\psi_n|\psi_n\rangle = \delta_{mn}$ and we have that $\hat{H}\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$. We have therefore that

$$\left\langle\psi_m\right|\hat{H}\left|\psi_n\right\rangle = \left\langle\psi_m\right|E_n\left|\psi_n\right\rangle = E_n\delta_{mn}$$

where $\delta_{mn} = \begin{pmatrix}1 & & \\ & \dots & \\ & & 1\end{pmatrix}$ $\hat{H} = \begin{pmatrix}E_1 & & \\ & E_2 & \\ & & \dots\end{pmatrix}$ We have that

$$H_{m,n} = \left\langle\psi_m\right|\hat{H}\left|\psi_n\right\rangle$$

in the (ψ_n) basis. Other operators we have are

$$\hat{x}\left|\psi_n\right\rangle = x\sqrt{\frac{2}{a}}\sin\left(n\pi\frac{x}{a}\right)$$

which is not proportional to ψ_n. This is the same for

$$\hat{p}\left|\psi_n\right\rangle = \frac{d}{\mathrm{d}x}\sin\left(n\pi\frac{x}{a}\right)\cos\left(npi\frac{x}{a}\right)$$

$$x_{\min} \approx \left\langle\psi_m\right|\hat{x}\left|\psi_n\right\rangle = \frac{2}{a}\int_0^a x\sin\left(m\pi\frac{x}{a}\right)\sin\left(n\pi\frac{x}{a}\right)\,\mathrm{d}x$$
$$= \frac{1}{a}\int_0^a x\left[\cos\left((m-n)\pi\frac{x}{a}\right) - \cos\left((m+n)\pi\frac{x}{a}\right)\right]\,\mathrm{d}x$$

Evaluating this we have

Lecture 8

Stationary States and Operator Expectation Values

Feb 24 01:10

A stationary state $\left|\psi_n\right\rangle$ satisfies

$$\hat{H}\ \left|\psi_n\right\rangle\ =\ E_n\ \left|\psi_n\right\rangle.$$

In general, a state $\left|\psi\right\rangle$ can be expanded in the energy eigenbasis:

$$\left|\psi\right\rangle\ =\ \sum_n c_n\ \left|\psi_n\right\rangle.$$

Operators and Expectation Values. Let $\hat{O}$ be any operator. In the energy-eigenbasis $\{\left|\psi_n\right\rangle\}$, its matrix representation is $\left(\hat{O}\right)_{mn} = \left\langle\psi_m\right|\hat{O}\left|\psi_n\right\rangle$. The expectation value of $\hat{O}$ in a state $\left|\psi\right\rangle$ is

$$\langle\hat{O}\rangle\ =\ \left\langle\psi\right|\hat{O}\left|\psi\right\rangle\ =\ (\left\langle\psi\right|\hat{O})\left|\psi\right\rangle\ =\ \text{[row] [matrix] [col]}.$$

Commutators and Simultaneous Diagonalization

Review of Commutators. For two operators $\hat{O}$ and $\hat{Q}$, their commutator is

$$[\hat{O}, \hat{Q}] \;=\; \hat{O}\,\hat{Q} \;-\; \hat{Q}\,\hat{O}.$$

If $[\hat{x}, \hat{p}]$ is a constant (specifically $i\hbar$ in quantum mechanics), then x and p cannot be simultaneously diagonalized.

Simultaneous Eigenstates. If $[\hat{O}, \hat{Q}] = 0$, then we can find a basis of states which are eigenstates of both $\hat{O}$ *and* $\hat{Q}$. In that case,

$$\hat{O}\;|\alpha_n\rangle = o_n\;|\alpha_n\rangle\,, \quad \hat{Q}\;|\alpha_n\rangle = q_n\;|\alpha_n\rangle\,,$$

for the *same* set of states $|\alpha_n\rangle$.

