Solutions, Practice Problems for Exam 1, CHM 3411

1. A photon of wavelength 465 nm encountering the surface of an unknown metal ejects an electron with a kinetic energy of 3.252×10^{-19} J.

(a) What is the minimum frequency of radiation required to eject an electron from the metal surface?

$$E_K = h\nu - \Phi$$

$$\nu = \frac{c}{\lambda} = \frac{2.99 \times 10^{8}\ m/s}{465 \times 10^{-9} m} = 6.43 \times 10^{14}\ s^{-1}$$

$$\Phi = h\nu - E_K = 4.261 \times 10^{-19} - 3.252 \times 10^{-19} = 1.009 \times 10^{-19}\ J$$

$$\Phi = h\nu_{min} \qquad \boxed{\nu_{min} = \frac{\Phi}{h} = 1.522 \times 10^{14}\ s^{-1}}$$

(b) What about this is contradictory to classical expectation?

Classically, there would be no minimum frequency.

2. For a particular diatomic molecule, absorption of light of wavelength 4292 nm causes a transition from the ground vibrational state (v=0) to the first excited vibrational state (v=1). Compute the zero-point energy for vibration of the molecule.

$$\Delta E = h\nu \qquad \Delta E = \hbar\omega \quad \Rightarrow \hbar\omega = h\nu$$

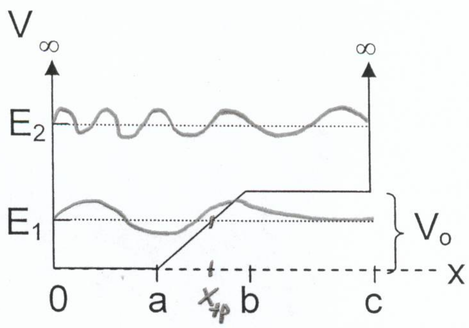
$$\Delta E = E(v=1) - E(v=0) = (1+\tfrac{1}{2})\hbar\omega - (0+\tfrac{1}{2})\hbar\omega$$

$$= \hbar\omega$$

$$\text{zero-pt energy} = \tfrac{1}{2}\hbar\omega = \tfrac{1}{2}h\nu = \tfrac{1}{2}h\frac{c}{\lambda} = \boxed{2.308 \times 10^{-20}\ J}$$

*Note that a QM particle cannot enter a region where potential energy is infinite, so the tunneling region ends at c. Also note that the particle with energy E_2 does not exhibit tunneling.

3. Consider the potential energy function sketched below. Two particular energy levels for consideration are labeled E_1 and E_2. The potential energy is infinite for $x < 0$ and $x > L$.



(a) On the figure above, sketch the wave functions for particles with energies E_1 and E_2. No calculations are needed, but the wave functions should qualitatively show the important features. [The finely dashed lines at E_1 and E_2 are drawn for your convenience; offset the wave functions so that each is zero along the corresponding finely dashed line.]

(b) Define three regions (ranges of x), and give the Schrödinger equation for each region.

Reg. I $\quad 0 < x \le a \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \psi = \psi_I$ in Reg I

" $\quad$ II $\quad a < x \le b \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_o\left(\frac{x-a}{b-a}\right)\psi = E\psi \quad \psi = \psi_{II}$ " " II

" $\quad$ III $\quad b < x < c \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_o\psi = E\psi \quad \psi = \psi_{III}$ " " III

(c) What boundary conditions are needed to obtain specific solutions to the Schrödinger equation for a particle confined to this "box" (i.e., the potential energy function sketched)?

continuity: $\psi_I(0) = 0 \quad \psi_I(a) = \psi_{II}(a) \quad \psi_{II}(b) = \psi_{III}(b) \quad \psi_{III}(c) = 0$

smoothness: $\frac{d\psi_I}{dx}(0) = 0 \quad \frac{d\psi_I}{dx}(a) = \frac{d\psi_{II}}{dx}(a) \quad \frac{d\psi_{II}}{dx}(b) = \frac{d\psi_{III}}{dx}(b) \quad \frac{d\psi_{III}}{dx}(c) = 0$

normalization: $\int_0^c \psi^*\psi \, dx = 1$

*

(d) Discuss the concept of tunneling and how it relates to the wave functions you drew in part (a). Be sure to identify any tunneling regions for a particle with energy E_1 or energy E_2.

