MATERIALS PHYSICS II FALL 2007 HOMEWORK PROBLEMS 10

Return to Robert (mailbox Physics 2nd floor) by Tuesday 4.12.2007 at noon. **two weeks to work !**

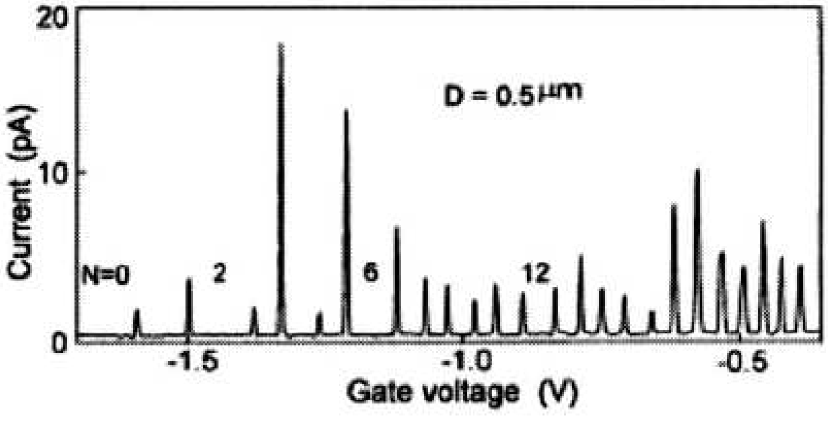
Comment: working through the weekly problems as team work is completely acceptable and even recommended, as far as each person writes down and returns his/her own solutions!

1. *Simple model for quantum dots.* Show that the eigenenergies of a two-dimensional harmonic potential are $\varepsilon_l = \hbar\omega(l+1)$, and degeneracies $d_l = l+1$ with $l = 0, 1, 2, \ldots$ (Hint: Show that the Hamiltonian separates into a sum of two one-dimensional Hamiltonians and use the energies of one-dimensional harmonic oscillator.)

In the capacitive model of a quantum dot the addition energy is

$$\Delta_2(N) = \varepsilon_{N+1} - \varepsilon_N + e^2/C,$$

where ε_N is the energy of the single-electron level occupied by the Nth electron and e^2/C is the capacitive charging energy. Use the simple model of a quantum dot where the non-interacting electrons occupy the levels of the two-dimensional harmonic oscillator, and plot the addition energies $\Delta_2(N)$ as a function of electron number N, for N=1…13. For simplicity use units where $\hbar\omega = e = 1$ and $C = N$, thus assume that the capacitance increases with the electron number. Compare your plot with the experimental one (from Tarucha *et al.* Phys. Rev. Lett. **77** (1996) 3613):



What are the qualitative differences and similarities?
(4 points)

2. *Pauli spin susceptibility.* Let $n^+ = \frac{1}{2}n(1+\xi)$ and $n^- = \frac{1}{2}n(1-\xi)$ be the consentrations of spin-up and spin-down elctrons, respectively. Show that in a magnetic field B the total energy of the spin-up electrons in a free-electron gas is

$$E^+ = E_0(1+\xi)^{5/3} - \frac{1}{2}n\mu_B B(1+\xi),$$

where $E_0 = \frac{3}{10} n \varepsilon_F$, in terms of the Fermi energy ε_F in zero magnetic field. Find a similar expression for E^-. Minimise $E = E^+ + E^-$ with respect to ξ and solve for the equilibrium value of ξ in approximation $\xi \ll 1$. Show that the magnetisation is $M = 3n\mu_B^2 B/2\varepsilon_F$. **(3 points)**

