Quantum Physics I

Exam 01 Summary

In-class Friday Feb Tues Feb 27

1 hour 50 min

Accommodations students contact me

1 page (2 sides) note sheet permitted

Topics:

- Compelling Experiments
- Math
  - Superposition of waves (phasors), Complex numbers, Distribution functions
- Quantum state functions
  - Properties of wavefunctions – Physical rules
  - Space and momentum functions
  - Probability current
  - Wavepackets
  - Expectation values
  - Operators
  - Eigenvalue equations
- The Time Independent Schrodinger Equation: 1-D cases
  - Particle in a box
    - Eigenvalues and Eigenfunctions
    - Superposition and <u>Eigenfunction expansions</u>
  - Finite square well
  - Delta function
  - Simple Harmonic Oscillator

Exam structure

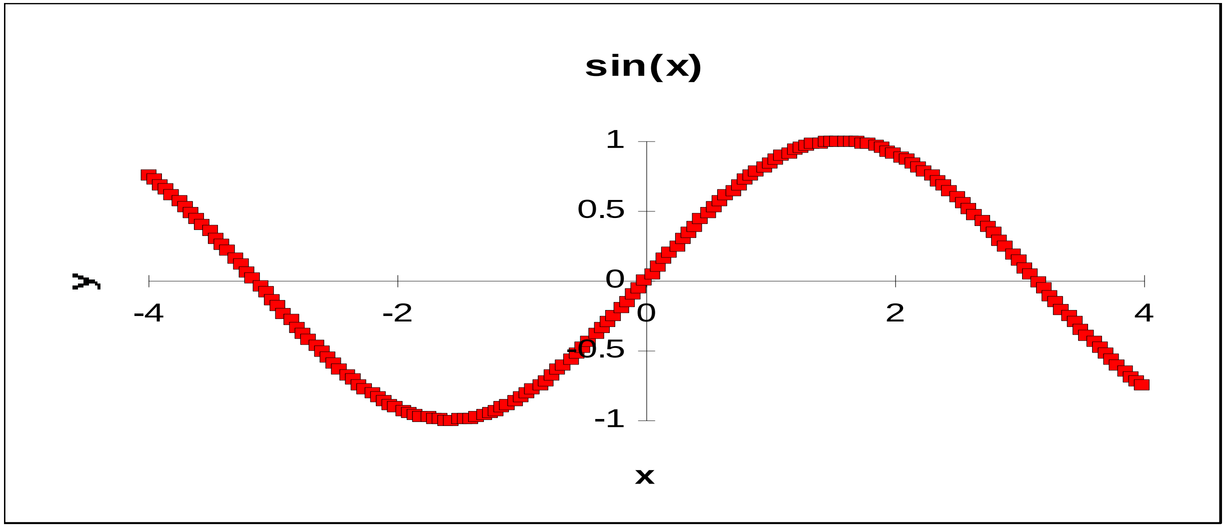
- Multiple choice ~20 pts
- Multiple choice with short explanation ~20 pts
- Short response/numerical calculation~ 20 pts
- Free response symbolic ~40 pts

Recommended resources

- Lecture notes
- In-class activities
- Homework (see solutions)
- Text (Townsend); (rec’d)Eisberg and Resnick
- Office hours

Harmonic waves

y=A sin($k(x \pm vt)+\varphi$) or y=Asin($kx \pm \omega t+\varphi$)



$$\lambda = wavelength; \quad k = \frac{2\pi}{\lambda}$$

$$T = period; \quad \omega = \frac{2\pi}{T} = 2\pi\nu$$

Complex Representation of Travelling Waves

Doing arithmetic for waves is frequently easier using the complex representation using:

$$e^{i\theta} = \cos\theta + i\sin\theta$$

So that a harmonic wave is represented as

$$\psi(x,t) = A\cos(kx - \omega t + \varepsilon)$$
$$\psi(x,t) = \mathrm{Re}\left[Ae^{i(kx-\omega t+\varepsilon)}\right]$$

Born's Postulate

If, at time t, a measurement is made to locate the particle associated with the wavefunction $\Psi(\vec{r}, t)$, then the probability $P(\vec{r}, t)dv$ that the particle will be found in the volume dv around position $\vec{r}$ is equal to:

$$\boldsymbol{P(\vec{r}, t)dv = \Psi^*(\vec{r}, t)\Psi(\vec{r}, t)dv}.$$

Where $\Psi^*(\vec{r}, t)$ denotes the complex conjugate of $\Psi(\vec{r}, t)$.

Principle of Superposition

If Ψ_1 and Ψ_2 represent two physically realizable states of a system, then the linear combination
$\Psi = c_1\Psi_1 + c_2\Psi_2$
is also a physically realizable state of the system.

Normalization

- Sometimes you will be given wave functions that lead to an integrated probability that is not already 1. (or that have an unspecified multiplicative constant.)
- Before you try to do any calculation with a wavefunction, you should make sure it is properly normalized.*

Given an un−normalized wavefunction Ψ' such that $\int_{-\infty}^{\infty} \Psi' * (\vec{r},t)\Psi'(\vec{r},t)dv = M$

just multiply Ψ' by the constant $\frac{1}{\sqrt{\mathrm{M}}}$ to create a new function:

$\Psi(\mathrm{x,t}) = \frac{\Psi'(\mathrm{x,t})}{\sqrt{M}}$ that will be normalized.

