SISSA ISAS

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Fall 2005 – Entrance Examination: Condensed Matter

Solve at least one of the following problems. Write out solutions clearly and concisely. State each approximation used. Diagrams welcome. Number page, problem, and question clearly. Do not write your name on the problem sheet, but use extra envelope.

Problem 1. Electrons in square 2D box and 3D cylinder.

Consider electrons moving in a two-dimensional (2D) square box of linear size a, with rigid walls.

1. Give the 4 lowest energy levels and wavefunctions.
2. Using only the Pauli principle, fill these levels with 3 electrons obtaining their total ground state energy E_{tot}, spin S, and degeneracy d.
3. Deforming the square box to a rectangle of sides $(a+\delta, a-\delta)$, find the change of E_{tot} assuming $\delta/a \ll 1$. Does the result depend on the sign of δ? Is there also a change of d?
4. Returning to the square box, fill it now with 4 electrons. Describe the ground state energy degeneracy and spin in the absence of electron interactions.
5. In the presence of electron interactions, the degeneracy of different spin states is lifted, the largest S achieving the lowest E_{tot}. What will be the ground state spin of the 4 interacting electrons?
6. Allow the electron in the square box to move freely along a third orthogonal direction z, i.e., inside a square-based rigid infinite $3D$ cylinder. Describe the resulting wavefunctions and energy bands.
7. Fill up these bands with free electrons of linear density ρ. Determine the Fermi level $E_F(\rho)$ for small ρ, where only one band is filled. Find the critical value ρ_c of ρ, where more than one band begins to be filled.

Problem 2. One-electron atom in an external magnetic field.

Let's consider an electron (mass m and charge e) of an hydrogenoid atom with nuclear charge Z, inside an external magnetic field B parallel to the z axis. The Hamiltonian of the electron is given by:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{r} + \frac{\mu_B}{\hbar}\left(L_z + 2S_z\right)B, \tag{1}$$

where μ_B is the Bohr magneton and L_z and S_z are the projection of the orbital and spin angular momentum along the z axis, respectively.

1. Find the exact energy levels of this Hamiltonian in terms of the $B = 0$ energy levels E_n of the hydrogenoid atom, and discuss the magnetic field induced splittings of a p level.

2. Let us consider the effect of spin-orbit coupling on these levels. Add to the Hamiltonian a spin-orbit term of the form:

$$H_{SO} = \left(\frac{Ze^2}{2m^2c^2}\right)\frac{1}{r^3}\mathbf{L}\cdot\mathbf{S}, \tag{2}$$

   where $\mathbf{L}$ and $\mathbf{S}$ are the orbital and spin angular momentum vectors and c is the velocity of light. Assume that H_{SO} is a small perturnation with respect to the Hamiltonian (1) and find the change of the energy levels to first order in perturbation theory.
   Hint: The expectation value of $1/r^3$ on the hydrogenoid wave-functions of principal quantum number n and angular momentum l is $\left\langle \frac{1}{r^3}\right\rangle = \frac{Z^3}{a_0^3 n^3 l(l+1/2)(l+1)}$ where a_0 is the Bohr radius.

3. Now consider the opposite limit where H_{SO} is much larger than the magnetic field term in H, while still being a small perturbation of the $B = 0$ Hamiltonian. The unperturbed ($B = 0$) energy levels are eigen-functions of the total angular momentum (J^2 and $J_z = L_z + S_z$). A level that in absence of spin-orbit has orbital angular momentum $l > 0$, splits into levels of total angular momentum $j = l + 1/2$ and $j = l - 1/2$, with energies $E_{n,l,j}$. The eigen-functions of the total angular momentum for $j = l + 1/2$ and $j = l - 1/2$ are respectively:

$$\begin{aligned}
\tilde{Y}^{j,m_j}_{l,1/2} &= \left(\frac{l+m_j+1/2}{2l+1}\right)^{1/2} Y_{l,m_j-1/2}\chi_{1/2} + \left(\frac{l-m_j+1/2}{2l+1}\right)^{1/2} Y_{l,m_j+1/2}\chi_{-1/2} \\
\tilde{Y}^{j,m_j}_{l,1/2} &= -\left(\frac{l-m_j+1/2}{2l+1}\right)^{1/2} Y_{l,m_j-1/2}\chi_{1/2} + \left(\frac{l+m_j+1/2}{2l+1}\right)^{1/2} Y_{l,m_j+1/2}\chi_{-1/2}
\end{aligned}$$

   where $-j \le m_j \le j$, $Y_{l,m}$ are spherical harmonics, and $\chi_{\pm 1/2}$ are the spin eigen-functions. Using first order perturbation theory, treating the B term as a small perturbation of the $B = 0$ energy levels of $H + H_{SO}$, find the splitting of $E_{n,l,j}$ due to the magnetic field. Hint: You do not need to calculate the value of $E_{n,l,j}$ at $B = 0$. Assume it is given to you by some other calculation.

4. Discuss the relationship between the energy levels found at point 2) and those found at point 3.

Problem 3. Two interacting particles in one dimension.

Two identical particles with spin $s = 3/2$ are confined in a one dimensional geometry, with an external field $\mathbf{B}$. The Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{2} \frac{p_i^2}{2m} + U\,\delta(x_1 - x_2) - g\mu_B \mathbf{B} \cdot (\mathbf{S}_1 + \mathbf{S}_2) \;,$$

where U describes a point-like interaction between the particles.

1. Calculate eigenvalues and eigenfunctions for both $U > 0$ (repulsion) and $U < 0$ (attraction);

2. Do the same calculation in the case in which the two identical particles have spin $s = 1$.

Consider now just the case of an attraction $U < 0$ and calculate:

3. the ground state degeneracy at zero magnetic field, $\mathbf{B} = 0$, both for $s = 3/2$ and $s = 1$ particles;

4. the zero-temperature magnetization M along the direction of the field $\mathbf{B}$

$$\langle\, (\mathbf{S}_1 + \mathbf{S}_2) \cdot \frac{\mathbf{B}}{|\mathbf{B}|} \,\rangle$$

as function of the modulus $|\mathbf{B}|$, again for both $s = 3/2$ and $s = 1$ particles.

Problem 4. Binding energy and potential.

A spinless particle of mass m moves in a short range central potential $V(r)$, in the three dimensional space. The wavefunction describing the ground state of the particle is

$$\psi(r) = A\frac{e^{-\alpha r} - e^{-\beta r}}{r}$$

where A is a normalization factor, while $0 < \alpha < \beta$ are positive constants.

1. What is the angular momentum of this particle? (Justify your answer.)
2. What is the binding energy of this state?
3. What is the potential $V(r)$ that produced this state?