

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

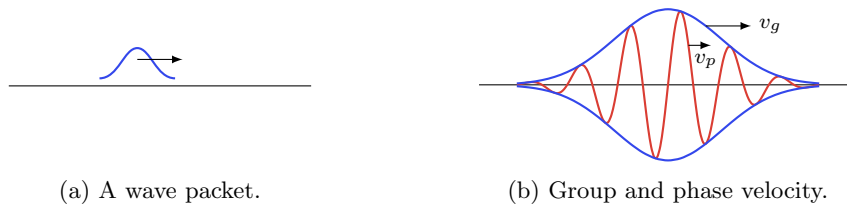
$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

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

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

- Example of the uncertainty principle: For a plane wave, we know the momentum but not the position. That is, $\Delta x \rightarrow \infty$ and $\Delta p_x \rightarrow 0$.
- 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*

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



(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

$$\begin{aligned}\omega(k) &= \omega(k_0) + \left. \frac{d\omega}{dk} \right|_{k=k_0} (k - k_0) + \dots \\ &= \omega(k_0) + \left. \frac{\hbar k}{m} \right|_{k=k_0} (k - k_0) + \dots \\ &= \omega(k_0) + \underbrace{\frac{\hbar k_0}{m}}_{\omega'_0} (k - k_0) + \dots\end{aligned}$$

- Define $s := k - k_0$.
- Then $k = k_0 + s$ and $dk = ds$, so

$$\begin{aligned}\psi(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k_0 + s) e^{i((k_0 + s)x - (\omega(k_0) + \omega'_0 s)t)} ds \\ &= \frac{1}{\sqrt{2\pi}} e^{i(k_0 x - \omega(k_0)t)} \int_{-\infty}^{\infty} \phi(k_0 + s) e^{is(x - \omega'_0 t)} ds\end{aligned}$$

- It follows that

$$|\psi(x, t)|^2 = \frac{1}{2\pi} \left| \int_{-\infty}^{\infty} \phi(k_0 + s) e^{is(x - \omega'_0 t)} ds \right|^2 = f(x - \omega'_0 t)$$

- 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 to the classical velocity

$$\left. \frac{d\omega}{dk} \right|_{k=k_0} = \frac{p_0}{m}$$

- **Group velocity:** A measure of the velocity of a wave packet. Denoted by \mathbf{v}_g , $\mathbf{v}_{\text{group}}$. Given by

$$v_{\text{group}} = \left. \frac{d\omega}{dk} \right|_{k=k_0}$$

- **Phase velocity:** A measure of the velocity of the ripples. Denoted by \mathbf{v}_p , $\mathbf{v}_{\text{phase}}$. 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

$$\psi_0(x, t) = \left(\frac{2}{\pi\sigma^2} \right)^{1/4} \exp \left[-\frac{(x - v_g t)^2}{\sigma^2} \right] e^{i(k_0 x - v_p t)}$$

- 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 $t = 0$,

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

- 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

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

- 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 $e^{-1/2}$.
 - Altogether, we get

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

so

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

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

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.

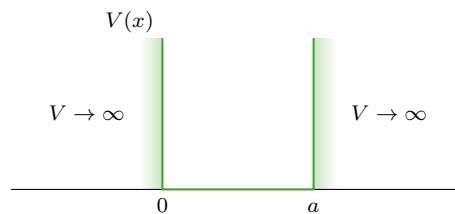


Figure 3.2: Infinite square well.

- **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

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

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

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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad \psi(0) = \psi(a) = 0$$

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

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

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

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

- 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.

