SISSA ISAS

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Fall 2003 – 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: Electron in a two–dimensional box

Consider an electron moving in two dimensions inside a generally rectangular box of potential $V(x,y) = 0$ when both $-a < x < a$ and $-b < y < b$
and $V(x,y) = \infty$ outside.

1. Assuming initially a square rigid box $a = b = a_0$, calculate the eigenfunctions and eigenvalues of the few lowest energy levels, specifying their respective symmetries and degeneracies.
2. Calculate the force F – due to the electron energy dependence upon the box size a_0 – exerted on the box walls by the electron, when it is
   (a) in the ground state
   (b) in the first excited state
3. Assume now the box to be elastically deformable, with a deformation energy
$$U = \frac{k}{2}[(a - a_0)^2 + (b - a_0)^2]$$
   for a general rectangular shape. Determine the nature and the (approximate) magnitude of the box deformation from the initial state $a = b = a_0$,
   (i) when the electron is in the ground state
   (ii) when the electron is in the first excited state.

   [Hint: assume the box deformation to be very small]

Problem 2: Motion of an electron in a harmonic trap

An electron is confined in an elipsoidal trap by the harmonic potential:

$$V(x,y,z) = \frac{m\omega_\perp^2}{2}(x^2+y^2) + \frac{m\omega_{||}^2}{2}z^2.$$

1. Determine the ground state energy of the electron and sketch its energy levels (assume $\omega_{||} << \omega_\perp$).

2. Consider now turning on slowly a transverse electric field, $\Delta V = eEx$, up to a finite value, E_0, and calculate the ground state energy of the perturbed system.

3. How are the excitation energies of the system modified by the presence of the electric field ?

4. The electron is in the new ground state when the electric field is suddenly switched off. Compute the energy of the electron immediately after the electric field is removed.

5. Compute the time evolution of the average electron position after the electric field is removed.

Problem 3: An atomic chain

Consider a one dimensional atomic chain composed by two types of atoms A and B, arranged in the infinite periodic sequence ...$ABABAB$.... The unit cell, of length a, contains two atoms at a distance $a/2$. Define a tight-binding model taking an orbital ϕ_A on each atom A and an orbital ϕ_B on each atom B, and neglecting the overlap between the two orbitals. The matrix elements of the Hamiltonian H between nearest-neighbor ϕ_A and ϕ_B orbitals are equal to $-t$. The on-site energies are $\langle\phi_A|H|\phi_A\rangle = \varepsilon_A$ and $\langle\phi_B|H|\phi_B\rangle = \varepsilon_B$. Neglect the other matrix elements of the Hamiltonian.

1. Sketch the band structure of this one-dimensional chain.
2. Calculate the energy gap and the band-widths.
3. Now consider Bloch states with complex $\kappa = k + i\alpha$ vector. Find for which k and α the eigenvalues of the Hamiltonian are real.
4. Sketch the complex band structure of the chain.
5. Optional: Find the relationship between the energy and the imaginary part of κ for eigenvalues in the gap of the real band structure.

Problem 4: Non interacting electron gas in a box

$2N$ non interacting electrons are confined within a cubic box of side L. Assume vanishing boundary conditions at the box faces.

1. Find the eigenvalues and normalized eigenfunctions of the Schrœdinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r}) = E\,\Psi(\vec{r}),$$

$\vec{r} = (x, y, z)$, with the appropriate boundary conditions.

2. Calculate the total energy of the $2N$ electrons in the limit of large L when sums over the discrete eigenvalues can be transformed into integrals (keep $N/L = \rho$=constant).

3. Calculate, in the same large L limit, the ground state spin magnetization in the presence of a Zeeman term which splits spin up from spin down eigenvalues by $\Delta E_B = -\mu_B B$, B being a uniform magnetic field along the z-direction.

4. The normal component of the current on any face of the box vanishes by boundary conditions. Is the pressure exterted on the box finite ? If yes, what is its value ?

5. Suppose one adds a δ-function wall perpendicular to the x-direction, namely the following perturbation to the Hamiltonian

$$\delta\hat{H} = U\,\delta(x-a),$$

where $a \in [0, L]$ is the position of the wall along the x-direction. Derive the eigenvalue equation which solves the Schrœdinger equation still keeping the above boundary conditions. Discuss whether it is energetically favorable or not to put the wall in the middle of the box, i.e. $a = L/2$.

Problem 5: Two electrons on a sphere

Consider two electrons (mass m, charge $-e$) constrained onto the surface of a sphere of radius R (no kinetic energy is associated to the, forbidden, radial motion).

1. Assume first $e = 0$: discuss the energy spectrum of the Hamiltonian giving the eigenvalues, eigenvectors, quantum numbers, and degeneracy of the ground and first few excited states.

2. Suppose now that e is small, but finite. Discuss qualitatively the spectrum of the Hamiltonian and indicate how the degeneracy of the states found in (1) is partially lifted by the interaction.

3. Discuss qualitatively the condition to be fulfilled in order for low-order perturbation theory to give an accurate estimate of the ground-state energy.

4. Using the identity:

$$\frac{1}{|\mathbf{r_1} - \mathbf{r_2}|} = 4\pi \sum_{l=0}^{\infty} \frac{1}{2l+1} \sum_{m=-l}^{l} Y^*_{lm}(\hat{r}_1) Y_{lm}(\hat{r}_2) \frac{R^l_<}{R^{l+1}_>}, \tag{1}$$

   where $\hat{\mathbf{r}}$ indicates the unit vector along $\mathbf{r}$ and $R_<$ ($R_>$) is the minimum (maximum) between $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$, calculate the first-order correction to the ground state.

5. Optional: Carry on as much as you can the calculation of the second-order correction.