Generalized Uncertainty Principle

Variance definitions. Suppose $|\psi\rangle$ is normalized, and let $\hat{O}$ and $\hat{Q}$ be Hermitian observables with real eigenvalues. Define their variances in state $|\psi\rangle$:

$$\sigma_O^2 \;=\; \langle(\hat{O} - \langle\hat{O}\rangle)^2\rangle, \quad \sigma_Q^2 \;=\; \langle(\hat{Q} - \langle\hat{Q}\rangle)^2\rangle.$$

We often let

$$|f\rangle \;=\; (\hat{O} - \langle\hat{O}\rangle)\;|\psi\rangle\,, \quad |g\rangle \;=\; (\hat{Q} - \langle\hat{Q}\rangle)\;|\psi\rangle\,.$$

Because $\hat{O}$ is Hermitian, $\langle f \mid f\rangle = \sigma_O^2$, and similarly for $\hat{Q}$.

Cauchy–Schwarz and Commutators. We use the fact that

$$|\langle f \mid g\rangle|^2 \;\le\; \langle f \mid f\rangle\,\langle g \mid g\rangle \;=\; \sigma_O^2\,\sigma_Q^2.$$

Moreover, the imaginary part of $\langle f \mid g\rangle$ is related to the commutator:

$$\mathrm{Im}\big(\langle f \mid g\rangle\big) \;=\; \tfrac{1}{2i}\,\langle\psi \mid [(\hat{O} - \langle\hat{O}\rangle), (\hat{Q} - \langle\hat{Q}\rangle)] \mid \psi\rangle \;=\; \tfrac{1}{2i}\,\langle[\hat{O}, \hat{Q}]\rangle.$$

Hence,

$$\sigma_O^2\,\sigma_Q^2 \;\ge\; \big|\mathrm{Im}(\langle f \mid g\rangle)\big|^2 \;=\; \tfrac{1}{4}\,\big|\langle[\hat{O}, \hat{Q}]\rangle\big|^2.$$

Therefore,

$$\sigma_O\,\sigma_Q \;\ge\; \tfrac{1}{2}\,\big|\langle[\hat{O}, \hat{Q}]\rangle\big|.$$

This is the *generalized uncertainty principle.*

Example:

For the canonical pair $\hat{x}$ and $\hat{p}$ with $[\hat{x}, \hat{p}] = i\hbar$, one obtains

$$\sigma_x\,\sigma_p \;\ge\; \tfrac{\hbar}{2}.$$

Similarly for energy and time (though t is not exactly an operator in the same sense), one often writes $\sigma_E\,\sigma_t \approx \hbar/2$.

Observables and Probabilities

A general state can be expanded as

$$|\Psi\rangle = \sum_i a_i\;|\phi_i\rangle\,.$$

If $\hat{H}\;|\phi_i\rangle = E_i\;|\phi_i\rangle$ (*i.e.* $|\phi_i\rangle$ are energy eigenstates), then the probability of measuring energy E_i is $|a_i|^2$. In general,

$$\langle\Psi \mid \hat{H} \mid \Psi\rangle \;=\; \sum_i |a_i|^2\,E_i.$$

Thus $|a_i|^2$ is interpreted as the probability (born rule) associated with outcome E_i.

Finite Square Well (FSQ) — Brief Sketch

Consider a 1D potential well of depth $V_0 > 0$ extending from $x = -\frac{a}{2}$ to $x = +\frac{a}{2}$. Inside the well ($|x| < a/2$), $V = 0$, so the wavefunction is oscillatory. Outside the well ($|x| > a/2$), $V = V_0$, so the wavefunction may be exponentially decaying (for $E < V_0$) or have free-particle–like behavior (for $E > V_0$).

Case $0 < E < V_0$: Inside: wave is sinusoidal with $k = \sqrt{2mE}/\hbar$.
Outside: decays exponentially since $E - V_0 < 0$.

Case $E > V_0$: Outside region is like a free particle with $k' = \sqrt{2m(E - V_0)}/\hbar$, allowing partial reflection and transmission. Repeated wells can create resonance and "band" structures in a solid-state context.

