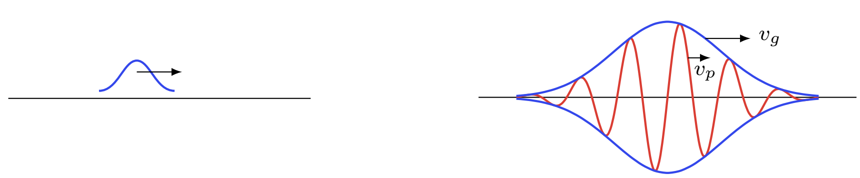
Week 3

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

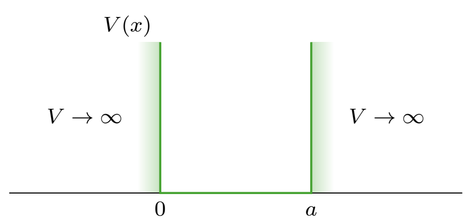


Figure 3.2: Infinite square well.

- **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.

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

- Therefore, the complete eigenfunctions and eigenvalues are

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

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

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

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

Proof. Observe that given any individual eigenstate of energy

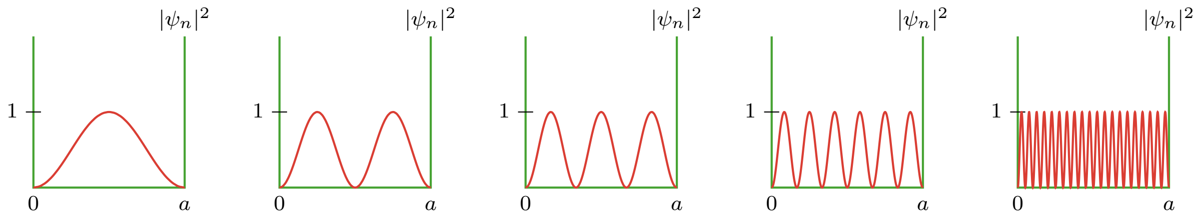
$$\psi_n(x,t) = \psi_n(x)\mathrm{e}^{-iE_n t/\hbar}$$

we have that

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

$\square$

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

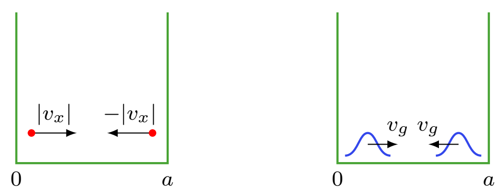


(a) $n = 1$. (b) $n = 2$. (c) $n = 3$. (d) $n = 6$. (e) $n \gg 1$.

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
$$\sin\left(\frac{\pi n x}{a}\right) = \frac{1}{2i}(\mathrm{e}^{i\pi nx/a} - \mathrm{e}^{-i\pi nx/a})$$
  - 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 $|\psi_0(x,t)|^2 = (1/\pi\sigma^2)^{1/2}\mathrm{e}^{-(x-v_g t)^2/2\sigma^2}$ 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.

3.2 Harmonic Oscillator

1/19:

- The harmonic oscillator is one of the most important problems in physics because we can solve it exactly.
- It used to approximate solutions near the bottom of smooth potential wells. It does so via

$$V(x) \approx V(x_0) + \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x_0}(x-x_0) + \frac{1}{2}\left.\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right|_{x_0}(x-x_0)^2 + \cdots$$

  - Mathematically, this represents small departures from x_0.
  - Recall that the first derivative goes to zero (because we are at a minimum) and the second one is a constant we can call k, yielding

$$V(x) = V(x_0) + \frac{1}{2}k(x-x_0)^2$$

  - This is now a potential with which we are familiar from classical mechanics.

- Recall what happens in classical mechanics.
  - We get an equation with a second derivative of $u = x - x_0$:

$$m\frac{\mathrm{d}^2u}{\mathrm{d}t^2} = -ku$$

  - This problem is solved in classical mechanics by defining $\omega^2 := k/m$ and solving the differential equation for

$$u = A\sin(\omega t) + B\cos(\omega t)$$

  - From this general solution, we can get to particular solutions using initial conditions.
  - For example, if $u(0) = 0$, then $B = 0$ and

$$u = A\sin(\omega t)$$

  - What happens if we multiply the original equation of motion by $v = \mathrm{d}u/\mathrm{d}t$? We get the conservation of energy!

$$mv\frac{\mathrm{d}v}{\mathrm{d}t} = -ku\frac{\mathrm{d}u}{\mathrm{d}t}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{mv^2}{2} + \frac{ku^2}{2}\right) = 0$$

  - Note that we associate the left term above with $KE = p^2/2m$ and the right term above with $V(u)$.