* exception: pure momentum wave

Physical constraints on wavefunctions

- A physical wavefunction must be normalizable. (The particle must be somewhere.)
- A physical wavefunction must be single valued. (It can't have two probabilities of being at the same point.)
- A physical wavefunction must be continuous.
- The spatial derivatives must be continuous unless there is an infinite potential energy step.

Expectation value

- In quantum mechanics, the ensemble average of an observable for a particular state of the system is called the **expectation value** of that observable.

$$\langle Q \rangle = \frac{\int_{-\infty}^{\infty} \Psi^* Q \Psi dv}{\int_{-\infty}^{\infty} \Psi^* \Psi dv}$$

- The **uncertainty** in the observable is the square root of the variance

$$\Delta Q = [\langle (Q - \langle Q \rangle)^2 \rangle]^{1/2}$$
$$= [\langle Q^2 \rangle - \langle Q \rangle^2]^{1/2}$$

Important results so far

Einstein− deBroglie relations: $p = \hbar k = \dfrac{h}{\lambda}; \quad E = \hbar\omega = hf$

The probability interpretation: $P(x)dx = \Psi^*\Psi dx$

$$\langle q \rangle = \int \Psi^* q(x) \Psi dx$$

The general form for a wave packet using waves with

well−defined momentum: $\Psi(x,t) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk$

where $A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$

Probability Current

- The probability current density
$$-\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\Psi\frac{\partial\Psi^*}{\partial x}\right)\equiv j_x(x)$$
is a useful concept that helps in thinking about traveling particles.

Momentum Probability Amplitude

Note that $A(k)$ clearly contains information about momentum because $k = p/\hbar$.

It is useful (later) to be able to describe the state function directly in terms of momentum states.

$\Phi(p) \equiv \frac{1}{\sqrt{\hbar}} A\left(\frac{p}{\hbar}\right)$ (the momentum probability amplitude)

Then we can rewrite the wavefunction as;

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp \quad \text{and}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ipx/\hbar} dx.$$

Note that the factor of $1/\sqrt{\hbar}$ is required for proper normailzation of Ψ and Φ.

Operators

Mathematically, an operator serves to map a function onto another function:

Example: $\boldsymbol{O_{op}f(x) = af(x)^2 + x}$

An operator that produces the momentum expectation value from the spatial wavefunction is

$$\boldsymbol{p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}}$$

Kinetic energy: $\hat{T}\psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi$

Position: $\hat{x} = x$

Constant: $\hat{C} = C$

Eigenvalue Equations

- The eigenvalue equation is a special class of operator equation where the operator operating on a function yields the original function times a constant.

  Example: $H\Psi = E\Psi$

The Schrodinger Equation

$$\hat{H}\psi = \hat{E}\psi$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x,t)\psi = i\hbar\frac{\partial\psi}{\partial t}$$

and if V(x) is constant in time,

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

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

Solving the Schrodinger Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi}{\partial t}$$

If the potential energy is independent of time, then we can start solving this equation using the separation of variables technique:

- Assume that $\Psi(x,t)=\psi(x)f(t)$

$$-f(t)\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)f(t)=i\hbar\psi(x)\frac{\partial \mathrm{f(t)}}{\partial t}$$

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=i\hbar\frac{1}{f(t)}\frac{\partial \mathrm{f(t)}}{\partial t}$$

And the only way the two sides can be equal for a x and t is if they are equal to a constant (which we will call *E*)

Solving the Schrodinger Equation

$$-\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$$

Solving $i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t}=E$, $\frac{df(t)}{f(t)}=-i\frac{E}{\hbar}dt$ and integrating both sides:

$$\ln\big(f(t)\big)-\ln\big(f(0)\big)=-i\frac{E}{\hbar}t$$

$$f(t)=Ce^{-i\frac{E}{\hbar}t}=Ce^{-i\omega t}$$

And the left hand side:

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

Is known as the time-independent Schrodinger Equation

Solution for $\psi(x)$ for constant V(x)

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

And setting $k^2 = \frac{2m}{\hbar^2}(E - V)$ for $E > V$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0$$

Which has solutions:

$\psi(x) = Ae^{ikx}$and Be^{-ikx}

So the overall solution is:

$\Psi(x,t) = Ae^{-i(kx+\omega t)} + B\, e^{i(kx-\omega t)}$

Traveling waves!