Lecture 9

Finite Square Well (FSQ) Notes

Feb 26 01:10

Potential Setup:

$$V(x) = \begin{cases} V_0, & x < -\frac{a}{2}, \\ 0, & -\frac{a}{2} \le x \le \frac{a}{2}, \\ V_0, & x > \frac{a}{2}. \end{cases}$$

We assume $V_0 > 0$ and define the well to extend from $-\frac{a}{2}$ to $+\frac{a}{2}$. We want to solve the time-independent Schrödinger equation,

$$\hat{H}\,\psi_n(x) \;=\; E_n\,\psi_n(x), \quad \hat{H} \;=\; -\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2} \;+\; V(x).$$

The full time-dependent wavefunction can be written as $\psi(x,t) = \psi_n(x)\, e^{-\frac{iE_n t}{\hbar}}$.

Two energy regimes:

- $E > V_0$
- $E < V_0$

Both cases lead to piecewise solutions (exponential vs. oscillatory) in the outer regions depending on whether $E < V_0$ or $E > V_0$.

Case: $E < V_0$

Region I: $x < -\frac{a}{2}$ (where $V = V_0$)

The Schrödinger equation in Region I is

$$-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}\,\psi_n(x) \;+\; V_0\,\psi_n(x) \;=\; E_n\,\psi_n(x).$$

Rearrange to

$$-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}\,\psi_n(x) \;=\; \big(E_n - V_0\big)\,\psi_n(x).$$

Since $E_n < V_0$, define

$$\kappa \;=\; \sqrt{\frac{2m\big(V_0 - E_n\big)}{\hbar^2}},$$

so the equation becomes

$$\frac{d^2}{dx^2}\,\psi_n(x) = \kappa^2\,\psi_n(x).$$

The general solution is

$$\psi_n^{(I)}(x) \;=\; A\,e^{\kappa\,x} \;+\; B\,e^{-\kappa\,x}.$$

But as $x \to -\infty$, we must avoid an unbounded solution; hence typically we set

$$\psi_n^{(I)}(x) \;=\; A\,e^{\kappa\,x} \quad \text{(assuming the } e^{-\kappa x} \text{ term blows up).}$$

Region II: $-\frac{a}{2} \le x \le \frac{a}{2}$ (where $V = 0$)

Here,

$$-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}\,\psi_n(x) = E_n\,\psi_n(x).$$

Define

$$k \;=\; \sqrt{\frac{2mE_n}{\hbar^2}}.$$

The general solution is

$$\psi_n^{(II)}(x) \;=\; C\,\cos\bigl(k\,x\bigr) \;+\; D\,\sin\bigl(k\,x\bigr).$$

Region III: $x > \frac{a}{2}$ (where $V = V_0$)

Same form as Region I:

$$-\frac{\hbar^2}{2m}\,\frac{d^2}{dx^2}\,\psi_n(x) \;=\; \bigl(E_n - V_0\bigr)\,\psi_n(x) \;=\; -\bigl(V_0 - E_n\bigr)\,\psi_n(x),$$

with the same κ as above. The general solution is

$$\psi_n^{(III)}(x) \;=\; F\,e^{\kappa\,x} + G\,e^{-\kappa\,x}.$$

But for $x \to +\infty$, finiteness requires $e^{\kappa x}$ must vanish, so typically

$$\psi_n^{(III)}(x) = G\,e^{-\kappa\,x}.$$

Boundary conditions: We require continuity of $\psi_n(x)$ and of its derivative $\psi_n'(x)$ at $x = \pm\frac{a}{2}$. These lead to transcendental equations that determine the allowed energies E_n.

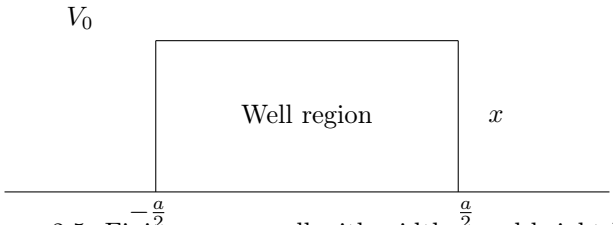

Figure 2.5: Finite square well with width a and height V_0.

