Lecture 5, Jan 20, 2022

Particle in a Box (Infinite Square Well)

- Particle of mass m in a 1-dimensional box box length L
- In side the box potential is 0, outside the box potential is infinite
- Inside the box the TISE reduces to $-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$ since there is zero potential
- Solution of the form $\psi = A\sin(kx) + B\cos(kx) \implies \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi$, and $E = \frac{\hbar^2 k^2}{2m}$ (the energy of a state depends on k)
- However since the potential is infinite outside the well we impose boundary conditions $|\psi|^2 = 0 \implies \psi = 0$ for $x \leq 0$ or $x \geq L$, and the normalization condition
  - At $x = 0$, the sine term is zero, so we conclude the cosine term should always be zero (i.e. $\psi = A\sin(kx)$ for all x)
  - At $x = L$, $\psi = 0$ means $A\sin(kL) = 0 \implies \sin(kL) = 0$ so $kL = n\pi$ (note $n \neq 0$ because that would make the wavefunction always zero), so now energies are quantized!
    - i.e. $k = \frac{n\pi}{L}$ where $n = 1, 2, 3, \cdots$
- $E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2}{8mL^2}n^2$ (note we switched from $\hbar$ to h)
- We also need to normalize, so $\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$
  - $1 = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right)\,\mathrm{d}x \implies A = \sqrt{\frac{2}{L}}$
- These wavefunctions are standing waves; n is the quantum number; ψ_n has $n-1$ nodes
- Note the ground state doesn't have zero energy (zero point energy ZPE)
- Kinetic energy is proportional to the curvature of the wavefunction; more kinetic energy leads to higher curvature and faster oscillating wavefunctions
- A smaller box increases E and makes the wavefunction oscillate faster