Particle in a well with infinite walls

- $V(x) = 0\ for\ 0 < x < L$ and infinity for $|x| > L$.
- Inside the well:
  $\Psi(x,t) = (Ae^{-i(kx)} + B\ e^{i(kx)})\ e^{-i\omega t}$
- Boundary conditions:

$\psi(x) = 0\ at\ x = 0\ and\ x = L$

$\psi(0) = 0\ \rightarrow\ A + B = 0$ so $-A = B$

$\psi(x) = A(e^{-i(kx)} - e^{i(kx)}) = -Asin(kx)$

$\psi(L) = 0\ \rightarrow\ Asin(ka) = 0\ \rightarrow\ ka = n\pi$

$k_n = n\frac{\pi}{a}$ where n is an integer. (quantization)

Particle in a well

$k^2 = \frac{2m}{\hbar^2} E \quad and \quad k^2 = \frac{n^2\pi^2}{L^2}$ so

$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2}$ (quantized)

Another way of finding this result:

λ that meets the boundary conditions must be such that $\frac{n\lambda_n}{2} = L$ and since $p = \frac{h}{\lambda}$ and $E = \frac{p^2}{2m}$ we have $E = \frac{h^2 n^2}{8mL^2}$.

The formal TISE approach allows us to deduce a lot more physics.

Particle in a well with infinite walls

- $V(x) = 0\ for\ 0 < x < L$ and infinity for $|x| > L$.
- Inside the well:
  $\Psi(x,t) = (Ae^{-i(kx)} + B\ e^{i(kx)})\ e^{-i\omega t}$
- Boundary conditions:

$\psi(x) = 0\ at\ x = 0\ and\ x = L$

$\psi(0) = 0\ \rightarrow\ A + B = 0$ so $-A = B$

$\psi(x) = A(e^{-i(kx)} - e^{i(kx)}) = -Asin(kx)$

$\psi(L) = 0\ \rightarrow\ Asin(kL) = 0\ \rightarrow\ kL = n\pi$

$k_n = n\frac{\pi}{L}$ where n is an integer. (quantization)

Normalization

Normalization requires that

$$P[0, L] = 1 = \int_0^L A^2 \sin^2 \frac{n\pi x}{L} \, dx$$

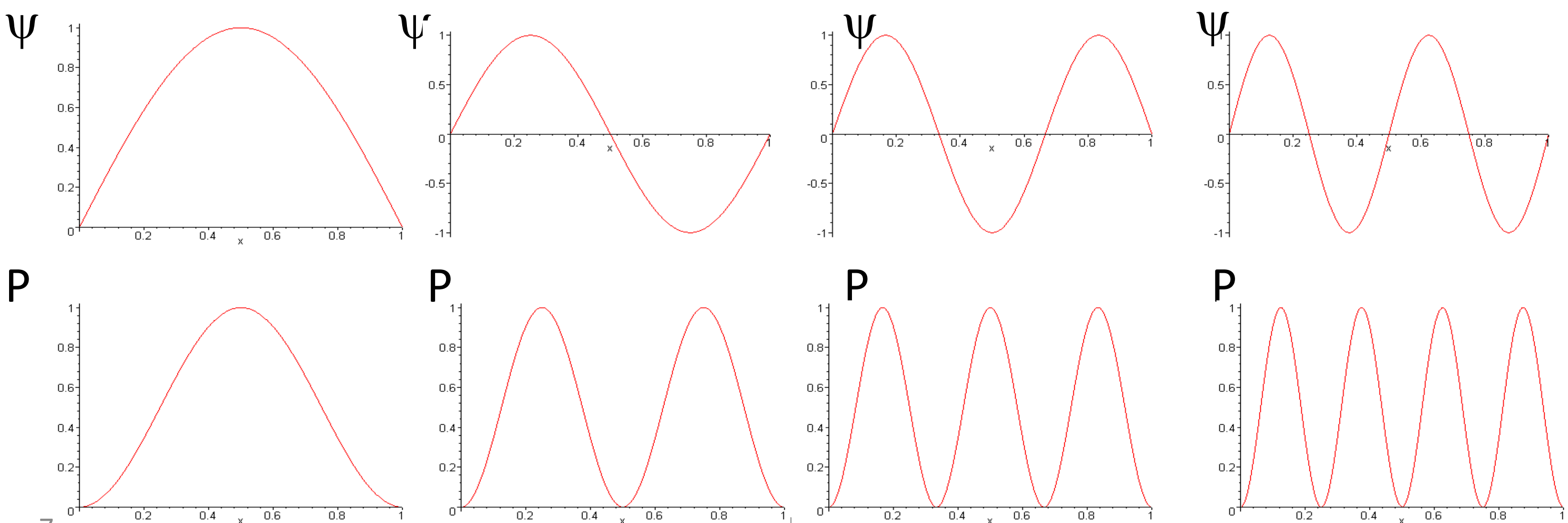
which leads to $A = \sqrt{\frac{2}{L}}$.

Particle in a well

$$k^2 = \frac{2m}{\hbar^2}E \quad and \quad k^2 = \frac{n^2\pi^2}{L^2} \text{ so}$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2} \text{ (quantized)}$$

$$\Psi(x,t) = \sqrt{\frac{2}{L}}\, sin\left(\frac{n\pi x}{L}\right) e^{\frac{iE_n t}{\hbar}}$$



Square well centered at x=0

- If we center the square well at x=0 so that it extends from –L/2 to L/2, then the general solutions remain the same but the boundary conditions change.
- $E_n, k_n, and\ A$ remain unchanged.
- The solutions are then the same as those found in the text.

$$\psi_n(x) = A\cos\left(\frac{n\pi x}{L}\right) for\ n = odd$$

$$\psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right) for\ n = even$$

Square well continued

- Next: Compute momentum distribution, averages and standard deviations of position, momentum, and energy.
- We will just do the computations for the even states ($\cos\left(\frac{n\pi x}{L}\right)$) of the well centered at 0 because the arithmetic is easier. We can generalize for the odd states.

