Week 3

Time-Independent Problems in One-Dimensional Systems

3.1 Infinite Well Motion

1/17:

- We begin today by building up to the uncertainty principle another, more general way.
- Recall that what we are aiming for is

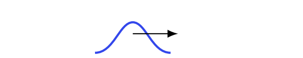
$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

where $\Delta p_x, \Delta x$ are the uncertainties in the determination of the momentum and position, respectively:

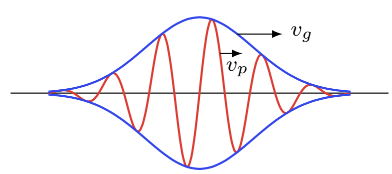
$$(\Delta p_x)^2 = \langle(\hat{\vec{p}}_x - \langle\hat{\vec{p}}_x\rangle)^2\rangle = \langle\hat{\vec{p}}_x{}^2\rangle - \langle\hat{\vec{p}}_x\rangle^2 \qquad (\Delta x)^2 = \langle\hat{\vec{x}}^2\rangle - \langle\hat{\vec{x}}\rangle^2$$

- Example of the uncertainty principle: For a plane wave, we know the momentum but not the position. That is, $\Delta x \to \infty$ and $\Delta p_x \to 0$.
- More generally, for a **wave packet**, we know only approximately the position and momentum.
- **Wave packet**: A continuous sum of waves of different frequencies. *Given by*

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \mathrm{e}^{i(kx-\omega(k)t)} \,\mathrm{d}k$$



(a) A wave packet.



(b) Group and phase velocity.

Figure 3.1: Wave packets.

  - Note that the above formula only applies to the one dimensional case.
- Let's investigate the case of a wave packet of free particles.
  - In this case,

$$\omega(k) = \frac{\hbar k^2}{2m}$$

- This is derived from
$$\hbar\omega = E = \frac{p^2}{2m} = \frac{(\hbar k)^2}{2m}$$
by cancelling an $\hbar$ from both sides.

- Let's assume that $\phi(k)$ is a narrowly peaked function around a certain value k_0.
- Then we can expand

$$\begin{aligned}
\omega(k) &= \omega(k_0) + \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} (k-k_0) + \cdots \\
&= \omega(k_0) + \left.\frac{\hbar k}{m}\right|_{k=k_0} (k-k_0) + \cdots \\
&= \omega(k_0) + \underbrace{\frac{\hbar k_0}{m}}_{\omega_0'}(k-k_0) + \cdots
\end{aligned}$$

- Define $s := k - k_0$.
- Then $k = k_0 + s$ and $\mathrm{d}k = \mathrm{d}s$, so

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k_0+s)\mathrm{e}^{i((k_0+s)x-(\omega(k_0)+\omega_0's)t)} \,\mathrm{d}s \\
&= \frac{1}{\sqrt{2\pi}}\mathrm{e}^{i(k_0x-\omega(k_0)t)} \int_{-\infty}^{\infty} \phi(k_0+s)\mathrm{e}^{is(x-\omega_0't)} \,\mathrm{d}s
\end{aligned}$$

- It follows that
$$|\psi(x,t)|^2 = \frac{1}{2\pi}\left|\int_{-\infty}^{\infty} \phi(k_0+s)\mathrm{e}^{is(x-\omega_0't)} \,\mathrm{d}s\right|^2 = f(x-\omega_0't)$$
  - In words, the probability density is a function of $x - \omega_0't$, so the packet moves with **group velocity** $\omega_0' = \hbar k_0/m = p_0/m$.
- Implication: The wave packet moves with a velocity that is equal ot the classical velocity
$$\left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0} = \frac{p_0}{m}$$

- **Group velocity**: A measure of the velocity of a wave packet. *Denoted by* $\boldsymbol{v_g}$, $\boldsymbol{v_{\text{group}}}$. *Given by*
$$v_{\text{group}} = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0}$$
- **Phase velocity**: A measure of the velocity of the ripples. *Denoted by* $\boldsymbol{v_p}$, $\boldsymbol{v_{\text{phase}}}$. *Given by*
$$v_{\text{phase}} = \frac{\omega(k_0)}{k_0} = \frac{\hbar k_0}{2m} = \frac{v_{\text{group}}}{2}$$
- Explicit example of a wave packet: A **Gaussian wave packet**.
- **Gaussian wave packet**: A one-dimensional wave packet of the following form. *Given by*
$$\psi_0(x,t) = \left(\frac{2}{\pi\sigma^2}\right)^{1/4} \exp\left[-\frac{(x-v_gt)^2}{\sigma^2}\right]\mathrm{e}^{i(k_0x-v_pt)}$$
  - This means that we must have used the following definition of $\phi(k)$ in the original definition.
$$\phi(k) = \left(\frac{\sigma^2}{2\pi}\right)^{1/4} \exp\left[-\frac{\sigma^2(k-k_0)^2}{4}\right]$$

