Problem 1 (Schodinger Equation)

The 1D time-independent Schrödinger Equation is defined as

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

where $\hbar$ is Planck's constant $h/2\pi$, m is the mass of a particle, $U(x)$ is the potential energy, and E is the system energy. To solve the 1D Schrödinger Equation, consider an electron, which is confined to move back and forth between rigid walls that are a distance, ℓ, apart from one another. Consider also de Broglie's *wave particle duality*: the electron and its motion can be described by a wave function ψ. Classically, this situation is analogous to standing-wave oscillations of a stretched string clamped at each end between massive supports, which are a distance ℓ apart. The supports constrain the vibrating string such that the nodes are always at these points, thus limiting the possible wavelengths of the standing waves.

a) What are the possible wavelengths of the standing waves in the string?

A possible solution of the standing wave is

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

Boundary conditions are applied to the possible solution.

At $x=0$: $\quad y(0)=B=0$

At $x=l$: $\quad y(l)=A\sin kl=0 \qquad \because B=0$

From the boundary condition at $x=l$, $k=\dfrac{n\pi}{l}$ where n is 1, 2, 3, ...

Therefore, the possible wavelength is $\dfrac{2l}{n}$ where n is 1, 2, 3, ...

b) Each point on the stretched string oscillations with simple harmonic motion. Let y_{max} be the maximum amplitude anywhere along the string. Derive the amplitude function of the standing wave? I.e. Show that $y_n(x)$ depend on x, n, and ℓ, where n= 1, 2, 3, …?

Since the problem defined that the standing wave, $y_n(x)=A\sin\left(\dfrac{n\pi}{l}x\right)$, has the maximum amplitude y_{max}, the wave function (the amplitude function) is

$$y_n(x)=y_{max}\sin\left(\frac{n\pi}{l}x\right)$$

c) The string is analogous to an electromagnetic wave trapped between two perfectly reflecting mirrors that are separated by a distance ℓ. The electromagnetic wave will also exhibit a standing wave pattern. What is the amplitude function $E_n(x)$ of the electromagnetic wave?

$$E(x,t) = E_m \sin(kx - \omega t)$$

From the boundary condition, $k = \frac{n\pi}{l}$ where n is 1, 2, 3, ...

Therefore, $E_n(x,t) = E_m \sin(\frac{n\pi}{l}x - \omega t)$

d) Now go back to our original goal which is to solve the 1D time-independent Schrödinger Equation. What is ψ?

In a one dimensional infinite square well, the potential $U(x) = 0$ in the well.

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

$$\frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where} \quad k = \frac{\sqrt{2mE}}{\hbar}$$

A possible solution of the above equation is

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

Boundary conditions are applied to the possible solution.

At $x = 0$: $\psi(0) = B = 0$

At $x = l$: $\psi(l) = A\sin kl = 0$ $\quad \because B = 0$

From the boundary condition at $x = l$, $kl = n\pi$ where n is 1, 2, 3, ...

Therefore, the wave function is

$$\psi_n(x) = A\sin\left(\frac{n\pi}{l}x\right)$$

By normalization,

$$\int_0^l |\psi_n(x)|^2 dx = 1 \rightarrow \psi_n(x) = \sqrt{\frac{2}{l}}\sin\left(\frac{n\pi}{l}x\right)$$

Therefore, the entire wave packet is

$$\psi(x) = \sum_n a_n \psi_n(x) = \sum_n a_n \sqrt{\frac{2}{l}} \sin\left(\frac{n\pi}{l} x\right) \qquad \text{where } a_n = \int_0^l \psi_n \psi(x) dx$$

e) Quantization of the wavelength of a particle trapped between rigid walls leads to the quantization of its kinetic energy. Show that

$$E_n = n^2 \frac{h^2}{8ml^2}$$

From the Schrodinger equation $\frac{d^2\psi}{dx^2} = -k^2\psi$ where $k = \frac{\sqrt{2mE}}{\hbar}$,