Expectation values of position

$$\langle x \rangle = \int \Psi^* x \Psi dx = \frac{2}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} x cos^2\left(\frac{n\pi x}{L}\right) dx = 0$$

(Why didn't I have to carry out the integration?)

$$\langle x^2 \rangle = \frac{2}{L}\int_{-L/2}^{L/2} x^2 \cos^2\left(\frac{n\pi x}{L}\right) dx$$

$$= \frac{1}{L}\int_{-L/2}^{L/2} x^2 (1 - \cos\left(\frac{2n\pi x}{L}\right)) dx$$

$$= \frac{1}{L}\left(\frac{x^3}{3} - \int_{-\frac{L}{2}}^{\frac{L}{2}} x^2 \cos\left(\frac{2n\pi x}{L}\right)\right) = L^2\left(\frac{1}{3} - \frac{1}{2n^2\pi^2}\right)$$

$$\sigma_x = \frac{L}{2n\pi}\left(\frac{n^2\pi^2}{3} - 2\right)^{\frac{1}{2}}$$ (=0.18, 0.26, 0.279, 0.283…0.289)

Momentum in the square well

$$\Psi(x,t) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right)e^{i\omega t}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\Psi(x,0)e^{-ipx/\hbar}dx = \frac{1}{\sqrt{L\pi\hbar}}\int_{-L/2}^{L/2}\cos\left(\frac{n\pi x}{L}\right)e^{ipx/\hbar}dx$$

$$= \frac{1}{\sqrt{L\pi\hbar}}\int_{-L/2}^{L/2}\cos\left(\frac{n\pi x}{L}\right)(\cos(px/\hbar) + i\sin(px/\hbar))dx$$

$$= \frac{1}{\sqrt{L\pi\hbar}}\int_{-L/2}^{L/2}\cos\left(\frac{n\pi x}{L}\right)\cos(\frac{px}{\hbar})dx$$

$$= \frac{1}{2\sqrt{L\pi\hbar}}\int_{-L/2}^{L/2}\left[\cos\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)x\right) + \cos\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)x\right)\right]dx$$

$$= \frac{1}{2\sqrt{L\pi\hbar}}\left[\frac{\sin\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)x\right)}{\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\right)} + \frac{\sin\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)x\right)}{\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)\right)}\right]_{-L/2}^{L/2}$$

$$= \frac{1}{\sqrt{L\pi\hbar}}\left[\frac{\sin\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\frac{L}{2}\right)}{\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\right)} + \frac{\sin\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)\frac{L}{2}\right)}{\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)\right)}\right]$$

Momentum in square well

$$\Phi(p) = \frac{L}{2}\frac{1}{\sqrt{L\pi\hbar}}\left[\frac{\sin\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\frac{L}{2}\right)}{\left(\left(\frac{n\pi}{L}-\frac{p}{\hbar}\right)\frac{L}{2}\right)}+\frac{\sin\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)\frac{L}{2}\right)}{\left(\left(\frac{n\pi}{L}+\frac{p}{\hbar}\right)\frac{L}{2}\right)}\right]$$

$$\Phi(p) = \sqrt{\frac{L}{4\pi\hbar}}\left[\frac{\sin\left(\left(\frac{n\pi}{2}-\frac{L}{2\hbar}p\right)\right)}{\left(\frac{n\pi}{2}-\frac{L}{2\hbar}p\right)}+\frac{\sin\left(\frac{n\pi}{2}+\frac{L}{2\hbar}p\right)}{\left(\frac{n\pi}{2}+\frac{L}{2\hbar}p\right)}\right]$$

$$A(k)=\sqrt{\frac{L}{4\pi\hbar}}\left[\frac{\sin\left(\left(\frac{n\pi}{2}-\frac{kL}{2}\right)\right)}{\left(\frac{n\pi}{2}-\frac{kL}{2}\right)}+\frac{\sin\left(\frac{n\pi}{2}+\frac{kL}{2}\right)}{\left(\frac{n\pi}{2}+\frac{kL}{2}\right)}\right]$$

