Announcement

- Homework 6 is due March 10, next Friday.
- Homework 7 is due March 22, the Wednesday after the spring break.
- Prof. Tanner's office hour next Monday is over zoom, next Friday no office hour.

Last time

- Expectation values and uncertainty principles for 1D infinite potential well
- 1D finite potential well
- 2D/3D infinite potential well $\Psi(x, y, z) = X(x)Y(y)Z(z)$

Today's class

- Harmonic oscillator

Classical harmonic oscillator

- Classical harmonic oscillator: Potential energy $U = \frac{1}{2}kx^2$

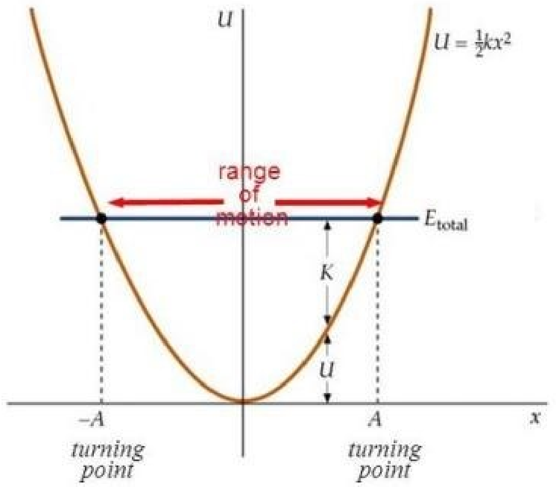
k : spring constant

$\omega_0^2 = k/m$ ω_0 : classical oscillation frequency

$|x| \leq x_{max}$

$E = \frac{1}{2}k x_{max}^2 = \frac{1}{2} m \omega_0^2 x_{max}^2$

$x_{max} = \sqrt{\frac{2E}{m\omega_0^2}}$ classical turning point



Why is harmonic oscillator important?

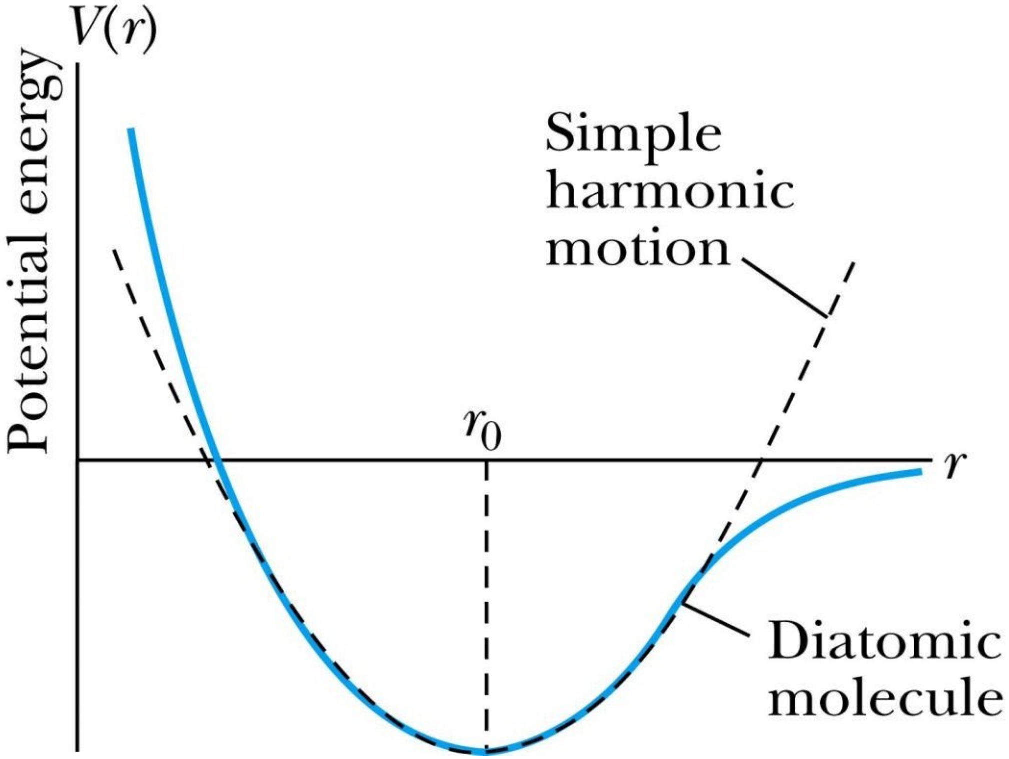
$$U(r) = U(r_0) + U'(r_0)(r-r_0) + U''(r_0)\frac{(r-r_0)^2}{2} + \cdots\cdots$$

