Suppose:

- $\Phi(x,t)$ is a general solution of the Schrödinger Equation (SE)
- $\psi_n(x)$ are the solutions ($n = 1, 2, 3 \ldots$) for the time-independent SE
- In the expressions below, c_n are suitable expansion coefficients, E_n are the energies for various solutions $\psi_n(x)$ and E is the average energy of the system.

Which one of the following statements is correct?

a) $\Phi(x,t) = [\sum_n c_n \psi_n(x)] e^{\frac{-iEt}{\hbar}}$

b) $\Phi(x,t) = \sum_n c_n \psi_n(x) e^{\frac{-iE_n t}{\hbar}}$

c) $\Phi(x,t) = \sum_n \psi_n(x) e^{\frac{-E_n t}{\hbar}}$

d) $\Phi(x,t) = \sum_n \psi_n(x) e^{\frac{-iE_n t}{\hbar}}$

CHM 305 The Quantum World
Lecture 4: Free & Confined Particles

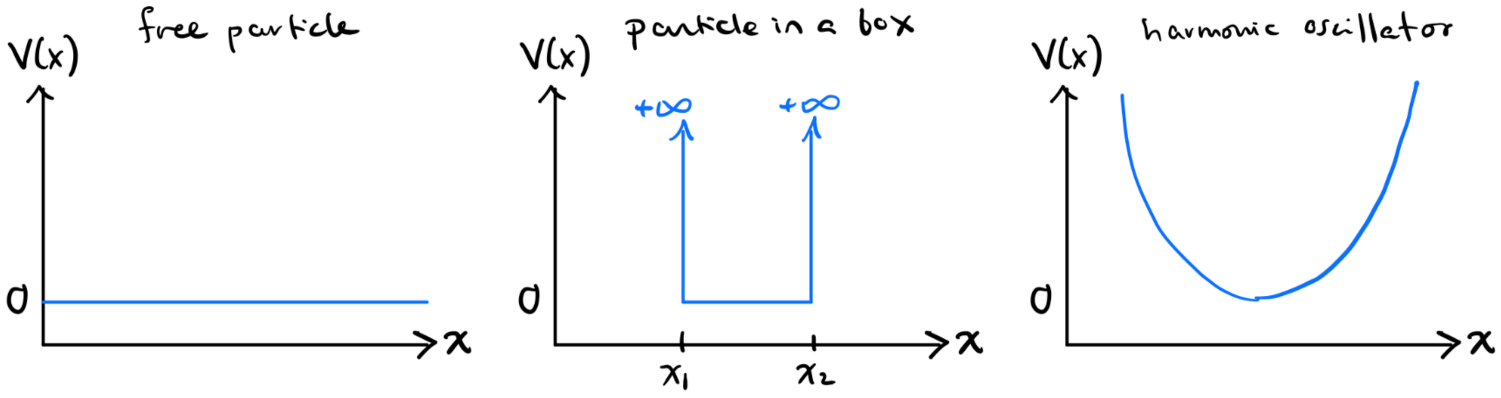
Reading: McQuarrie Chap. 3

Quick review of what we learned last time…

- Motivation of the Schrödinger equation from classical waves plus the deBroglie relation

- The time-*dependent* Schrödinger equation and how it governs the temporal and spatial evolution of quantum wavefunctions

- The time-*independent* Schrödinger equation and how we can solve it to find a stationary state solutions and their corresponding energies for a given potential, V(x)



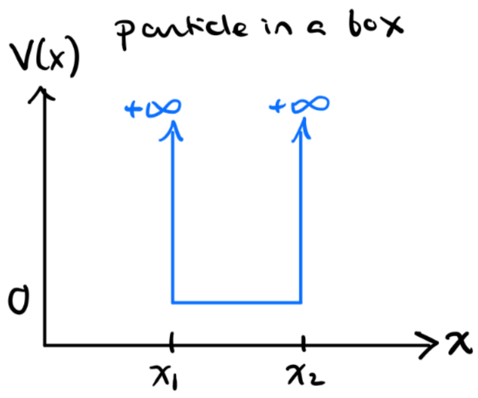
Road map for today's lecture

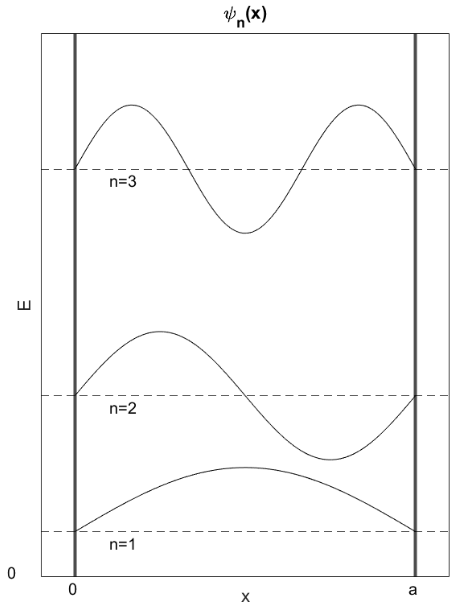
Review the rules for solving the Schrödinger equation

Description of the simplest quantum system: the *free particle* in a potential with V(x) = 0

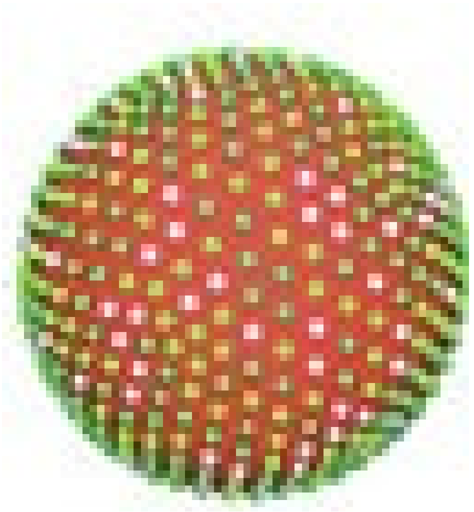
Description of the next simplest quantum system: the particle in a box