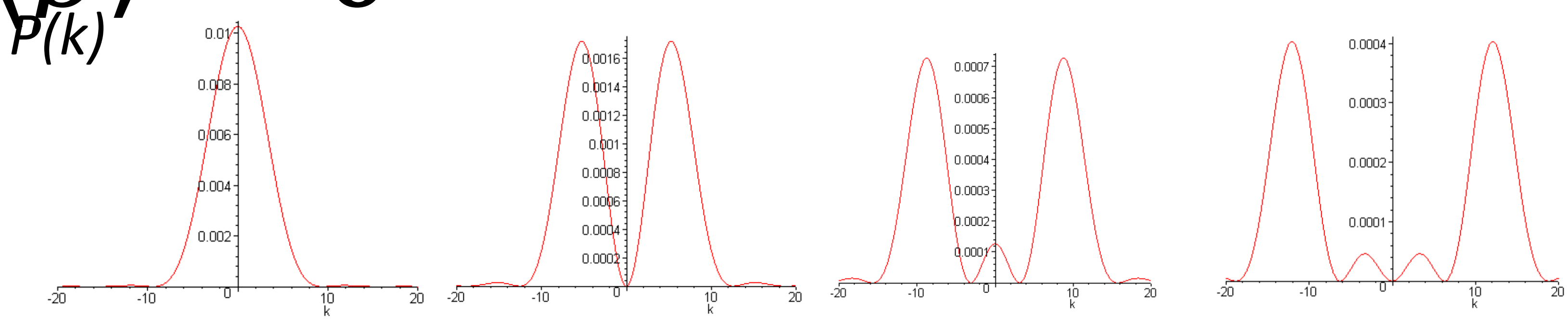
Momentum in square well

Now to calculate expectation value of momentum,

$$\langle \mathrm{p} \rangle = \int_{-\infty}^{\infty} \Phi^* p \Phi dp = \int_{-\infty}^{\infty} \sqrt{\frac{L}{4\pi\hbar}} \left[\frac{\sin\left(\left(\frac{n\pi}{2} - \frac{L}{2\hbar}p\right)\right)}{\left(\frac{n\pi}{2} - \frac{L}{2\hbar}p\right)} + \frac{\sin\left(\frac{n\pi}{2} + \frac{L}{2\hbar}p\right)}{\left(\frac{n\pi}{2} + \frac{L}{2\hbar}p\right)} \right]^2 p dp$$

(We don′t really want to calculate this awful thing, so let′s think about symmetry. We note that Φ is symmetric about $p = 0$. This means that $p\Phi$ is an odd function, and therefore the integral is zero.)

$$\langle p \rangle = 0$$



Expectation values for the square well: Momentum

$$\langle p_x \rangle = \int_{-a}^{a} \Psi^*(x,t)\hat{p}_x \Psi(x,t)dx = \int_{-a}^{a} \Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)dx$$

$$= \frac{-i\hbar 2}{L}\int_{-a}^{a} \cos\left(\frac{n\pi x}{L}\right)\frac{\partial}{\partial x}\left(\cos\left(\frac{n\pi x}{L}\right)\right)dx$$

$$= \frac{-i\hbar n 2\pi}{L^2}\int_{-a}^{a} \cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)dx = \frac{-i\hbar n 2\pi}{L^2}\int_{-a}^{a} u\,du = 0$$

$$\langle p_x^2 \rangle = -\int_{-a}^{a} \Psi^*(x,t)\left(\hbar^2\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)dx = \frac{\hbar^2\pi^2 n^2}{L^3}\int_{-a}^{a} \cos^2\left(\frac{n\pi x}{L}\right)dx$$

$$\langle p_x^2 \rangle = \frac{\hbar^2\pi^2 n^2}{L^3}\frac{L}{2} = \frac{\hbar^2\pi^2 n^2}{2L^2}$$

Expectation values in the square well: Momentum uncertainty

We just found that $\langle p \rangle = 0$ and $\langle p_x^2 \rangle = \frac{\hbar^2 \pi^2 n^2}{2L^2}$.

The standard deviation of the momentum is thus

$$\sigma_p = \frac{\hbar \pi n}{\sqrt{L}}$$

Particle in a box
Expectation value and uncertainty in energy

The kinetic energy operator is: $\hat{T} = \dfrac{\hat{p}^2}{2m}.$

Since we previously solved for $\left\langle p_n^2 \right\rangle$ we can easily solve for $\left\langle T \right\rangle$.

$$\left\langle T_n \right\rangle = \frac{\left\langle p_n^2 \right\rangle}{2m} = \frac{1}{2m}\left(\frac{n\pi\hbar}{L}\right)^2$$

The lowest allowed state has n=1,

so expectation value of the kinetic energy is always > zero.

Another remarkable observation is that: $\left\langle T^2 \right\rangle - \left\langle T \right\rangle^2 = 0.$

There is no uncertainty in the energy!

Particle in a box – Probability current

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) e^{-i\omega_n t}$$

$$j(x,t) \equiv \frac{-i\hbar}{2m}\left[\Psi^* \frac{\partial}{\partial x}\Psi - \Psi \frac{\partial}{\partial x}\Psi^*\right]$$

$$= \frac{-i\hbar}{2m}\frac{2}{L}[k \sin k_n\, x \sin k_{nx} - k \sin k_n\, x \sin k_{nx}]$$

$$= 0$$

NOTE: The probability current is zero for any real space function.

