Nanophotonic Modeling
Lecture 1.1: Introduction

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Bandstructure Problem

- Amounts to solving an eigenvalue equation of the form: $\mathcal{H}\Psi = E\Psi$
- Examples include:
  - Electronic bandstructure: $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\Psi(x) = \hbar\omega\Psi(x)$
  - Photonic bandstructure: $\nabla \times [\epsilon^{-1}(\nabla \times H)] = \left(\frac{\omega}{c}\right)^2 H$
  - Phononic bandstructure: $\nabla \times [C(\nabla \times u)] = -\rho\omega^2 u$

Schrodinger's Equation

- Wavefunction Ψ describes extent of particle
- Also eigenfunction of Schrodinger's equation:
$$\mathcal{H}\Psi = E\Psi$$
- Hamiltonian consists of kinetic and potential terms: $\mathcal{H} = T + V$
- Classically, $T = \frac{p^2}{2m}$; if $p = -i\hbar\nabla$, $T = -\frac{\hbar^2}{2m}\nabla^2$
- Probability of finding at x given by $|\Psi(x)|^2$

Free Particle

- A free particle has zero potential everywhere
- Schrodinger's equation becomes:

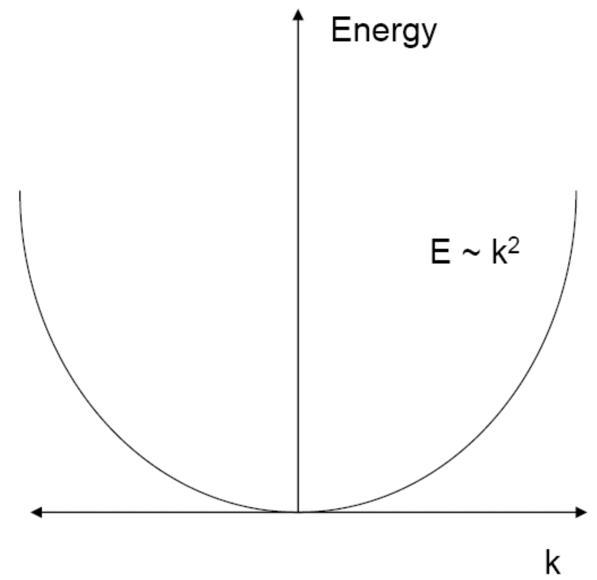
$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

- Eigenfunction can be obtained analytically:

$$\Psi(x) = Ae^{\pm ikx}$$

- Energy eigenvalue thus given by:

$$E = \frac{\hbar^2 k^2}{2m}$$

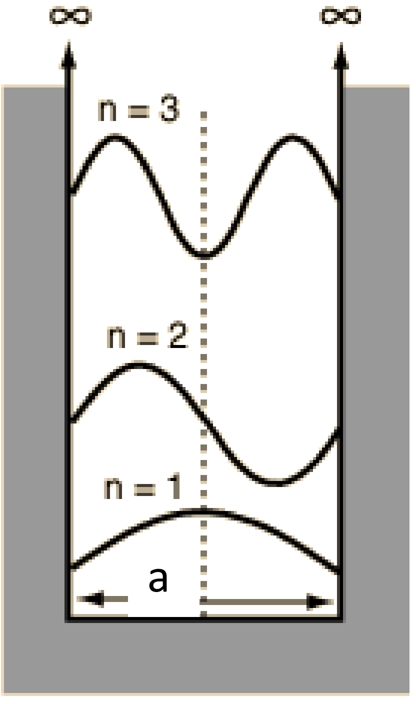


Infinite Quantum Well

- Example: proton in iron nucleus
- Potential $V(x) = \begin{cases} 0, & |x| < a/2 \\ \infty, & |x| \geq a/2 \end{cases}$
- Boundary condition:

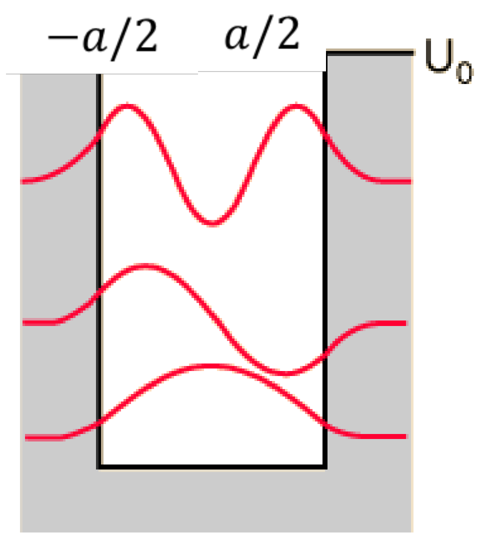
$$\Psi(\pm a/2) = 0$$

- Eigenfunctions are standing waves: $\Psi(x) = A\left[e^{ikx} + e^{-ikx}\right]$
- By BC's, $k = \frac{n\pi}{a}$; $E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$



Finite Quantum Well

- Example: α-particle in U-235 nucleus
- Potential $V(x) = \begin{cases} 0, & |x| < a/2 \\ U, & |x| \geq a/2 \end{cases}$
- Eigenfunctions inside box like before; outside region decays exponentially



Kronig-Penney Potential

- Example: 1D atomic crystal
- Potential $V(x) =$
$$\begin{cases} 0, & 0 < x < a/2 \\ U, & a/2 < x < a \end{cases}$$
- And, $V(x + a) = V(x)$
- Boundary conditions:
$$\Psi(x + a) = \Psi(x)?$$
- Will each electron be stuck in its own little well?