Classically, a particle can never have negative kinetic energy. This prevents a classical particle ~~mass~~ with energy E_1 from entering the region to the right of the point marked x_{tp} on the figure. However, the Q.M. particle can enter this region; this behavior is called tunneling. The tunneling region for the particle with energy E_1 is $x_{tp} < x < c$

4. Consider a particle of mass m in a box of length L = 1 (neglecting units) which is in a state that is a superposition of sine functions:

$$\psi(x) = c_1\phi_1(x) + c_2\phi_2(x)$$

where c_1 and c_2 are constants, and $\phi_1(x)$ and $\phi_2(x)$ are orthonormal functions (over the interval $0 < x < 1$) defined by:

$$\phi_1(x) = \sqrt{2}\sin(\pi x)$$
$$\phi_2(x) = \sqrt{2}\sin(2\pi x)$$

(a) Show that $\phi_1(x)$ and $\phi_2(x)$ are eigenfunctions of the kinetic energy operature, $\hat{E}_K$, but $\psi(x)$ is not.

$$\hat{E}_K = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \qquad \text{use } \hbar = \frac{h}{2\pi}$$

$$\hat{E}_K\phi_1 = \frac{\pi^2\hbar^2}{2m}\sqrt{2}\sin(\pi x) = \frac{h^2}{8m}\phi_1$$

$$E_K\phi_2 = \frac{4\pi^2\hbar^2}{2m}\cdot\sqrt{2}\sin(2\pi x) = \frac{h^2}{2m}\phi_2$$

$$E_K\psi = \frac{h^2}{2m}\left(\frac{1}{4}c_1\phi_1 + c_2\phi_2\right)$$ cannot be expressed as constant times ψ

(b) The constants c_1 and c_2 must satisfy a relationship in order for required $\psi(x)$ to be normalized. Determine this relationship. Hint: recalling that $\phi_1(x)$ and $\phi_2(x)$ are orthonormal will save some work.

$$1 = \int_0^1 \psi^*\psi\,dx = \int_0^1 (c_1\phi_1 + c_2\phi_2)^*(c_1\phi_1 + c_2\phi_2)\,dx$$

$$= |c_1|^2 \underbrace{\int_0^1 \phi_1^*\phi_1\,dx}_{1} + |c_2|^2 \underbrace{\int_0^1 \phi_2^*\phi_2\,dx}_{1} + c_1^*c_2 \overbrace{\int_0^1 \phi_1^*\phi_2\,dx}^{0} + c_2^*c_1 \underbrace{\int_0^1 \phi_2^*\phi_1\,dx}_{0}$$

$$\boxed{1 = |c_1|^2 + |c_2|^2}$$

(c) What is the expectation value of T (in terms of m)?

$$\langle E_K\rangle = \int_0^1 \psi^*\hat{T}_x\psi\,dx = \int (c_1\phi_1 + c_2\phi_2)^*\hat{T}_x(c_1\phi_1 + c_2\phi_2)\,dx$$

$$= |c_1|^2\left(\frac{h^2}{8m}\right)\underbrace{\int_0^1 \phi_1^*\phi_1\,dx}_{1} + |c_2|^2\left(\frac{h^2}{2m}\right)\underbrace{\int_0^1 \phi_2^*\phi_2\,dx}_{1} + 0 + 1$$

$$= \boxed{\frac{h^2}{2m}\left(\frac{1}{4}|c_1|^2 + |c_2|^2\right)}$$

(d) Suppose a single measurement of the kinetic energy, E_{Ki} is made. What possible values can be obtained (your answer should be in terms of m)?

Either of the two eigenvalues:

$$\frac{h^2}{8m}, \quad \frac{h^2}{2m}$$