Completeness

Any physically admissible wavefunction can be expanded in the complete set of eigenfunctions, provided that the wavefunction obeys the same boundary conditions as the eigenfunctions.

$$\psi(x) = \sum_i c_i \psi_i$$

We find the coefficients using orthogonality!

$$\int \psi(x)\psi_n(x)dx = \int \sum_i c_i \psi_i \psi_n \, dx = c_i$$

Mixed States

- A wavefunction that satisfies the Schrodinger Equation and obeys the same boundary conditions as the eigenfunctions can be expressed as the sum of eigenstates (called an expansion in eigenfunctions)

$$\Psi(x,t) = c_1\psi_1(x,t) + c_2\psi_2(x,t) \ldots$$

- We can find the expansion coefficients $c_1, c_2 \ldots$ by using the orthogonality of eigenfunctions.

$$c_n = \int \Psi(x,0)\psi_n(x,0)dx$$

(Integrated over the range of the eigenfunctions.)

Time evolution

- Once the expansion coefficients are known, we can calculate the time evolution of the wavefunction.

$$\psi_i(x,t) = \psi_i(x,0)e^{i\omega_i t}$$

$$\Psi(x,t) = \sum_i c_i \psi_i(x,t)$$

- Finding the coefficients:
PHYS2210Spring2022_Class08_1DWavefunctionCoefficients.ipynb
- Viewing time evolution:
Falstad.com/qm1d

Calculating energy using Eigenfunction Expansion

- $\langle E \rangle = \int \Psi^* \widehat{H} \Psi dx$
- $\int (c_1\psi_1 + c_2\psi_2)^* H (c_1\psi_1 + c_2\psi_2)$dx
- $\int (c_1\psi_1 + c_2\psi_2)^* (E_1 c_1\psi_1 + E_2 c_2\psi_2)$dx
- $\langle E \rangle = c_1^2 E_1 + c_2^2 E_2$

Piecewise potentials 1

Solution to the TISE in a region where V is a constant and E>V:

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

Guess: $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m} = (E - V) \Rightarrow k = \pm\sqrt{\frac{2m(E - V)}{\hbar^2}}$$

$$\psi = Ae^{ikx} + Be^{-ikx}$$

Piecewise potentials 2

Solution to the TISE in a region where V is a constant and E<V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - |E-V|\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E-V| \qquad \Rightarrow \qquad k = \pm i\sqrt{\frac{2m|E-V|}{\hbar^2}}$$

Let $K = ik = \pm\sqrt{\frac{2m|E-V|}{\hbar^2}}$ (∴ K is a real number)

$\psi = Ae^{Kx} + Be^{-Kx}$ (exponential growth or decay)

Some “intuitive” rules for sketching wavefunctions*

1. Solutions for the Schrodinger equation curve toward the x-axis in classically allowed $(E > V\ )$ regions and away from the axis in classically forbidden regions.
2. For bound states, the wavefunction must go to zero for large distances outside the well. (must be normalizable)
3. Curvature increases for larger $|E - V(x)|$.
4. Solutions are continuous and smooth if the potential has no infinite steps.
5. Energy eigenfunctions have an integer number of antinodes on classically allowed regions.
6. The wavefunction amplitude is usually larger in regions with small E>V.

* From https:’’www.asc.ohio-state.edu/physics/ntg/H133/handouts/wavefunctions.pdf

Illustrated “intuitive” rules

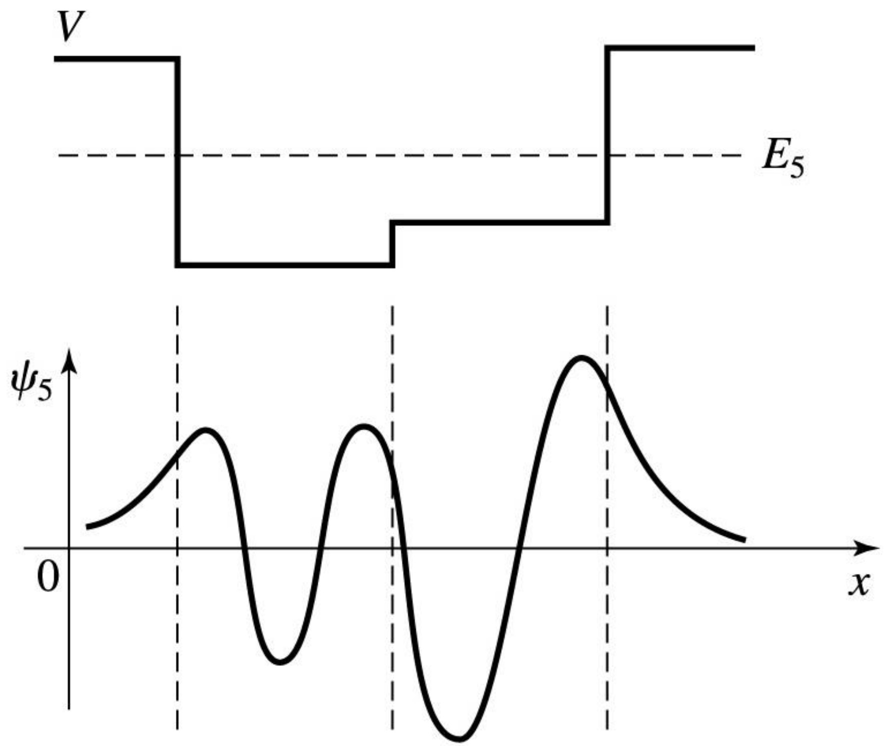


Figure 4.10 copyright 2009 University Science Books

1. Curvature direction.
2. Goes to zero outside well.
3. Curvature magnitude.
4. Continuity/smoothity.
5. Integer antinodes.
6. Wavefunction amplitude