Even/Odd (Symmetric/Antisymmetric) Solutions

Because the potential is symmetric about $x = 0$, we can classify solutions by parity:

$$\hat{P}\,\psi_n(x) \;=\; \psi_n(-x) \;=\; \pm\,\psi_n(x).$$

Thus we look for either *even* solutions (+ sign) or *odd* solutions (− sign).

Even solutions. An *even* wavefunction means

$$\psi_n(-x) = \psi_n(x).$$

In Region II, an even solution can be taken in the form

$$\psi_n^{(II)}(x) \;=\; A_s\,\cos\big(k\,x\big).$$

Matching at $x = \pm\frac{a}{2}$ gives conditions leading to a transcendental equation (often written as $\tan(k\,a/2) = \dots$).

Odd solutions. An *odd* wavefunction means

$$\psi_n(-x) = -\,\psi_n(x),$$

which in Region II is typically

$$\psi_n^{(II)}(x) \;=\; A_a\,\sin\big(k\,x\big).$$

Similarly, matching the boundary conditions yields a different transcendental equation (often involving $-\cot(k\,a/2)$).

Outside regions (I and III) then get exponentials of the form $e^{\kappa x}$ or $e^{-\kappa x}$ with appropriate amplitudes chosen to preserve the even or odd symmetry (i.e. the same magnitude outside $\pm a/2$, possibly with a sign flip in the odd case).

Graphical Solution and Quantization Conditions

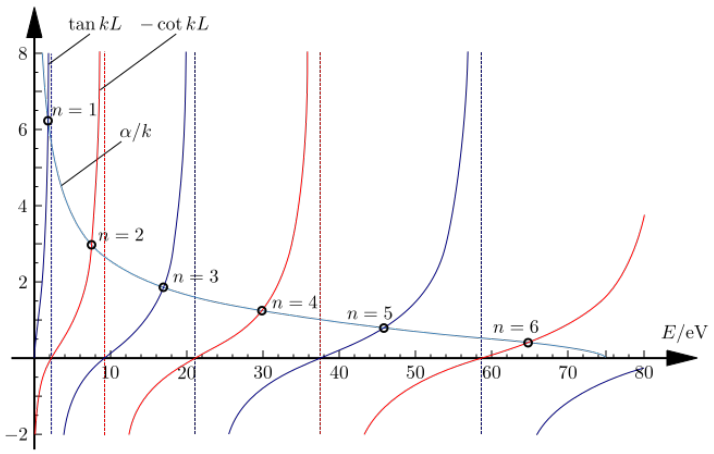

Figure 2.6

By enforcing continuity of ψ_n and ψ_n', one arrives at equations typically written in the form:

$$k = \sqrt{\frac{2m\,E}{\hbar^2}}, \quad \kappa = \sqrt{\frac{2m\,(V_0 - E)}{\hbar^2}}.$$

Then for *even* solutions:

$$\tan\big(k\,\tfrac{a}{2}\big) = \frac{\kappa}{k},$$

while for *odd* solutions:

$$-\cot\big(k\,\tfrac{a}{2}\big) = \frac{\kappa}{k}.$$

These transcendental equations can be solved numerically or by graphical methods. One typically plots the left-hand sides (tan or $-\cot$) alongside the right-hand side κ/k and finds the intersections that give the allowed k (and hence the allowed E).

As limits:
- If $V_0 \to \infty$, this reduces to the *infinite* square well of width a.
- If $a \to \infty$, one recovers a *free particle*.
- If $a \to 0$ with $V_0\,a = \text{const}$, one can get a delta-function-like potential.

