Quantum Mechanics

September 19, 2008

Work 4 of the 5 problems. Please put each problem solution on a separate sheet of paper and your name on each sheet.

Problem 1

Derive the Russell-Saunders terms $^{(2S+1)}L_J$ for two p-electrons in the cases of the electrons being

a. distinguishable

b. indistinguishable (Hint: Construct a table of the possible values of M_L and M_S).

Problem 2

Given are a wave packet for a free electron of mass m in one dimension,

$$\psi(x,t) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dk\, c(k) \exp\left[i(kx - \omega_k t)\right]$$

where $\omega_k = \hbar k^2/2m$, and a Gaussian $c(k)$,

$$c(k) = N \exp\left(-\frac{1}{2}\Delta^2 (k-k_0)^2\right) ,$$

where N, Δ, k_0 are constants.

a. State how to find N, and then show that $N = (\Delta^2/\pi)^{1/4}$.

b. Show that

$$\psi(x,t) = \chi(x - \hbar k_0 t/m, t) \exp\left[i(k_0 x - \omega_{k_0} t)\right]$$

where

$$\chi(\xi, t) = N\Lambda^{-1}(t) \exp(-\xi^2/2\Lambda^2)$$

and $\Lambda^2(t) \equiv (\Delta^2 + i\hbar t/m)$. Identify the phase and group velocities directly from the expression for ψ.

c. Show that

$$\rho = \psi^* \psi = \frac{1}{\sqrt{\pi\sigma^2}} \exp(-\xi^2/\sigma^2) , \qquad \sigma^2 \equiv \Delta^2 \left[1 + \left(\frac{\hbar t}{m\Delta^2}\right)^2\right]$$

and verify directly that $\langle\psi|\psi\rangle = 1$.

d. What Heisenberg uncertainty should this wave packet predict? If you have time, start with

$$(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle , \qquad (\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle$$

where $\langle x \rangle = \langle \psi | x | \psi \rangle$, etc., and $p = -i\hbar\partial_x$, and derive the uncertainty relation. Hint: $(\Delta x)^2 = \sigma^2/2$.

e. Suppose $\Delta = \hbar/mc$, the Compton wave length, so that the electron is very well localized at $t = 0$. Show that then $(\Delta x)^2 \approx c^2 t^2/2$ for $t \gtrsim 10\hbar/mc^2 \approx 10^{-20}s$. What happens for large Δ? Explain. Discuss this result in comparison with ordinary (Einstein) diffusion, if you can.

Problem 3

The representation of the elastic scattering amplitude for two spin-zero particles, even in the case where some inelastic channels may exist, is given by

$$f(\theta) = \frac{1}{2ik} \sum_{\ell=0}^{\infty} (2\ell + 1)(S_\ell - 1) P_\ell(\cos\theta). \tag{1}$$

It is sometimes convenient to write the S-matrix as

$$S_\ell = \eta_\ell e^{2i\delta_\ell}; \quad 0 < \eta_\ell < 1 \tag{2}$$

a) Calculate the integrated elastic cross section, that is, the total cross section for elastic scattering.
b) Use the result obtained in part a, along with the optical theorem for the total cross section, $\sigma_T = \frac{4\pi}{k} Im f(0)$, to obtain an expression for the reaction cross section.
c) Suppose that a single value of $\ell = L$ dominates the sum, so that only that partial wave need be considered, and that there is a resonance in that partial wave. In that case an appropriate form for S_L is

$$S_L = \frac{E - E_0 + \frac{i}{2}(\Gamma_i - \Gamma_e)}{E - E_0 + \frac{i}{2}\Gamma} \tag{3}$$

where $\Gamma = \Gamma_i + \Gamma_e$ and Γ_e is called the "elastic width" and Γ_i is called the "inelastic width". Find an expression for the integrated elastic cross section for these conditions.
d) Find an expression for the inelastic cross section for the conditions of part c.
e) For the conditions of part c, give a description of what happens physically at the peak of the resonance if $\Gamma_i = \Gamma_e$.

Problem 4

A neutral tritium atom (^{3}H; a heavy hydrogen atom with one proton and two neutrons in its nucleus) is initially in its ground state when it undergoes β^--decay into a singly-charged, helium-3 ion (^{3}He$^+$, with two protons and one neutron in the nucleus). Assuming that the change of the nuclear charge is very sudden and ignoring any effects from the emitted β^- particle, calculate the probability that the ^{3}He$^+$ ion will end up in the $2s$ excited state.

Problem 5

The π-orbitals of benzene, C_6H_6, may be modeled using the wave functions and energies of a particle on a ring. This problem consists of two parts: Treat the problem of a particle on a ring and then apply it to benzene.

a. Suppose that a particle of mass m is constrained to move on a circle of radius r in the xy plane and that the particle's potential energy is constant (zero is a good choice). Write down the Schrödinger equation in the normal Cartesian coordinate representation. Transform this Schrödinger equation to cylindrical coordinates, where $x = r\cos\varphi$, $y = r\sin\varphi$, and $z = z$. Holding r constant, write down the general solution, $\Psi(\varphi)$. The boundary conditions require that $\Psi(\varphi) = \Psi(\varphi + 2\pi)$. Apply this boundary condition to the general solution. Write down the final expressions for the normalized wave functions and quantized energies, labeled by an appropriate quantum number. Give the physical significance of this quantum number, which can have both positive and negative values. Draw an energy diagram representing the first five energy levels (label appropriately).

b. Treat the six π-electrons of benzene as particles free to move on a ring of radius 1.40 Å and calculate the energy of the lowest electronic transition (ensure that the Pauli principle is satisfied). What wave length does this correspond to? Suggest at least two reasons why this differs from the observed wave length of 2600 Å.