The energy of the wave function is

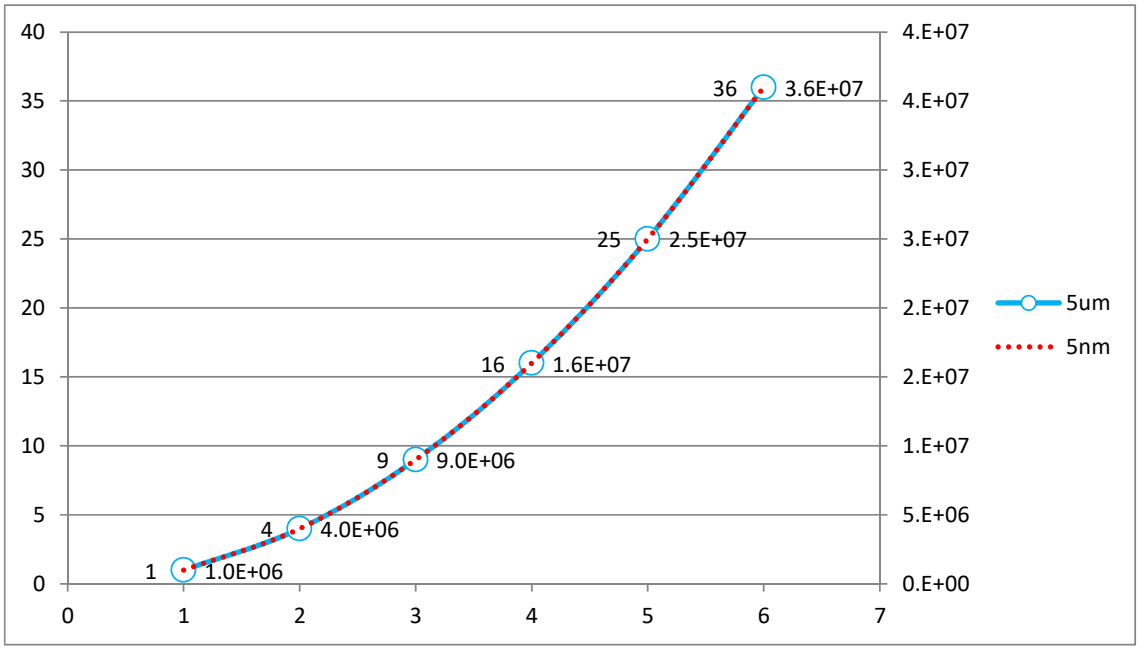
$$E = \frac{\hbar^2 k^2}{2m}$$

From the boundary condition at $x = l$, $kl = n\pi$ where n is 1, 2, 3, ...

Therefore, the quantized energy is

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{l}\right)^2 = \frac{\hbar^2 n^2 \pi^2}{2ml^2} = \frac{h^2 n^2}{8ml^2}$$

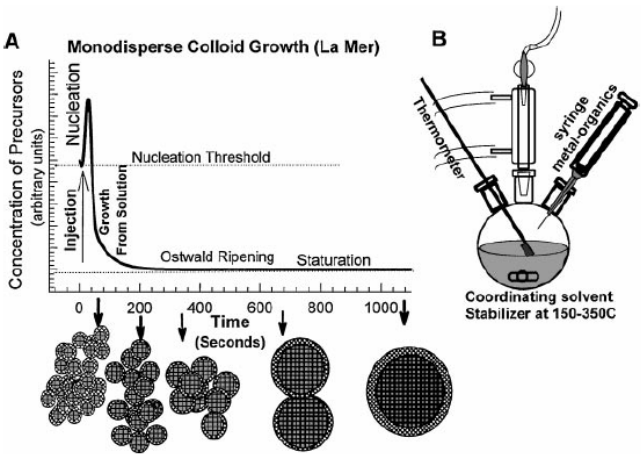
f) Plot E_n (in normalized units, assuming the same mass) vs n for ℓ = 5 μm and 5 nm



Problem 2 (QD Synthesis)

Name conditions that can control the size of quantum dots and also the trends that relate to quantum dot size.