* from Townsend Ch 4

Piecewise potentials 1

Solution to the TISE in a region where V is a constant and E>V:

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

Guess: $\psi = e^{ikx}$

$$-\frac{\hbar^2 k^2}{2m}=(E-V)\Rightarrow k=\pm\sqrt{\frac{2m(E-V)}{\hbar^2}}$$

$$\psi = Ae^{ikx}+Be^{-ikx}$$

Piecewise potentials 2

Solution to the TISE in a region where V is a constant and E<V:

$$\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} - |E-V|\psi(x) = 0$$

Guess: $\psi = e^{ikx}$

$$\frac{\hbar^2 k^2}{2m} = -|E-V| \qquad \Rightarrow \qquad k = \pm i\sqrt{\frac{2m|E-V|}{\hbar^2}}$$

Let $K = ik = \pm\sqrt{\frac{2m|E-V|}{\hbar^2}}$ ($\therefore$ K is a real number)

$\psi = Ae^{Kx} + Be^{-Kx}$ (exponential growth or decay)

The physical requirement that the wavefunction must be normalizable means that it cannot blow up at $\pm\infty, so$

$$\psi(x) = \begin{cases} Ce^{Kx} \ for \quad x < -\frac{a}{2} \\ A \sin k\,x + B \cos k\,x \ \text{ for } -\frac{a}{2} < x < \frac{a}{2} \\ Ge^{-Kx} \ for \quad x > \frac{a}{2} \end{cases}$$

Symmetry of the potential leads to the requirement that the probability density for an eigenfunction be an even function of x. This leads to the requirement that the eigenfunctions be either even or odd.

$$\psi_{even}(x) = \begin{cases} Ce^{Kx} \ \ for \ \ x < -\frac{a}{2} \\ B\cos k\,x \ \text{ for } -\frac{a}{2} < x < \frac{a}{2} \\ Ce^{-Kx} \ for \ \ x > \frac{a}{2} \end{cases}$$ (Note that we set C=G.)

$$\psi_{odd}(x) = \begin{cases} Ce^{Kx} \ \ for \ \ x < -\frac{a}{2} \\ B\sin kx \ \text{ for } -\frac{a}{2} < x < \frac{a}{2} \\ -Ce^{-Kx} \ for \ \ x > \frac{a}{2} \end{cases}$$ (Note that we set C=-G.)

From these equations alone, we can find the allowed energies:

$$\frac{\mathrm{K}}{\mathrm{k}} = \tan\left(\frac{kL}{2}\right) \text{ for odd n (even parity)}$$

$$\frac{\mathrm{K}}{\mathrm{k}} = -\cot\left(\frac{kL}{2}\right) \text{ for even n (odd parity)}$$

The even parity state will be the lowest energy state.

These equations cannot be solved in closed form, but we can find the numerical solutions using "solve" in Maple

or by plotting each side as a function of k.

On the next slide we'll switch to terms of energy because everyone does.

Let

$\xi = \frac{ka}{2}$ (a measure of kinetic energy in the well)

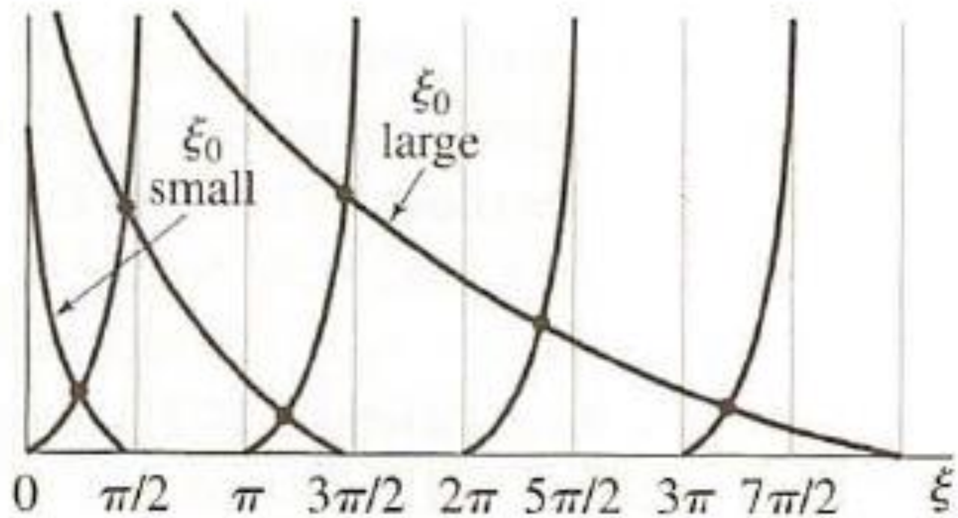
$\xi_0 = \frac{a}{\hbar}\sqrt{\frac{mV}{2}}$ (a measure of the depth of the well)

Then

$$\tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$$

$$-\cot\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$$

Even solutions: Plot both the left hand and right hand side of $\tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$ as a function of ξ.



