Quantum Mechanics

September 22, 2006

Work 4 of the 5 problems. Please put each problem solution on a separate sheet of paper (except for problem 5 which you should answer directly on the problem sheet) and your name on each sheet.

Problem 1

A conjugated bond framework consists of covalently bonded atoms with alternating single and double bonds. This results in a delocalization of the electrons, and hence the electron density, thereby increasing stability by lowering the overall energy of the molecule. An electron moving in a conjugated bond framework may be viewed as a "particle in a box". An externally applied electric field of strength E interacts with the electron in a fashion described by the perturbation

$$V = eE(x - L/2)$$

where x is the position of the electron in the box, e is the electron's charge, and L is the length of the box.

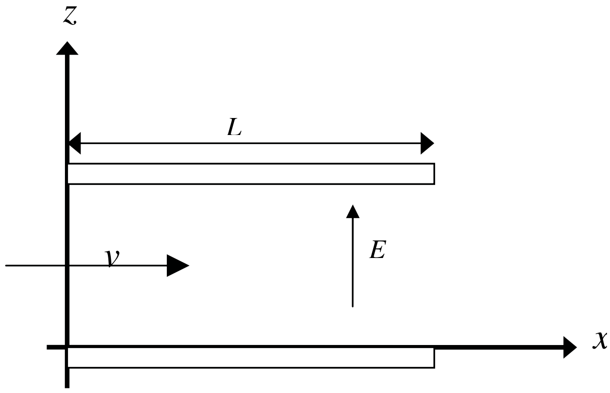
(A) Compute the first-order correction to the energy of the $n = 1$ state and the first-order wave function for the $n = 1$ state (In the wave function calculation, one only needs to compute the contribution to $\psi_1^{(1)}$ made by $\psi_2^{(0)}$).

(B) Use the answer to arrive at the induced dipole moment caused by polarization of the electron density due to the electric field effect,

$$\mu_{induced} = -e \int \psi^*(x - L/2)\psi \, dx$$

Problem 2

A beam of excited hydrogen atoms in the $2s$ state passes between the plates of a capacitor in which a uniform electric field $\vec{E}$ exists over a distance L. The hydrogen atoms have velocity v along the x-axis and the electrical field of magnitude E is directed along the positive z-axis as shown in the figure.



(A) What is the perturbing Hamiltonian H_I due to the perturbing electrical field?

(B) Show that the only non-vanishing matrix elements are $\langle 2l'm'|H_I|2lm\rangle$ for $l' = l + 1$ and $m' = m = 0$.

(C) Which of the $n = 2$ states are mixed (to first order) due to the applied electrical field?

(D) Give a concise argument that shows that $\langle 210|H_I|200\rangle = \langle 200|H_I|210\rangle$ and determine the eigenstates to first order in H_I. Use this information to draw an energy level diagram for the perturbed and unperturbed systems and identify clearly the energy and the eigenstate(s) that belong to each energy level.

(E) For a system that is in the $2s$ state at $t = 0$, express the wave function at a time $t \leq L/v$, where L is the width of the capacitor and v is the velocity of the electron beam (see also figure above).

(F) Find the probability that the emerging beam contains hydrogen in the various $n = 2$ states.

Hint: $\langle 210|H_I|200\rangle = 3eEa$, where e is the electrical charge, E is the strength of the applied field, and a is the Bohr radius ($a = 0.529177\,\text{Å}$). Also, here are a few low-order spherical harmonics:

$$Y_{00}(\theta,\varphi) = \sqrt{\frac{1}{4\pi}} \qquad Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{1\pm1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}}e^{\pm i\varphi}\sin\theta$$

Problem 3

Consider the Schrödinger equation in one dimension for a particle of mass m and energy $E > 0$ which is initially moving from $x = -\infty$ in a wave with unit incident amplitude. The wave function for large negative x is

$$\psi(x) = e^{ikx} + Re^{-ikx},$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$.

1) If the wave is totally reflected from a barrier to the right show $|R|$=1. (1 point)
2) If it is reflected from an infinite barrier at $x = 0$ what is R? (1 point)
3) If it is reflected from an infinite barrier at $x = -b$ what is R? (1 point)
4) Now consider a system of potentials ($V_0 > E$)

$$\begin{array}{lll} V = 0 & \text{for} & x < -b \\ V = V_0 & \text{for} & -b \leq x \leq -a \\ V = 0 & \text{for} & -a < x \leq 0 \\ V = \infty & \text{for} & x > 0. \end{array}$$

For $V_0 \to \infty$ the region between $x = -a$ and $x = 0$ will have bound state solutions. What is the energy of the lowest bound state? (1 point)