- Uncertainty analysis of a Gaussian wave packet.
  - The uncertainties Δx and Δk are associated with the widths of the Gaussians, as one can determine by computing. Indeed, at $t = 0$,

$$\langle \hat{\vec{x}} \rangle = 0 \qquad \langle \hat{\vec{x}}^{\,2} \rangle = (\Delta x)^2 \qquad \langle (k - k_0)^2 \rangle = (\Delta k)^2$$

    - Indeed, since $\langle k \rangle = k_0$, we know that $\langle (k-k_0)^2 \rangle = \langle k^2 \rangle - k_0^2$.
  - For Gaussians, normalized as $\int |\psi|^2 = 1$, we obtain

$$\left(\frac{1}{\pi\sigma^2} \right)^{1/2} \int_{-\infty}^{\infty} u^2 \exp\left(-\frac{u^2}{\sigma^2} \right) \mathrm{d}u = (\Delta u)^2 = \frac{\sigma^2}{2}$$

    - How do we get this??
  - It follows that the value of Δu coincides well with the departure from the central value for which the exponential in $|\psi|^2$ or $|\phi|^2$ is $\mathrm{e}^{-1/2}$.
  - Altogether, we get

$$\Delta x = \frac{\sigma}{2} \qquad \Delta k = \frac{1}{\sigma}$$

    so

$$\begin{aligned} \Delta x \Delta k &= \frac{1}{2} \\ \Delta x \Delta p_x &= \frac{\hbar}{2} \end{aligned}$$

    for a Gaussian wave packet.
  - Implication: The Gaussian function minimizes the product of the position and momentum uncertainties!
- We now move onto discussing the **infinite square well** potential, a one-dimensional time-independent potential for which we can solve the Schrödinger equation exactly.

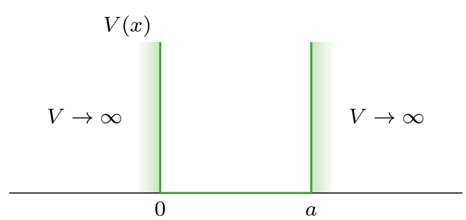


Figure 3.2: Infinite square well.

- **Infinite square well**: The potential energy function that vanishes for $0 < x < a$ and tends to infinity for $x \leq 0$ and $x \geq a$. *Given by*

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

- We would like to obtain energy eigenstates for this potential. That is, we seek eigenvalues and eigenfunctions for

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

  - Any such eigenstate ψ will have $\psi(x) = 0$ in the region of space where $V \to \infty$.

- Hence, the Schrödinger equation reduces to the boundary-value problem

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi \qquad\qquad \psi(0) = \psi(a) = 0$$

- The above ODE may be expressed in the following equivalent form

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -\left(\frac{2mE}{\hbar^2}\right)\psi$$

- Observe that this ODE is of the same form as the classical harmonic oscillator equation $\mathrm{d}^2x/\mathrm{d}t^2 = -(k/m)x$. Thus, it admits a similar set of solutions:

$$\psi_n(x) = C\sin\left(\sqrt{\frac{2mE_n}{\hbar^2}}x\right) \qquad\qquad \sqrt{\frac{2mE_n}{\hbar^2}}a = n\pi,\ n = 1, 2, \dots$$

- It follows that

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

- The coefficient C can be fixed via the normalization requirement, as follows.

$$\begin{aligned}
1 &= \int_0^a |\psi_n(x)|^2\,\mathrm{d}x \\
&= C^2\int_0^a \sin^2\left(\frac{\pi nx}{a}\right)\mathrm{d}x \\
&= C^2\int_0^a \frac{1-\cos\left(\frac{2\pi nx}{a}\right)}{2}\,\mathrm{d}x \\
&= \frac{C^2}{2}\left[\int_0^a \mathrm{d}x - \int_0^a \cos\left(\frac{2\pi nx}{a}\right)\mathrm{d}x\right] \\
&= \frac{C^2}{2}\left[a - \underbrace{\frac{a}{2n\pi}\sin\left(\frac{2\pi nx}{a}\right)\bigg|_0^a}_{0}\right] \\
&= \frac{aC^2}{2} \\
C &= \sqrt{\frac{2}{a}}
\end{aligned}$$

- Therefore, the complete eigenfunctions and eigenvalues are

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi nx}{a}\right) \qquad\qquad E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

- A general solution is therefore given by the following, where ψ_n, E_n are defined as above.

$$\psi(x,t) = \sum_n c_n\psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$$

- The probability density of the infinite square well potential is time-independent.