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

- Therefore, the complete eigenfunctions and eigenvalues are

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

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

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

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

Proof. Observe that given any individual eigenstate of energy

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

we have that

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

□

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

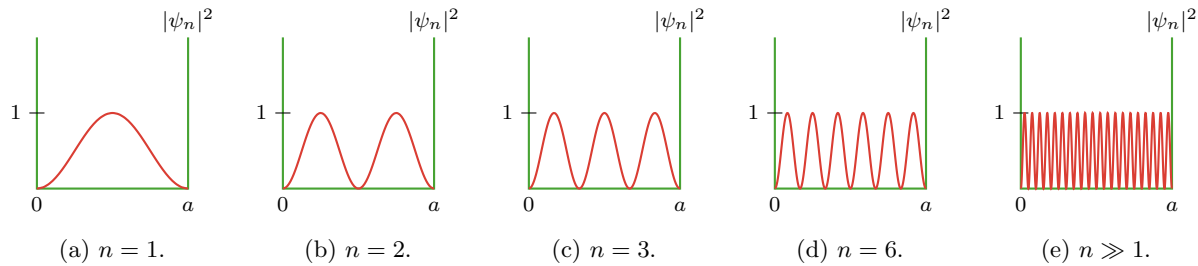


Figure 3.3: Infinite square well probability density.

- 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 $d/dt(\langle \psi | \hat{x} | \psi \rangle) \neq 0$

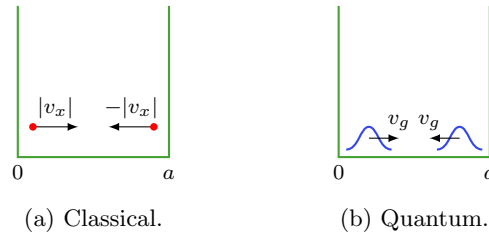


Figure 3.4: Infinite square well motion.

- 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

$$\sin\left(\frac{\pi n x}{a}\right) = \frac{1}{2i}(e^{i\pi n x/a} - e^{-i\pi n x/a})$$

- 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 $|\psi_0(x, t)|^2 = (1/\pi\sigma^2)^{1/2} e^{-(x-v_g t)^2/2\sigma^2}$ with $\phi(k) = k e^{-\sigma^2(k-k_0)^2}$, we would like to try

$$\phi(k_n) \propto e^{-\sigma^2(k_n - k_0)^2} =: c_n$$

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

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

- 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 $u = x - x_0$:

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

- 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 $v = du/dt$? We get the conservation of energy!

$$mv \frac{dv}{dt} = -ku \frac{du}{dt}$$

$$\frac{d}{dt} \left(\frac{mv^2}{2} + \frac{ku^2}{2} \right) = 0$$

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

- This gives us

$$V(u) = \frac{ku^2}{2} = \frac{k[A \sin(\omega t)]^2}{2} = \frac{kA^2}{2} \sin^2(\omega t)$$

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

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

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

- What do we know, qualitatively, about a solution to this ODE?

- Since $V(x)$ is time-independent, the eigenfunctions will be of the form

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

- We will be able to normalize these solutions via

$$\int dx \psi_m^*(x) \psi_n(x) = \delta_{nm}$$

- 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.

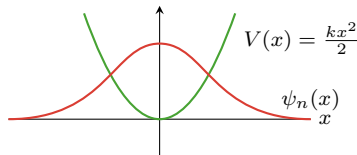


Figure 3.5: Solving the quantum harmonic oscillator with an asymptotic Schrödinger equation.

- 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

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

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

– We can then algebraically rearrange this equation into the form

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

– 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

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

– 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

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

and thus

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

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

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

- 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*

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

- 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 $f_1 = b_1x$ for some constant b_1 ?
 - Then the ODE simplifies to

$$\hbar\omega b_1x + \left(\frac{\hbar\omega}{2} - E_1\right) b_1x = 0$$

$$E_1 = \frac{3\hbar\omega}{2}$$

- 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 $H_n(\xi)$. Given by

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

- 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 **raising** 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 $d\langle\hat{r}\rangle/dt = \langle p\rangle/m$ and $d\langle p\rangle/dt = 0$.
 - Now the $\psi = \sum_n c_n \sin(k_n x)$.
 - The mean value of the momentum, once computed explicitly, is

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

- 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 ,

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

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