because $U'(r_0) = 0$

$$= U(r_0) + U''(r_0)\frac{(r-r_0)^2}{2}$$

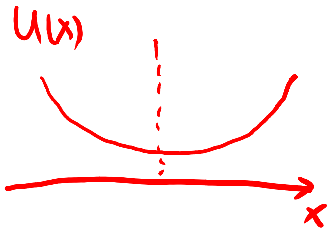
It's everywhere!

- Any stable potential can be approximated as harmonic oscillator near minimum



Real-life example:
A vibrating diatomic molecule

Simple harmonic oscillator



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\psi(x) = E\psi(x) \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

$\psi(x)$ $\quad$ $\underline{x \to +\infty \text{ or } -\infty \quad \psi(x) \to 0}$ $\qquad$ $e^{-x^2} \to \psi(x) = Ae^{-ax^2}$

$$\frac{d\psi}{dx} = -2axAe^{-ax^2}, \quad \frac{d^2\psi}{dx^2} = -2aAe^{-ax^2} - 2ax(-2ax)Ae^{-ax^2} = (-2a + 4a^2x^2)Ae^{-ax^2}$$

$$-\frac{\hbar^2}{2m}(-2a + 4a^2x^2)Ae^{-ax^2} + \frac{1}{2}kx^2 Ae^{-ax^2} = EAe^{-ax^2}$$

$$\frac{\hbar^2 a}{m} - \frac{2\hbar^2 a^2 x^2}{m} + \frac{1}{2}kx^2 = E$$

$$\frac{\hbar^2 a}{m} - E + x^2\left(\frac{k}{2} - \frac{2\hbar^2 a^2}{m}\right) = 0$$

valid for any x

$\omega_0 = \sqrt{k/m} \Rightarrow \omega_0^2 = k/m$

$k = m\omega_0^2$

$\sqrt{km} = m\omega_0$

$$E = \frac{\hbar^2 a}{m}, \quad \frac{2\hbar^2 a^2}{m} = \frac{k}{2} \Rightarrow a = \sqrt{\frac{km}{4\hbar^2}} = \frac{\sqrt{km}}{2\hbar} = \frac{m\omega_0}{2\hbar}$$

$$E = \frac{\hbar^2}{m}\cdot\frac{m\omega_0}{2\hbar} = \frac{1}{2}\hbar\omega_0$$

ground state

Simple harmonic oscillator

$$\psi(x) = A e^{-ax^2}$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} A^2 e^{-2ax^2} dx = A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 2A^2 \int_0^{\infty} e^{-2ax^2} dx = A^2 \sqrt{\frac{\pi}{2a}} = 1$$

from integral table $\int_0^{\infty} e^{-ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \xrightarrow{a \to 2a} \int_0^{\infty} e^{-2ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{2a}}$