Proof. Observe that given any individual eigenstate of energy

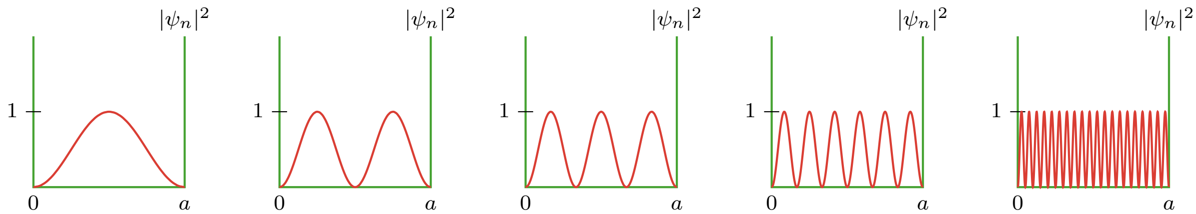
$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_nt/\hbar}$$

we have that

$$|\psi_n(x,t)|^2 = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\left(\frac{\pi nx}{a}\right)$$

□

- Let's investigate the form of the probability density for a few n.

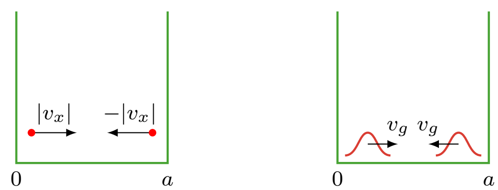


(a) $n = 1$. (b) $n = 2$. (c) $n = 3$. (d) $n = 6$. (e) $n \gg 1$.

Figure 3.3: Infinite square well probability density.

  – Recall that the average height of a sine wave is half its amplitude. Thus the average probability density is
$$\frac{1}{2} \cdot \frac{2}{a} = \frac{1}{a}$$

- Recovering "motion," in the sense that $\mathrm{d}/\mathrm{d}t\,(\langle\psi|\hat{\vec{x}}|\psi\rangle) \neq 0$



(a) Classical. (b) Quantum.

Figure 3.4: Infinite square well motion.

  – We obtain motion upon superimposing different eigenstate wave functions.
  – Guiding question: What would happen in the classical case of a particle in such a potential?
    - The particle would move first to the right with momentum $|p_x|$, then bounce against the wall at $x = a$ and change its momentum to $-|p_x|$, then bounce against the wall at $x = 0$ and change its momentum back to $|p_x|$, and so continue indefinitely.
  – In quantum mechanics, we can mimic the same behavior by forming a wave packet!
  – Since the particle moves free of forces between $0 < x < a$, one can try to build a Gaussian wave packet, similar to the one we discussed in the free particle case. The difference is that any wave function must vanish at $x = 0, a$, so it must be represented not by combinations of free waves e^{ikx} at $t = 0$ but by
$$\sin\left(\frac{\pi nx}{a}\right) = \frac{1}{2i}(\mathrm{e}^{i\pi nx/a} - \mathrm{e}^{-i\pi nx/a})$$
  – Define
$$k_n = \frac{\sqrt{2mE_n}}{\hbar} = \frac{\pi n}{a}$$
  – Now, what we want is a Gaussian with width Δx for $\Delta x \ll a$.
  – Recalling the free case $|\psi_0(x,t)|^2 = (1/\pi\sigma^2)^{1/2}\mathrm{e}^{-(x-v_gt)^2/2\sigma^2}$ with $\phi(k) = k\mathrm{e}^{-\sigma^2(k-k_0)^2}$, we would like to try
$$\phi(k_n) \propto \mathrm{e}^{-\sigma^2(k_n-k_0)^2} =: c_n$$
where $\sigma = \Delta x \ll a$, and hence $1/\sigma \gg 1/a$.

- Since
$$k_m - k_n = (m-n)\frac{\pi}{a}$$
we will obtain a "continuous" distribution of states with $|k_n - k_0| < 1/\sigma$ as well as a suppression of other modes.
- Left as an exercise to the student to derive further results about this system.