In colloidal synthesis, the size of quantum dots can be affected by temperature, concentration of precursor, reaction time, etc. As shown in the below figure, longer reaction of colloid growth increases the size of the quantum dots.



[C. B. Murray, C. R. Kagan, and M. G. Bawendi, *Annu. Rev. Mater. Sci.* 30, 545, 2000.]

Larger dots emit redder (lower energy) light, and smaller dots emit bluer (higher energy) light. The color is related to the energy levels of the quantum dot; the band gap energy determines the energy (wavelength), and it is inversely proportional to the size of the quantum dot. Since larger quantum dots have more energy levels, they are more closely spaced. Hence, the larger quantum dot emits less energy which is closer to red end of the spectrum

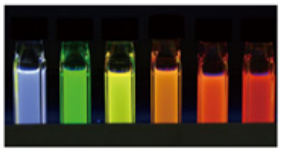


Figure 1: Fluorescence emitted from quantum dots. Blue fluorescence can be emitted from small particles of approximately 2 nm in diameter, green from ~3 nm particles, yellow from ~4 nm particles, and red from large particles of ~5 nm.
The wavelength of the excitation light is 365 nm.

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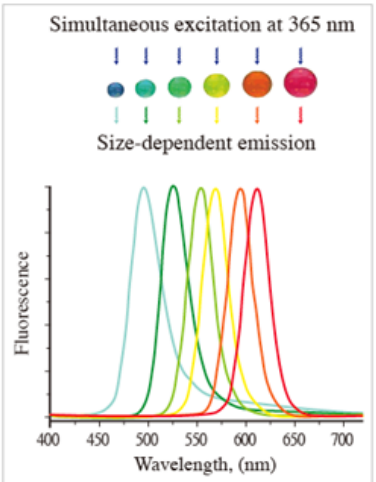

Figure 2: Fluorescence spectra depending on the size of quantum dots.

Problem 3 (QD Application)

Describe five applications of bio-conjugated quantum dots. Why are quantum dots preferred?

1. **Cell imaging**: The unique optical properties of QDs make them appealing as *in vivo* and *in vitro* fluorophores in a variety of biological investigations, in which traditional fluorescent labels based on organic molecules fall short of providing long-term stability and simultaneous detection of multiple signals.
   ["Quantum dot bioconjugates for imaging, labeling, and sensing", IL Medintz *et al.*, Nature materials, 2005]

2. **Immunohistochemistry**: Bioconjugated QDs can be used for multiplexed profiling of molecular biomarkers, and ultimately for correlation with disease progression and response to therapy.
   ["Bioconjugated quantum dots for multiplexed and quantitative immunohistochemistry", Y Xing *et al.*, Nature Protocols, 2007]

3. **Cell targeting**: The unique optical properties, such as size-dependent tunable absorption and emission in the visible and NIR regions, narrow emission and broad absorption bands, high photoluminescence quantum yields, large one- and multi-photon absorption cross-sections, and exceptional photostability shows excellent cell targeting performance.
   ["Delivering quantum dots to cells: bioconjugated quantum dots for targeted and nonspecific extracellular and intracellular imaging", V Biju *et al.*, Chem. Soc. Rev., 2010]

4. **Stem cell labeling**: The use of bioconjugated QDs acts as an effective probe for long-term labeling of stem cells.
   ["Labeling of Mesenchymal Stem Cells by Bioconjugated Quantum Dots", BS Shah et *al.*, Nano letters, 2007]

5. **Cell detection**: Highly luminescent semiconductor quantum dots covalently coupled to biomolecules for use in ultrasensitive biological detection. In comparison with organic dyes such as rhodamine, this class of luminescent labels is 20 times as bright, 100 times as stable against photobleaching, and one-third as wide in spectral linewidth.
   ["Quantum Dot Bioconjugates for Ultrasensitive Nonisotopic Detection", WCW Chan *et al.*, Science, 1998]