

Last time

$$I = \int_{y=-\infty}^{+\infty} e^{-y^2} dy = \sqrt{\pi}$$

Change variables: $y^2 = ax^2$, $y = \sqrt{a}x$, $dy = \sqrt{a}dx$

$\text{Re}(a) > 0$

$$y = \pm \infty \Rightarrow x = \pm \infty$$

$$I = \int_{x=-\infty}^{+\infty} e^{-ax^2} \sqrt{a} dx = \sqrt{\pi}$$

$$\int_{x=-\infty}^{+\infty} e^{-ax^2} dx = \frac{\sqrt{\pi}}{\sqrt{a}}$$

differentiate both sides
w.r.t. a

$$-\int_{x=-\infty}^{+\infty} x^2 e^{-ax^2} dx = \sqrt{\pi} \frac{d(a^{-1/2})}{da} = \sqrt{\pi} \left(-\frac{1}{2}\right) a^{-3/2}$$

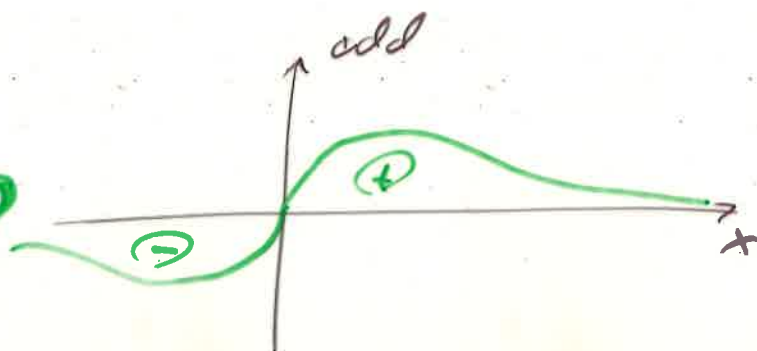
$$\int_{x=-\infty}^{+\infty} x^2 e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a^3}}$$

differentiate w.r.t. a

$$\int_{x=-\infty}^{+\infty} x^4 e^{-ax^2} dx = \frac{3}{4} \sqrt{\frac{\pi}{a^5}}$$

$$\int_{x=-\infty}^{+\infty} x^{2n} e^{-ax^2} dx = \text{known}$$

$$\int_{x=-\infty}^{+\infty} x^{2n+1} e^{-ax^2} dx = 0$$



$$\langle x \rangle = \int_{x=-\infty}^{+\infty} e^{-\frac{cx^2}{k_B T}} \left[\cancel{x} + \frac{gx^4}{k_B T} + \frac{fx^5}{k_B T} + \dots \right] dx$$

$$\int_{x=-\infty}^{+\infty} e^{-\frac{cx^2}{k_B T}} [1 + \dots] dx$$

$$\langle x \rangle = \frac{g}{k_B T} \int_{-\infty}^{+\infty} x^4 e^{-\left(\frac{c}{k_B T}\right)x^2} dx$$

$$= \frac{g}{k_B T} \frac{3}{4} \sqrt{\frac{\pi c^{-5/4}}{(k_B T)^{5/4}}}$$

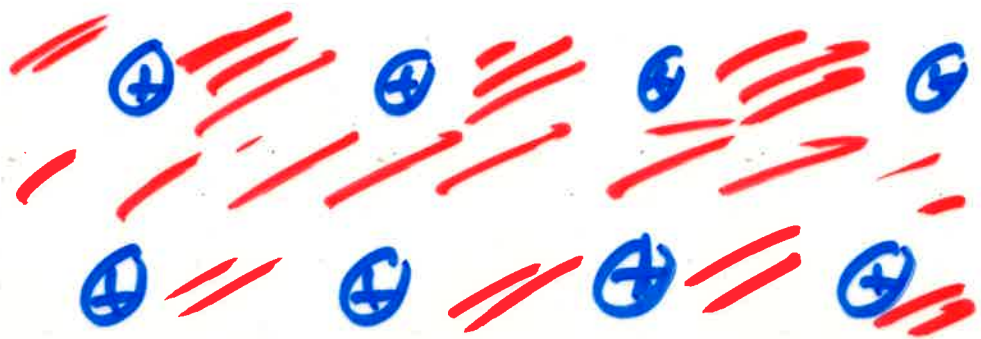
$$\frac{\int_{-\infty}^{+\infty} e^{-\left(\frac{c}{k_B T}\right)x^2} dx}{\sqrt{\frac{\pi k_B T}{c}}}$$

$$\langle x \rangle = \frac{3g}{4c^2} k_B T$$

If we kept the g and f terms in the denominator, this would be

$$\frac{3g}{4c^2} k_B T [1 + f(?)]$$

and gf is (small)².



Infinite square well approximation
(particle in a box)

Na⁺ e.g.

Schrodinger Equation is non-relativistic, spin-zero

$$T + V = H$$

$$\hat{x} = x$$

$$\frac{p^2}{2m} + V = H$$

$$\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial}{\partial t} \psi$$

$$H\psi = E\psi \text{ for stationary states}$$

Schrödinger (Schrödinger) Equation

Non-relativistic Spin-zero.

$$\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{x} = x, \quad \hat{H} = \hbar i \frac{\partial}{\partial t}$$

$$\frac{\hat{p}^2}{2m} \Psi(x,t) + V(\hat{x}) \Psi = \hat{H} \Psi$$

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

Look for "stationary states" = states
of definite energy = eigenstates of
energy.