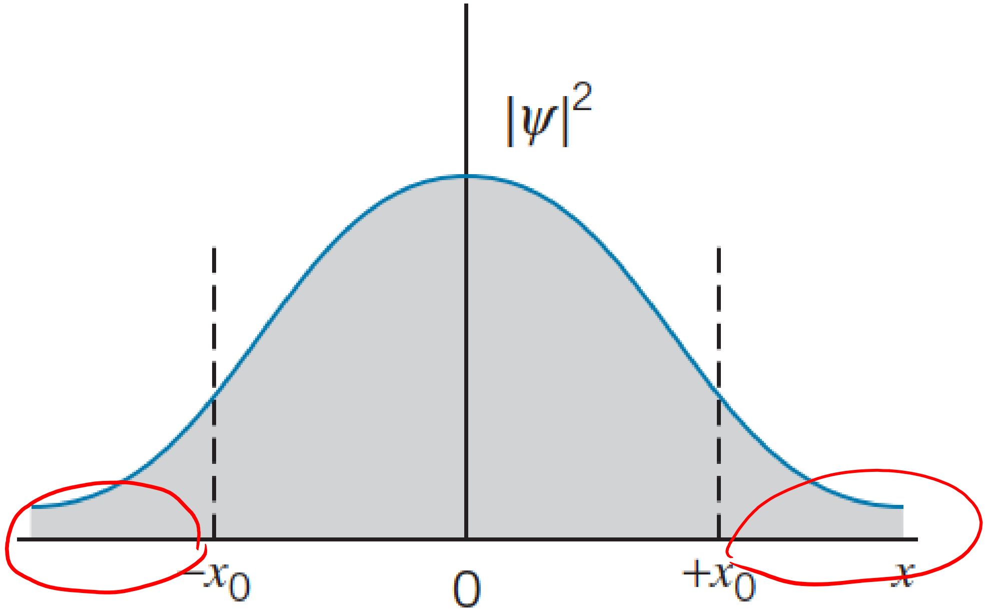
$$A^2 = \sqrt{\frac{2a}{\pi}} \Rightarrow A = \left(\frac{2a}{\pi}\right)^{\frac{1}{4}} = \left(\frac{\sqrt{km}}{\pi\hbar}\right)^{\frac{1}{4}} = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}}$$

$$a = \frac{\sqrt{km}}{2\hbar} = \frac{m\omega_0}{2\hbar}$$

$$\psi(x) = A e^{-ax^2} = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega_0}{2\hbar}x^2}$$

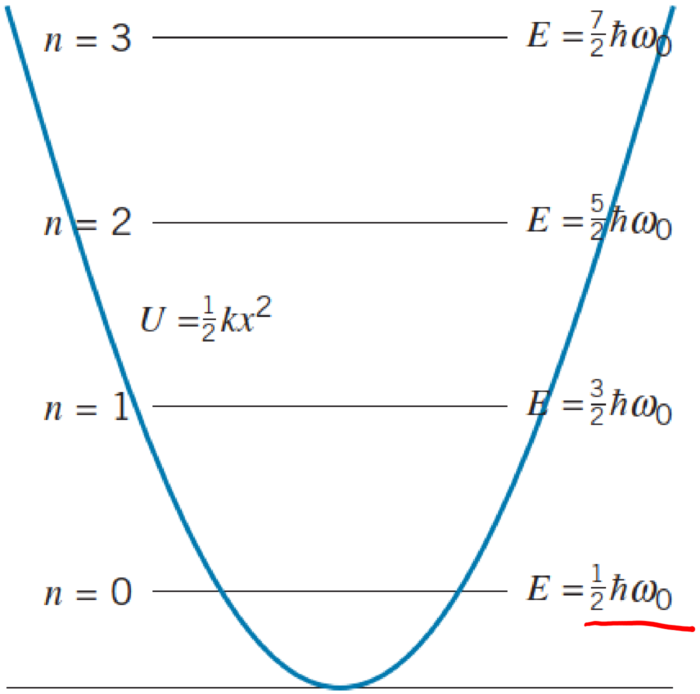
ground state

Tunneling



Ground state
Classical turning points are +/-x_0

Simple harmonic oscillator



$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0$$

Find <x>, <x²>, and <Δx> for the ground state simple harmonic oscillator.