– This gives us

$$V(u) = \frac{ku^2}{2} = \frac{k[A\sin(\omega t)]^2}{2} = \frac{kA^2}{2}\sin^2(\omega t)$$
$$K(u) = \frac{mv^2}{2} = \frac{m}{2}\left(\frac{\mathrm{d}}{\mathrm{d}t}[A\sin(\omega t)]\right)^2 = \frac{A^2m\omega^2}{2}\cos^2(\omega t) = \frac{kA^2}{2}\cos^2(\omega t)$$

so that

$$V(u) + K(u) = \frac{kA^2}{2}$$

for all u!

- The situation is different in quantum mechanics.
  – Here, we must begin from

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \frac{kx^2}{2}\psi_n(x) = E_n\psi_n(x)$$

- What do we know, qualitatively, about a solution to this ODE?
  – Since $V(x)$ is time-independent, the eigenfunctions will be of the form

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

  – We will be able to normalize these solutions via

$$\int \mathrm{d}x\, \psi_m^*(x)\psi_n(x) = \delta_{nm}$$

  – The general solution will then be a sum of the normalized solutions, like the following.

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

  – The normalization condition *here* will then yield

$$\sum_n |c_n|^2 = 1$$

  – Lastly, we will be able to calculate expected values, such as

$$\langle\psi|\hat{H}|\psi\rangle = \sum_m |c_m|^2 E_m$$

- We now work toward quantitative solutions $\psi_n(x,t)$, based on insight from the following picture.

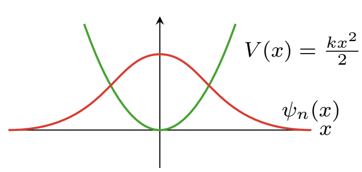


Figure 3.5: Solving the quantum harmonic oscillator with an asymptotic Schrödinger equation.

  – Although it may not be immediately obvious how to solve the Schrödinger equation in this case, we can see from Figure 3.5 that at large values of x, $\psi_n(x) = 0$. Thus, for large x, we will have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) + \frac{kx^2}{2}\psi_n(x) = 0$$

    - This tells us the **asymptotic** behavior of the equation.

  - We can then algebraically rearrange this equation into the form

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_n(x) - \frac{m^2\omega^2x^2}{\hbar^2}\psi_n(x) = 0$$

  - To solve it, use an ansatz proportional to the following.

$$\psi_n(x) \propto \exp\left[-\frac{m\omega}{2\hbar}x^2\right]$$

    - This works because

$$\begin{aligned}\frac{\mathrm{d}\psi_n}{\mathrm{d}x} &= -\frac{m\omega x}{\hbar}\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\\ \frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} &= \left(-\frac{m\omega}{\hbar} + \frac{m^2\omega^2x^2}{\hbar^2}\right)\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\end{aligned}$$

  - In particular, use the ansatz

$$\psi_n(x) = f_n(x)\exp\left[-\frac{m\omega}{2\hbar}x^2\right]$$

  - Now insert this ansatz into the original equation and solve for values of $f_n(x)$ that give an exact solution.
  - Start by calculating that

$$\frac{\mathrm{d}\psi_n}{\mathrm{d}x} = \frac{\mathrm{d}f_n(x)}{\mathrm{d}x}\exp\left[-\frac{m\omega}{2\hbar}x^2\right] - f_n(x)\frac{m\omega x}{\hbar}\exp\left[-\frac{m\omega}{2\hbar}x^2\right]$$

  and thus

$$\begin{aligned}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} &= \frac{\mathrm{d}^2f_n(x)}{\mathrm{d}x^2}\exp\left[-\frac{m\omega}{2\hbar}x^2\right] - 2\frac{\mathrm{d}f_n(x)}{\mathrm{d}x}\frac{m\omega x}{\hbar}\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\\ &\quad - f_n(x)\frac{m\omega}{\hbar}\exp\left[-\frac{m\omega}{2\hbar}x^2\right] + f_n(x)\frac{m^2\omega^2x^2}{\hbar^2}\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\\ &= \left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) - f_n(x)\frac{m\omega}{\hbar} + f_n(x)\frac{m^2\omega^2x^2}{\hbar^2}\right]\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\\ &= \left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) + \frac{m\omega}{\hbar}\left(\frac{m\omega x^2}{\hbar} - 1\right)f_n(x)\right]\exp\left[-\frac{m\omega}{2\hbar}x^2\right]\end{aligned}$$