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

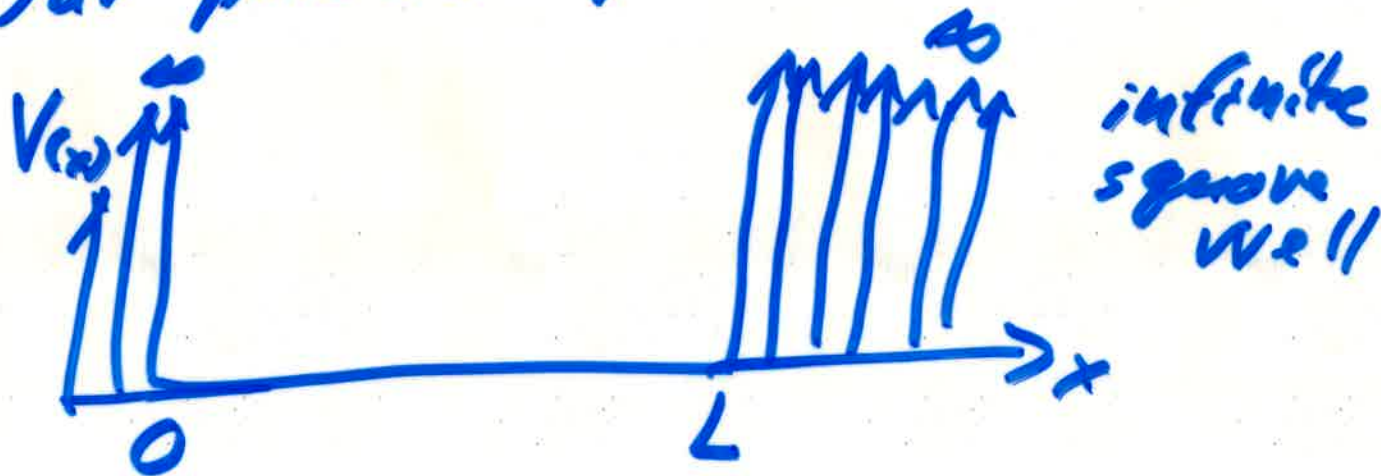
time dependence $e^{\frac{iEt}{\hbar}}$

$$\Psi(x,t) = e^{\frac{iEt}{\hbar}} \psi(x)$$

Time-independent Schrödinger Eq.

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

Our problem: particle in a box



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

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

$$\frac{d}{dx} \psi(x) = Ak \cos(kx) - Bk \sin(kx)$$

$$\begin{aligned} \frac{d^2}{dx^2} \psi(x) &= -Ak^2 \sin(kx) - Bk^2 \cos(kx) \\ &= -k^2 \psi(x) \end{aligned}$$

$$+\frac{\hbar^2}{2m} k^2 \psi(x) = E \psi(x) \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

Boundary Conditions $\psi(0) = 0 = \psi(L)$

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

$$\psi(0) = A \sin(0) + B \cos(0) = B = 0$$

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

$$\psi(L) = 0 = A \sin(kL)$$

$$A \neq 0 \Rightarrow \sin(kL) = 0$$

$$\Rightarrow kL = n\pi \quad n = 1, 2, 3, \dots$$

$$k_n = \frac{n\pi}{L}$$

↑
Quantum
Number

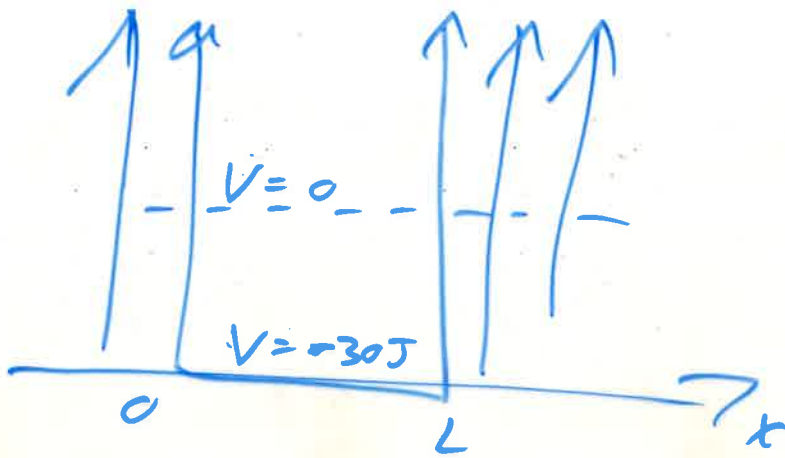
$$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

Normalize to get A : $\int_0^L \psi^* \psi dx = 1$
 $A = \sqrt{\frac{2}{L}}$

A SQUARE WELL

well



$$\psi_0 \rightarrow \psi_0 e^{i\theta}$$

introduces a phase into the wave function, but this phase is not physically measurable.

Physical Quantity

$$P(x) = |\psi(x)|^2 = \psi^*(x) \psi(x)$$

$$\langle \hat{p} \rangle = \langle \psi_0 | \hat{p} | \psi_0 \rangle$$

AVG
momentum