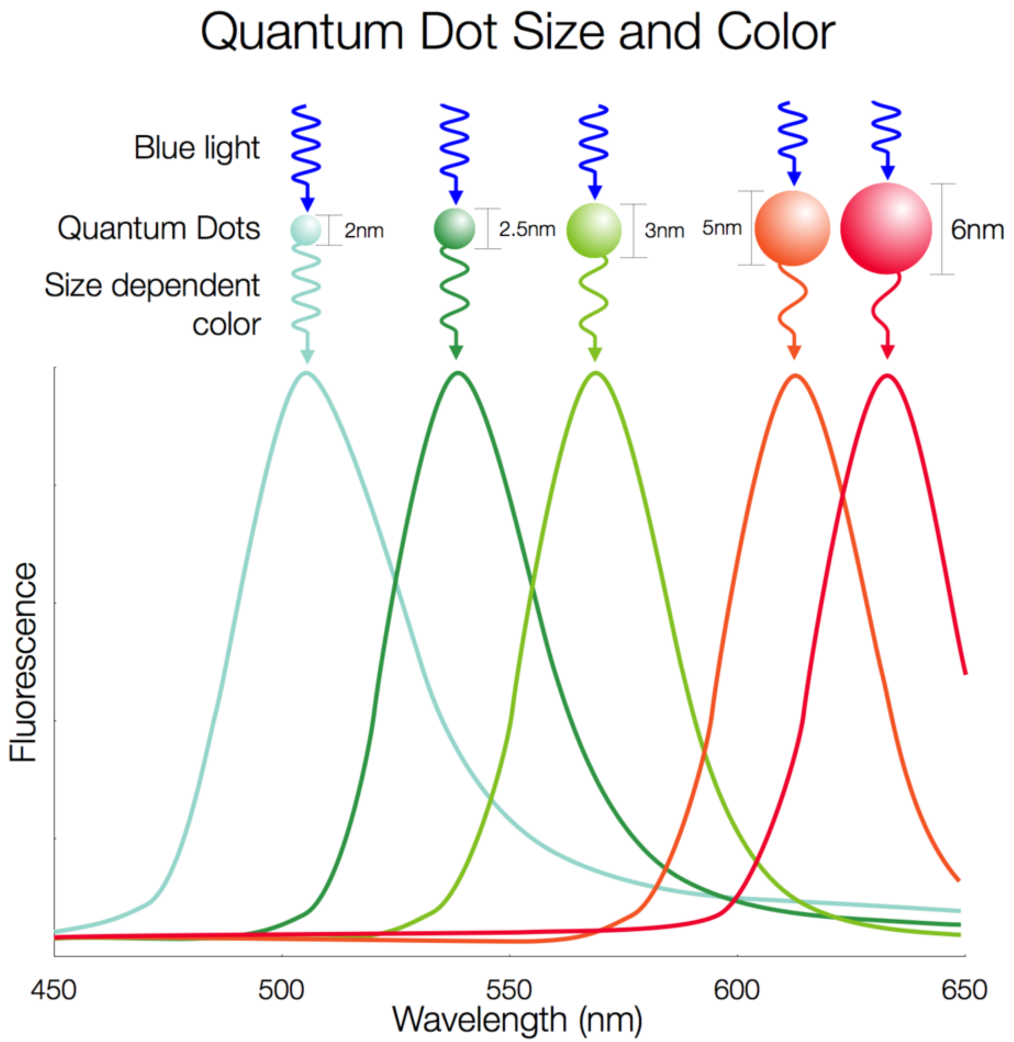
- Stationary states & energies for a 1D box
- Boxes of 2 and 3 dimensions





Quantum dots as 3D PIBs





Practice Problem #1

In solving the time-independent Schrodinger equation for a free particle, we are working with the expression:

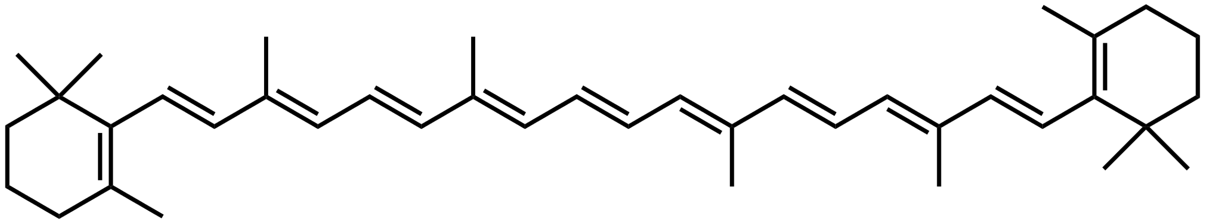
$$\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}E\psi(x)$$

Our solutions will be complex exponentials of the form:

$$\psi_k(x) = A_+ e^{ikx}$$

Write down an expression for *k* that solves the differential equation. Does it look familiar?

Practice Problem #2: beta carotene



β-carotene can be approximated as a 1D particle in a box.

This molecule has a conjugated region that is approximately 2.4 nm long and contains 11 π bonds. There are therefore 22 π electrons filling the lowest 11 orbitals of the π network.

Write down an expression for the lowest-energy electronic transition of β-carotene? What wavelength of light is needed to excite this transition?