  - Now we insert the above into the full original Schrödinger equation, cancelling the exponential term immediately to save space.

$$\begin{aligned}-\frac{\hbar^2}{2m}\left[f_n''(x) - \frac{2m\omega x}{\hbar}f_n'(x) + \frac{m\omega}{\hbar}\left(\frac{m\omega x^2}{\hbar} - 1\right)f_n(x)\right] + \frac{m\omega^2x^2}{2}f_n(x) &= E_nf_n(x)\\ -\frac{\hbar^2}{2m}\left(f_n'' - \frac{2m\omega x}{\hbar}f_n' - \frac{m\omega}{\hbar}f_n\right) &= E_nf_n\\ -\frac{\hbar^2}{2m}f_n'' + \hbar\omega xf_n' + \left(\frac{\hbar\omega}{2} - E_n\right)f_n &= 0\end{aligned}$$

- Thus, we have obtained an ODE that we can solve to find particular solutions.
- One obvious solution: the **minimal energy solution**.
- **Minimal energy solution** (to the quantum harmonic oscillator): Take f_n to be a constant C. *Given by*

$$\psi_0(x) = C\exp\left[-\frac{m\omega}{2\hbar}x^2\right] \qquad\qquad E_0 = \frac{\hbar\omega}{2}$$

  - Note that it is the above ODE that necessitates $E_0 = \hbar\omega/2$ if f_n is to be a constant.
  - The minimal energy solution classically is zero, but in quantum mechanics, there will always be some energy!
    - Zero energy is impossible because it would imply that the position and momentum are both zero. But there needs to be some uncertainty, in both, so the position and momentum *cannot* both be zero.
    - Essentially, the uncertainty principle *necessitates* a finite nonzero minimal energy. Stated another way, zero energy is *inconsistent* with the uncertainty principle.

- What if we postulate that $f_1 = b_1 x$ for some constant b_1?
  - Then the ODE simplifies to

$$\begin{aligned}\hbar\omega b_1 x + \left(\frac{\hbar\omega}{2} - E_1\right) b_1 x &= 0\\ E_1 &= \frac{3\hbar\omega}{2}\end{aligned}$$

  - Note that

$$E_1 - E_0 = \hbar\omega$$

    - This observation is important because we can actually prove that

$$E_{n+1} - E_n = \hbar\omega$$

      for all $n = 0, 1, 2, \dots$.
    - We will not prove this in this class, though; we will just postulate it.
    - Essentially, what we do is assume that

$$f_N(x) = \sum_{n=1}^{N} b_n x^n$$

      and solve.
    - All the solutions are either even or odd solutions based on whether N is even or odd. These "even" and "odd" solutions correspond to even and odd polynomial functions.
  - This means that

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

- In particular, if we let $\xi = x\sqrt{m\omega/\hbar}$, then the solutions f_N are the **Hermite polynomials**.
- **Hermite polynomial**: A polynomial of the following form. *Denoted by* $\boldsymbol{H_n(\xi)}$. *Given by*

$$H_n(\xi) = (-1)^n \exp(\xi^2) \frac{\mathrm{d}^n}{\mathrm{d}\xi^n}[\exp(-\xi^2)]$$

- Thus, the general solutions to the quantum harmonic oscillator

$$\psi_n(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4} \frac{H_n(\xi)}{\sqrt{2^n n!}} \exp\left[-\frac{\xi^2}{2}\right]$$

- On Monday, we will derive this result using **rasing** and **lowering** operators.