5) If we define $q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$, $L = -\frac{q}{k}\tan ka$ and $\alpha = \frac{L-1}{L+1}e^{2q(b-a)}$, show that

$$R = e^{-2ikb}\frac{k(1+\alpha) + iq(1-\alpha)}{k(1+\alpha) - iq(1-\alpha)}. \qquad \text{(5 points)}$$

6) For V_0 (and hence q) very large, discuss the behavior of the phase of R as a function of α. Is there a critical value of α and, if so, how is it related to the bound state in part 4 above? (1 point)

Problem 4

Consider a particle of mass m in a one-dimensional potential of the form

$$\begin{aligned} V &= \tfrac{K}{2}x^2 && 0 \le x \le L, \\ V &= \infty && x < 0 \text{ or } x > L. \end{aligned}$$

where $K \ll h^2/mL^4$.

(A) Derive an expression for the energy levels E_n. (8 points)

(B) Comment on the asymptotic form of E_n for large n. (2 points)

Problem 5

This is a multiple choice test. Do not show your work.

I. Consider the following matrix elements of type $\langle Y_{lm}|f(\vec{r})|Y_{l'm'}\rangle$. Decide, which of these matrix elements are zero:

a. $\langle Y_{00}|y|Y_{11}\rangle$ ◯ zero ◯ not zero

b. $\langle Y_{00}|x|Y_{10}\rangle$ ◯ zero ◯ not zero

c. $\langle Y_{10}|z|Y_{10}\rangle$ ◯ zero ◯ not zero

d. $\langle Y_{00}|x^2 - y^2|Y_{10}\rangle$ ◯ zero ◯ not zero

e. $\langle Y_{11}|x|Y_{1,-1}\rangle$ ◯ zero ◯ not zero

f. $\langle Y_{00}|xy|Y_{22}\rangle$ ◯ zero ◯ not zero

Hint: Use $e^{i\phi} = x+iy$ and express the corresponding operator in terms of $e^{im\phi}$. (3 points).

II. Consider now a particle subject to the Hamiltonian

$$H = \frac{1}{2m}\vec{p}^2 + V(r) + \gamma\vec{L}\cdot\vec{S} + \delta\vec{r}\cdot\vec{p},$$

where $\vec{S} = \frac{1}{2}\vec{\sigma}$ is the spin and γ and δ are constants. Decide, which of the following quantities are conserved

a. $\vec{L}\cdot\vec{S}$ ◯ conserved ◯ not conserved

b. $L_y + S_y$ ◯ conserved ◯ not conserved

c. parity ◯ conserved ◯ not conserved

(1.5 points)

Please turn over, this problem continues on the back.

III. Consider now a particle subject to the Hamiltonian

$$H = \frac{1}{2m}\vec{p}^2 + V(r) + \gamma z(x^2 + y^2),$$

where γ is a constant. State, which of these statements is correct

a. The ground state has even parity ○ true ○ false

b. The ground state has $\vec{L}^2 = 0$ ○ true ○ false

c. The ground state has $L_z = 0$ ○ true ○ false

d. The ground state has $L_y = 0$ ○ true ○ false

Here "has" means "is an eigenstate of the corresponding operator with the corresponding eigenvalue". (2 points)

IV. What is the ground state energy for a Schrödinger equation $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x)$ in a potential

$$V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & \text{for} \quad x \leq 0 \\ +\infty & \text{for} \quad x > 0 \end{cases}$$

(2 points)

V. The scattering amplitude for some hypothetical (actually somewhat unrealistic) model is given by

$$f(\theta) = \frac{1}{k}\left[e^{i2ka}\sin(2ka) + 3ie^{2ik^2a^2}\cos(2k^2a^2)\cos(\theta) + e^{ika}\sin(ka)\left(\frac{15}{2}\cos^2\theta - \frac{5}{2}\right)\right]$$

where a is a constant and $\frac{\hbar^2 k^2}{2m} = E$. Check the correct answers

1. The s-wave ($l = 0$) contribution to the total cross section in the zero energy limit $E \longrightarrow 0$ is

   a.) zero ○

   b.) finite, i.e. neither zero nor infinite ○

   c.) infinite ○

   (0.5 points)

2. The p-wave ($l = 1$) contribution to the total cross section in the zero energy limit $E \longrightarrow 0$ is

   a.) zero ○

   b.) finite, i.e. neither zero nor infinite ○

   c.) infinite ○

   (0.5 points)

3. The d-wave ($l = 2$) contribution to the total cross section in the zero energy limit $E \longrightarrow 0$ is

   a.) zero ○

   b.) finite, i.e. neither zero nor infinite ○

   c.) infinite ○

   (0.5 points)