Lecture 10

March 3 01:10

Chapter 3

Finite Barriers

3.1 Finite Square Well

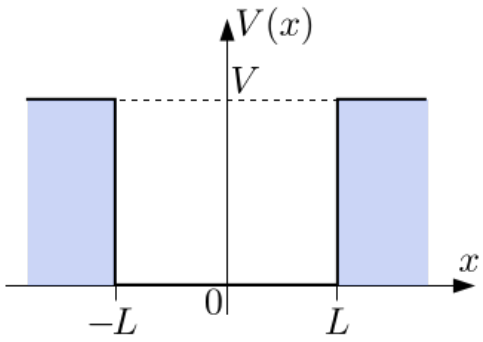

Figure 3.1

We look here at cases where

$$E > V_0$$

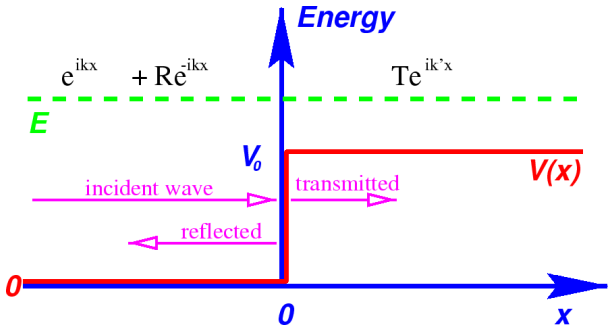

Figure 3.2

For the solution in between we have that we get to solutions of $\frac{1}{k_0}$ and $\frac{1}{k'}$. And in order to find a solution we have to match the boundary conditions at $\frac{a}{2}$. Thus, what we are doing is solving for a real k_0 with a moving wave packet. Suppose we had Region 1 and 2 where

$$\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$$

which represents the incoming and outcoming wave where $k = \sqrt{\frac{2mE}{\hbar^2}}$. We will now make the assumption that in region 2 we ignore the wave coming back where

$$\psi_2(x) = Ce^{ik_2 x}$$

Thus, we are asking the equation of how much of the wave is going to be coming through. The B coefficient is a reflection and the C coefficient is the transmission. We are assuming that there is no particle coming in, thus we ignore the D term. Therefore

$$k_2 = \sqrt{2m\frac{E - V_0}{\hbar^2}}$$

To solve, shift the solution to the left. Our first boundary condition is

$$\psi_1(x = 0) = \psi_2(x = 0) \Rightarrow A + B = C$$

$$\frac{\mathrm{d}\psi_1}{\mathrm{d}x}(x = 0) = \frac{\mathrm{d}\psi_2}{\mathrm{d}x}(x = 0) \Rightarrow ik_1(A - B) = ik_2C$$

Remark. Notice 2 equations and 3 unknowns. However, depending on the wavepacket for a given k we know what A is. Thus we are going to be computing ratios between A, B, C

$$A - B = \frac{k_2}{k_1}C$$

Solving we must have

$$2A = C\left(1 + \frac{k_2}{k_1}\right)$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

Let $\mathcal{R} = |\frac{B}{A}|^2$

$$\gamma = \frac{k_2}{k_1} \Rightarrow \mathcal{R} = \frac{(1 - \gamma)^2}{(1 + \gamma)^2}$$

To get the probability of transmission is simply

$$\mathcal{T} = 1 - \mathcal{R} = \frac{4\gamma}{(1 + \gamma)^2}$$

Notice that $\gamma = \sqrt{\frac{E - V_0}{E}}$. When this quantity $\neq 0$, then there is a finite reflection. Classically speaking, if a particle passes through there should be no reflection i.e. a particle rolling with enough energy. In the quantum case, this is not true. We can now graph these quantities to show

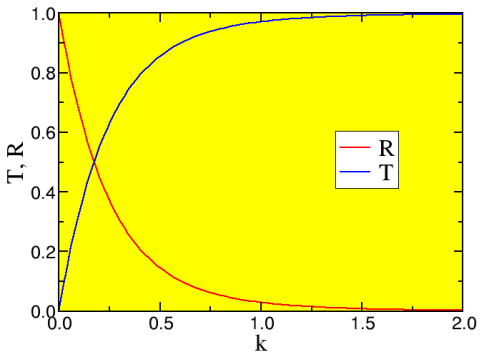

Figure 3.3

Remark. In the classical case, this would be a step function. Notice that we cannot calculate $\mathcal{T} = \frac{C}{A}$ due to the fact that the probabilities would not be conserved. Thus, we have to look at the probability current.