3.3 Office Hours (Wagner)

- PSet 2, Q1: Do you want us to rederive the wavefunction, or just answer the questions in the parts?
- Do we have to show our integration steps, or are integral calculators fine?
  - Show whatever we feel comfortable with.
  - Sounds like Wagner thinks we should be able to do all these calculations like we were born doing them, but integral calculators and skipping steps shouldn't lose us any points.
- Including Problem 3 was probably a mistake, but now that it's included, we have to do it.
- PSet 2, Q1d:
  - One way to do this problem is to remember that $\mathrm{d}\langle\hat{r}\rangle/\mathrm{d}t = \langle p\rangle/m$ and $\mathrm{d}\langle p\rangle/\mathrm{d}t = 0$.
  - Now the $\psi = \sum_n c_n \sin(k_n x)$.
  - The mean value of the momentum, once computed explicitly, is

$$\langle p\rangle \propto \int \mathrm{d}x \left[\sum_n c_n \sin(k_n x) \cdot \frac{\partial}{\partial x}\left(\sum_n c_n \sin(k_n x)\right)\right]$$

  - Then we integrate using the trick that

$$\sin x \cos y = \frac{1}{2}\sin(x+y) + \frac{1}{2}\sin(x-y)$$

    - Wagner briefly proves this trig identity.
  - Recall tricks like given an *even* function f,

$$\int_{-L}^{L} \mathrm{d}x\, x \cdot f(x) = 0$$

- PSet 2, Q2:
  - There is some part where we do not need to find exact solutions.

3.4 Chapter 2: Time-Independent Schrödinger Equation

From Griffiths and Schroeter (2018).

Section 2.2: The Infinite Square Well

1/29:
- Goes through the derivation from class.
- The boundary conditions will be justified in Section 2.5!
- Note that since A is complex, normalization technically only determines the magnitude $|A|$. However, the phase of A carries no physical significance, so there is no reason not to choose the simplest solution to $|A|^2 = 2/a$, which is just the positive real square root.
- Notice how, as promised, the TISE delivers a set $\{\psi_n(x)\}$ of solutions!
- **Ground state**: The wave functional solution to the TISE which carries the lowest energy.
- **Excited state**: Any wave functional solution to the TISE that is not the ground state.
- Four properties of the ψ_n of the infinite square well.

1. They are alternately even and odd, with respect to the center of the well.
2. As E_n increases, each successive state has one more **node**.
3. The $\{\psi_n\}$ are mutually orthogonal.
   - Griffiths and Schroeter (2018) proves that any ψ_n, ψ_m ($n \neq m$) are orthogonal.
4. The $\{\psi_n\}$ are **complete**.

- **Complete** (set of functions): A set of functions such that any other function $f(x)$ can be expressed as a linear combination of them.
  - Griffiths and Schroeter (2018) will not prove the completeness of the functions $\sqrt{2/a}\sin(\pi nx/a)$, but the mathematically inclined student may notice that an infinite sum of these is the **Fourier series** for $f(x)$, and the fact that any function can be expanded in this way is called **Dirichlet's theorem**.
  - To compute the c_n corresponding to an arbitrary f, use **Fourier's trick**:

$$\int \psi_m^*(x)f(x)\,\mathrm{d}x = \sum_{n=1}^{\infty} c_n \int \psi_m^*(x)\psi_n(x)\,\mathrm{d}x = \sum_{c_n} \delta_{mn} = c_m$$

  - Aside (from me): Dirac notation expresses the above statement as simply a consequence of taking the inner product of a vector and a member of the orthonormal basis.

$$\langle \psi_m | f \rangle = c_m$$

- Note on the four properties.
  - Property 1 is true whenever the potential is a symmetric function.
  - Property 2 is universal, regardless of the shape of the potential.
  - Orthogonality is quite general (we'll see exactly how much in Chapter 3).
  - Completeness holds for all potentials we are likely to encounter (but the proofs tend to be nasty).
    - "Most physicists simply *assume* completeness, and hope for the best" (Griffiths & Schroeter, 2018, p. 52).
- With what we know now, we can compute the time evolution of any particle in this system.
  - Simply start with its wave function at $t = 0$, which is $\psi(x, 0)$.
  - Compute expansion coefficients.
  - And take $\psi(x, t)$ to be the sum of stationary states.
- Griffiths and Schroeter (2018) proves — as at the end of class on 1/12 — that $\sum_n |c_n|^2 = 1$ and $\sum_n |c_n|^2 E_n = \langle H \rangle$.