Hint: $\int_{-\infty}^{\infty} x^2 e^{-ax^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{a^3}} \quad (a>0)$ $\xRightarrow{a \to 2a}$ $\int_{-\infty}^{\infty} x^2 e^{-2ax^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{(2a)^3}} = \frac{1}{2}\sqrt{\frac{\pi}{8a^3}}$

$\langle x \rangle = 0$ $\quad \langle x \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 x\,dx = \int_{-\infty}^{\infty} A^2 e^{-2ax^2} x\,dx = 0$ odd function

$\langle x^2 \rangle = \int_{-\infty}^{\infty} |\psi(x)|^2 x^2 dx = \int_{-\infty}^{\infty} A^2 e^{-2ax^2} x^2 dx = A^2 \int_{-\infty}^{\infty} x^2 e^{-2ax^2} dx = A^2 \cdot \frac{1}{2}\sqrt{\frac{\pi}{8a^3}}$

$= \frac{1}{2}\frac{\hbar}{m\omega_0}$

$\langle \Delta x \rangle = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{\hbar}{2m\omega_0}}$

Find <p>, <p^2>, and <Δp> for the ground state simple harmonic oscillator.

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

$$\langle p \rangle = 0$$

$$\langle p^2 \rangle = A^2 \hbar^2 \sqrt{\frac{\pi a}{2}}$$

$$\langle \Delta p \rangle = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\frac{m\omega_0 \hbar}{2}}$$

$$\Delta x \cdot \Delta p = \frac{\hbar}{2}$$ most compact

In-class exercise (5 min)

An electron is confined by a 1-D harmonic potential with an effective spring constant of 100 eV/nm^2.

k

a. What is the ground-state energy in eV? Hint: use $\hbar c$=197 eV·nm

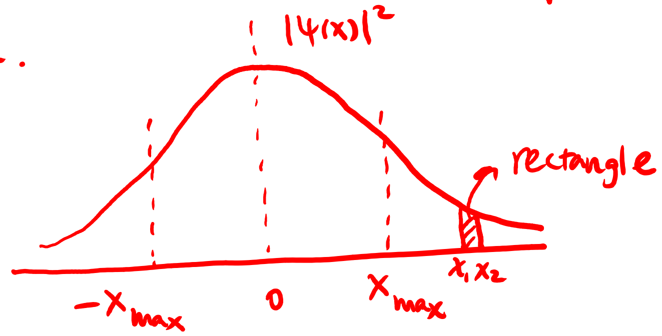
b. Where is the classical turning point?

c. What is the probability of finding this electron in a narrow interval of width 0.004 nm in the classical forbidden region located 0.01 nm further away from the classical turning point?

a. $E = \frac{1}{2}\hbar\omega_0 = \frac{1}{2}\hbar\sqrt{\frac{k}{m}} = \frac{1}{2}\hbar c\sqrt{\frac{k}{mc^2}} = \frac{1}{2}(197\,\text{eV}\cdot\text{nm})\sqrt{\frac{100\,\text{eV/nm}^2}{0.511\times10^6\,\text{eV}}} = 1.38\,\text{eV}$

b. $E = \frac{1}{2}kx_{max}^2 \Rightarrow x_{max} = \sqrt{\frac{2E}{k}} = \sqrt{\frac{2\times1.38\,\text{eV}}{100\,\text{eV/nm}^2}} = 0.166\,\text{nm}$

c.



$P(x) = \int_{x_1}^{x_2} |\psi(x)|^2 dx = |\psi(x)|^2 \Delta x = 0.0044 = 0.44\%$

$x = 0.166\,\text{nm} + 0.01\,\text{nm} = 0.176\,\text{nm}$, $\Delta x = 0.004\,\text{nm}$

$A =$, $a =$

New quantum perspective …

You will never look at these the same way…