3. Consider an alternative way of deriving the (Larmor) atomic diamagnetic susceptibility. Do the following steps: (i) Assume $\mathbf{B}_{ext}$ parallel to z-axis, take the vector potential $\mathbf{A} = -\frac{1}{2}(\mathbf{r} \times \mathbf{B}_{ext})$ and develop the kinetic part of the Hamiltonian, $H_{kin} = \frac{1}{2m_e} \sum_i (\mathbf{p} + e\mathbf{A})^2$ where the sum is over all the electrons in the atom. (ii) Evaluate the expectation value of the atomic magnetic moment in a state $|\phi>$:

$$\mu_m = -\frac{\partial}{\partial \mathbf{B}_{ext,z}} < \phi | H | \phi >$$

and separate from the result two parts, the first one proportional to $< \phi | \mathbf{L}_z | \phi >$ and the second one to $< \phi | \sum_i (x_i^2 + y_i^2) | \phi >$. From the second term, derive the result

$$\chi_{m,dia} = -\frac{n_{at}}{6m_e} e^2 \mu_0 \sum_i < \phi | r_i^2 | \phi > .$$

Compare the result to the one derived in the lecture: $\chi_{m,dia} = -n_{at} Z e^2 \mu_0 < r^2 > /6m_e$. **(3 points)**

4. *Landau Levels.* The Hamiltonian of a free electron without spin is

$$H = \frac{1}{2m}(-i\hbar\nabla + e\mathbf{A})^2.$$

The vector potential of a uniform magnetic field $B\mathbf{z}$ is $\mathbf{A} = -By\mathbf{x}$ in the Landau gauge. We will look for an eigenfunction of the Schrödinger equation $H\psi = \varepsilon\psi$ in the form

$$\psi(x, y, z) = \chi(y) \exp[i(k_x x + k_z z)].$$

Show that $\chi(y)$ satisfies the equation

$$-\frac{\hbar^2}{2m}\chi''(y) + 1/2m\omega_c^2 (y - y_0)^2 \chi(y) = (\varepsilon - \hbar^2 k_z^2/2m)\chi(y),$$

where $\omega_c = eB/m$ and $y_0 = -\hbar k_x/eB$. Show that this equation yields the energies of the Landau levels,

$$\varepsilon_\nu = \hbar\omega_c(\nu + 1/2) + \frac{\hbar^2 k_z^2}{2m}, \qquad \nu = 0, 1, 2, \ldots$$

(3 points)

5. *Diamagnetic susceptibility of atomic hydrogen.* The wave function of the hydrogen *1s* electron is $\psi = (\pi a_0^3)^{-1/2} \exp(-r/a_0)$, where $a_0 = \hbar^2/me^2$ is the Bohr radius. Show that for this state $\langle r^2 \rangle = 3a_0^2$ and calculate the molar diamagnetic (Larmor) susceptibility of atomic hydrogen. **(2 points)**

6. The electron has an internal symmetry described "internal" spin operators S_i that satisfy the commutation relations similar to those of the angular momenta:

$$[S_x, S_y] = i\hbar\, S_z \qquad [S_y, S_z] = i\hbar\, S_x \qquad [S_z, S_x] = i\hbar\, S_y$$

We now look for representations of these relations in terms of matrices. The simplest representation is one in terms of 2×2-matrices:

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In order to make these operators act on a wavefunction the wavefunction must depend on an extra variable, the so-called spin-variable σ. We therefore have a wavefunction $\Psi(\mathbf{r}, \sigma)$. The variable σ can attain two values such that Ψ can be written as a two-component vector. We write $\Psi(\mathbf{r}, \sigma) = (\Psi(\mathbf{r}, 1), \Psi(\mathbf{r}, -1))$ (the labelling $\sigma = \pm 1$ is completely arbitary but customary, we could also have chosen $\sigma = 1, 2$). Now a general electron wavefunction can always be written as

$$\begin{aligned} \Psi(\mathbf{r}, \sigma) &= (\Psi(\mathbf{r}, 1), \Psi(\mathbf{r}, -1)) = \Psi(\mathbf{r}, 1)(1, 0) + \Psi(\mathbf{r}, -1)(0, 1) \\ &= \Psi(\mathbf{r}, 1)\, \alpha(\sigma) + \Psi(\mathbf{r}, -1)\, \beta(\sigma) \end{aligned}$$

where $\alpha = (1, 0)$ and $\beta = (0, 1)$ satisfy $\alpha(1) = \beta(-1) = 1$ and $\alpha(-1) = \beta(1) = 0$. In Marders book the notation $\alpha(\sigma) = \chi_\uparrow(\sigma)$ and $\beta(\sigma) = \chi_\downarrow(\sigma)$ is used.

a) Check that α and β are eigenfunctions of S_z with eigenvalues $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$. What is the action of S_x and S_y on these spin functions?