- Intersections are allowed energies
- $\tan\xi$ goes to ∞ each time ξ goes through odd $\frac{\pi}{2}$.
- If well depth is small, then only one solution can be found.
- If well depth is large, solutions approach infinite well.

The Dirac Delta Function

- Definition: $\int_{-\infty}^{\infty} \delta(x - x_0) f(x) dx = f(x_0)$
- $\delta(x - x_0) = \begin{cases} 0 \; for \; x \neq x_0 \\ \infty \;\; for \; x = x_0 \end{cases}$
- $\int \delta(x - x_0) dx = 1$
- $\delta(x) \;\; is \; real$
- $\delta(x) \; is \; even$

The delta function potential

$$\hat{H}\psi = \hat{E}\psi$$

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

with λ negative, for an attractive potential.

http://galileo.phys.virginia.edu/classes/751.mf1i.fall02/OneDimSchr.htm

$\psi = Ae^{Kx} + Be^{-Kx}$
So for negative x, $\psi^- = Ae^{Kx}$
and for positive x, $\psi^+ = Be^{-Kx}$
Continuity of the wavefunction gives $\psi^- = \psi^+ \; so \; A = B$.
The slope on the two sides is discontinuous due to the infinite δ function.
$\left.\frac{d\psi}{dx}\right|_{-\beta} = KA$; $\left.\frac{d\psi}{dx}\right|_{\beta} = -KA$; for small β, so $\left.\frac{d\psi}{dx}\right|_{-\beta}$ $\left.\frac{d\psi}{dx}\right|_{\beta} - \left.\frac{d\psi}{dx}\right|_{-\beta}$
$= -2KA$;
Returning to the Schrodinger equation,
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + \lambda\delta(x)\psi = E\psi$$
We integrate both sides once in x, from $-\beta$ to $+\beta$.
$$-\int_{-\beta}^{\beta}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi dx + \int_{-\beta}^{\beta}\lambda\delta(x)\psi dx = \int_{-\beta}^{\beta}E\psi dx$$
The rhs goes to zero as $\beta \Rightarrow 0$ because the integrand is finite.

so, $\displaystyle\int_{-\beta}^{\beta} \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi dx = \int_{-\beta}^{\beta} \lambda\delta(x)\psi dx$

Doing both integrals separately, $\displaystyle\left.\frac{\hbar^2}{2m}\frac{\partial\psi}{\partial x}\right|_{-\beta}^{\beta} = \lambda\psi(0)$

and substituting $\displaystyle\left.\frac{\partial\psi}{\partial x}\right|_{-\beta}^{\beta} = -2AK$ (from the previous slide),

we have $\displaystyle -\frac{\hbar^2 K}{m} = \lambda$

$$K = -\frac{\lambda m}{\hbar^2} \quad \Rightarrow \quad E = \frac{\hbar^2 K^2}{2m} = -\frac{m\lambda^2}{2\hbar^2}$$

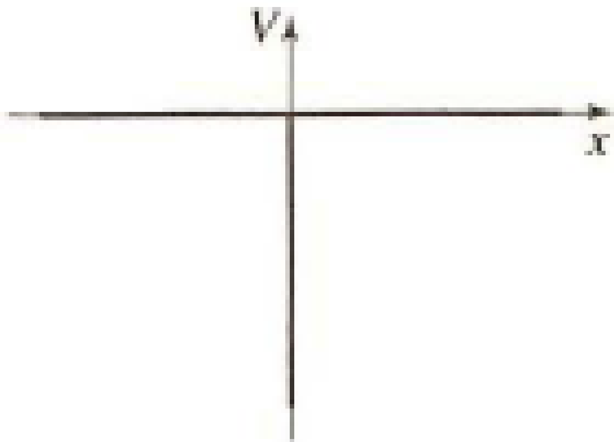


Figure 4.14 The Dirac delta function potential energy (4.77).

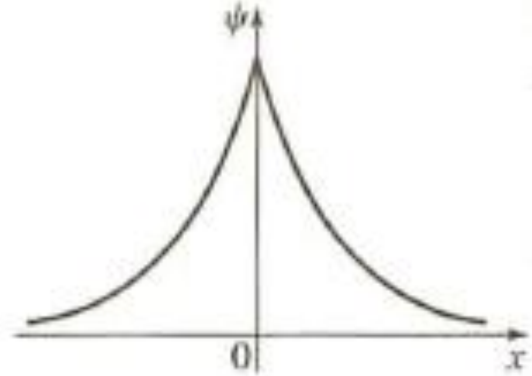


Figure 4.15 The wave function (4.85) for a particle bound in a Dirac delta function potential energy well.

$$\psi(x) = \mathrm{A}\exp\left(-\frac{\lambda m}{\hbar^2}|x|\right)$$

is the only bound state.