3.2 Probability Current

For the probability flowing we know that the incoming and outcoming currents should be $v_1|A|^2$ and $v_1|B|^2$. The probability leaving should be $v_2|C|^2$. Thus the continuity equation should be

$$v_1\left(|A|^2 + |B|^2\right) = v_2|C|^2$$

Thus we get that

$$\mathcal{T} = 1 - \mathcal{R} = \frac{v_2}{v_1}\frac{|C|^2}{|A|^2}$$

Consider the finite potential well again with

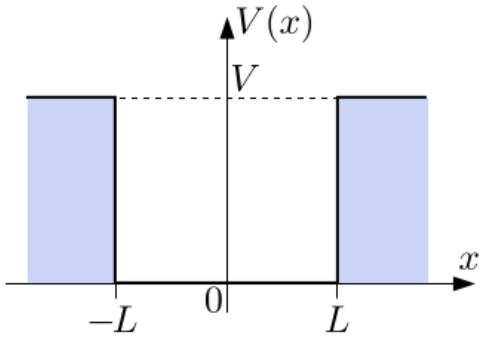

Figure 3.4

denoted as Region I, II, and III with $L = \frac{a}{2}$. Then we must have the following:
Region 1:

$$Ae^{ik_1x} + Be^{-ik_1x}$$

Region 3:

$$Ee^{ik_1x}$$

Region 2:

$$C\sin k_2x + D\cos k_2x$$

We can now solve the boundary conditions where

$$k_1 = \sqrt{2m\frac{E - V_0}{\hbar^2}}, k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{\mathrm{d}\psi_1}{\mathrm{d}x}(x = -\frac{a}{2}) = \frac{\mathrm{d}\psi_2}{\mathrm{d}x}(x = -\frac{a}{2})$$

$$\psi_1(x = -\frac{a}{2}) = \psi_2(x = -\frac{a}{2})$$

$$\frac{\mathrm{d}\psi_2}{\mathrm{d}x}\left(x = \frac{a}{2}\right) = \frac{\mathrm{d}\psi_3}{\mathrm{d}x}\left(x = \frac{a}{2}\right)$$

$$\psi_2\left(x = \frac{a}{2}\right) = \psi_3\left(x = \frac{a}{2}\right)$$

Plugging in we have

$$Ae^{-ik_1\frac{a}{2}} + Be^{ik_1\frac{a}{2}} = -C\sin k_2\frac{a}{2} + D\cos k_2\frac{a}{2}$$

$$ik_1\left[Ae^{-ik_1\frac{a}{2}} - Be^{ik_1\frac{a}{2}}\right] = k_2\left[C\cos k_2\frac{a}{2} + D\sin k_2\frac{a}{2}\right]$$

and the same with the other teams. Solving the algebra we will get the following:

$$E = e^{-2ik_1\frac{a}{2}} \cdot \frac{A}{\cos k_2 a - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin k_2 a}$$

$$\mathcal{T} = |\frac{E}{A}|^2$$

which gives an oscillating probability

Plotting the transmission as a function of energy will give

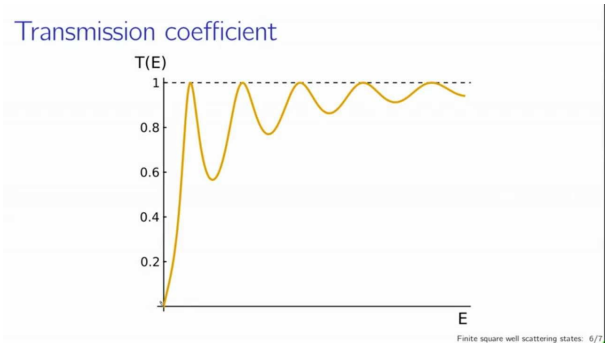

Figure 3.5

We see we get a resonance where the particle can go through the potential. where the resonance will be where

$$k_2 = n\frac{\pi}{a}$$

This is such that the transmitting and reflecting wave match up to get a resonance.

Example. Notice with semiconductors we can do this quite easily. When we inject an electron we can get a resonance tunneling where there is no resistance except the metal. Thus, the semiconductor doesn't exist.