Now we consider the following spin functions for two electrons

$$\begin{aligned} \theta_{0,0}(\sigma_1, \sigma_2) &= \frac{1}{\sqrt{2}}(\alpha(\sigma_1)\beta(\sigma_2) - \beta(\sigma_1)\alpha(\sigma_2)) \\ \theta_{1,1}(\sigma_1, \sigma_2) &= \alpha(\sigma_1)\alpha(\sigma_2) \\ \theta_{1,0}(\sigma_1, \sigma_2) &= \frac{1}{\sqrt{2}}(\alpha(\sigma_1)\beta(\sigma_2) + \beta(\sigma_1)\alpha(\sigma_2)) \\ \theta_{1,-1}(\sigma_1, \sigma_2) &= \beta(\sigma_1)\beta(\sigma_2) \end{aligned}$$

b) Let $S_z = S_{z,1} + S_{z,2}$ be the total z-component of the spin of the two electrons (so $S_{z,i}$ acts of spin functions depending on spin coordinate σ_i where $i = 1, 2$). Show that the four spin functions $\theta_{0,0}, \theta_{1,1}, \theta_{1,0}, \theta_{1,-1}$ are eigenfunctions of S_z. What are the eigenvalues ?

c) We further consider the total spin vector $\mathbf{S} = \mathbf{S_1} + \mathbf{S_2}$ where $\mathbf{S_1}$ and $\mathbf{S_2}$ are the total spin vectors of electron 1 and 2. Show that the four spin functions $\theta_{0,0}, \theta_{1,1}, \theta_{1,0}, \theta_{1,-1}$ are eigenfunctions of

$$\mathbf{S}^2 = (\mathbf{S_1} + \mathbf{S_2})^2 = \mathbf{S_1}^2 + \mathbf{S_2}^2 + 2\,\mathbf{S_1} \cdot \mathbf{S_2}$$

with eigenvalues $\hbar^2 S(S+1)$ where $S = 0$ for $\theta_{0,0}$ (singlet) and $S = 1$ for $\theta_{1,1}, \theta_{1,0}$ and $\theta_{1,-1}$ (triplet)

d) Consider a two-electron Slater determinant with one electron described by orbital $\Psi_1(\mathbf{r}, \sigma) = \varphi(\mathbf{r})\alpha(\sigma)$ and the other electron by orbital $\Psi_2(\mathbf{r}, \sigma) = \varphi(\mathbf{r})\beta(\sigma)$. What are eigenvalues of the S_z and $\mathbf{S}^2$ for this two-electron wave function ?

e) Repeat question **d)** but now for electrons described by the orbitals $\Psi_1(\mathbf{r}, \sigma) = \varphi_1(\mathbf{r})\alpha(\sigma)$ and $\Psi_2(\mathbf{r}, \sigma) = \varphi_2(\mathbf{r})\alpha(\sigma)$. Why can we not choose $\varphi_1(\mathbf{r}) = \varphi_2(\mathbf{r})$?

f) Consider a two-electron Slater determinant for electrons described by the orbitals $\Psi_1(\mathbf{r}, \sigma) = \varphi_1(\mathbf{r})\alpha(\sigma)$ and $\Psi_2(\mathbf{r}, \sigma) = \varphi_2(\mathbf{r})\beta(\sigma)$. What is the eigenvalue of S_z ? In the case the wave function is not an eigenstate of $\mathbf{S}^2$. What other Slater determinant do we have to add in order to make this a an eigenstate of $\mathbf{S}^2$?

g) What can you say about the symmetries of the spatial and the spin parts of the two-electron wave functions discussed in **d), e), f)** ?

(5 points)