SISSA ISAS

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Fall 2004 – 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 two dimensions.

Consider electrons in a hypothetical crystal consisting of a 2-dimensional square lattice, with lattice parameter a.

1. Assuming at first free electron motion (i.e., negligible effect of the lattice) compare the electron energy $E(\mathbf{k})$ at three points the the 2D Brillouin Zone (BZ), namely (i) $E(0)$ at the center; (ii) $E(\mathbf{k}_1)$ at the midpoint of the BZ side face; (iii) $E(\mathbf{k}_2)$ at the BZ corner. Calculate the ratio of kinetic energies $r = [E(\mathbf{k}_2) - E(0)]/[E(\mathbf{k}_1) - E(0)]$.

   Assume now the opposite limit of tightly bound electrons, with an s-orbital per site, zero overlap between sites, and first-neighbor hopping energy $-|t|$.

2. Write down the electron band energy $E(\mathbf{k})$ in this case. Re-calculate $E(0)$, $E(\mathbf{k}_1)$, $E(\mathbf{k}_2)$, and compare the new ration r with the free electron case (1).

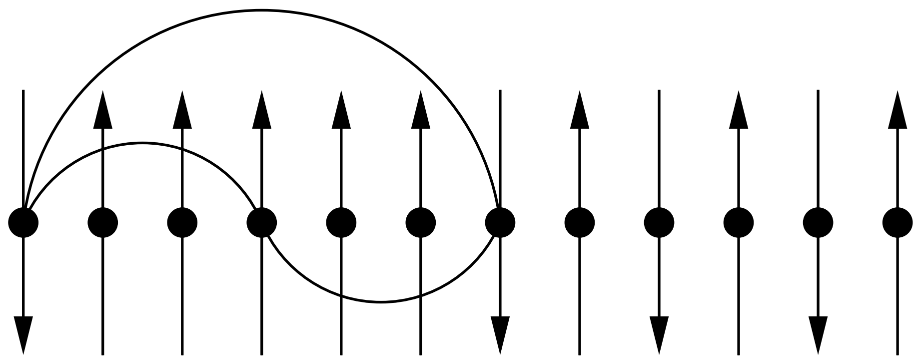
3. Assuming now a concentration $n = 1$ of electrons occupying the lattice sites, consider the 2D Fermi surface $E(\mathbf{k}) = E_F$ corresponding to free electrons (1), and to tightly bound electrons (2). Sketch qualitatively their respective shapes, and discuss their comparison.

Problem 2. One electron in an antiferromagnetic background.

Consider one particle propagating on the sites of a one-dimensional lattice $j = 1, \cdots L$ (with L even) in the presence of a background of classical spins $\sigma_j = \pm 1$. The particle can propagate only when the spins of the background are all parallel in a given region of the lattice, and the wave function of the particle $\psi(j)$ satisfies the Schrödinger equation:

$$-t[\psi(j+1) + \psi(j-1)] = E_t \psi(j),$$

the wave function vanishing when σ_j changes sign (see figure).



The magnetic energy of the background spins is given by:

$$E_J = J \sum_{j=1}^{L} [\sigma_j \sigma_{j+1} - 1],$$

and periodic boundary conditions $\sigma_{L+1} = \sigma_1$ are assumed.

The total energy is the sum of the two contributions $E_{tot} = E_t + E_J$.

1. Consider ferromagnetic interactions between spins, i.e., $J < 0$, and $|J| >> t$: what is the ground state of this systems and the first excited states?

   Optional: Discuss qualitatively what happens if $|J| << t$.

2. Take now the more interesting case of antiferromagnetic interactions, i.e., $J > 0$. Compute the minumum of the magnetic energy contribution E_J, by assuming that the particle propagates in one region with l (odd) parallel and consecutive spins, i.e., $j = 2, 3, \cdots l + 1 < L$.

3. Compute the energy levels of the particle in this region and in particular write down the ground state.

4. Finally, find the total ground state energy (minimum of E_{tot} as a function of l) and the degeneracy of the ground state. Discuss what happens to the spread l of the one particle wave function in the limit $J/t \to 0$. In this limit provide an analityc expression of the total energy as a function of J/t. (Hint: suppose l very large and verify this assumpion)

5. Optional: Discuss what happens if l is even.

Problem 3. Electric susceptibility of a harmonic oscillator.

A particle of mass m and charge q moves in a harmonic potential which depends only on the x coordinate: $V(x) = (k/2)x^2$. The particle is in an electric field E parallel to the x axis. Consider only the motion along x.

The Hamiltonian of the system is:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 - qEx, \tag{1}$$

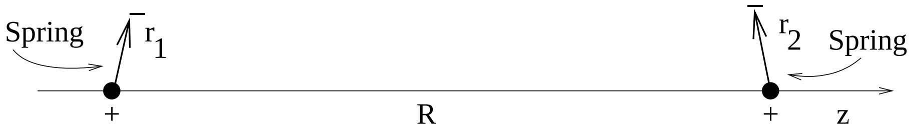
where $p = m\dot{x}$ is the momentum of the particle.

1. Write the classical equations of motion and solve them with the initial conditions that at $t = 0$ the particle is in x_0 with zero velocity.
2. Show that the classical motion is a harmonic oscillation with center in x_1. Find x_1 as a function of q, $\omega = \sqrt{\frac{k}{m}}$ and E.
3. Assume that at the origin there is an equal and opposite fixed charge so that the dipole moment induced by the electric field is $P = qx_1$. Show that P is proportional to E and find the electric susceptibility $\chi = P/E$.
4. Solve the same problem in Eq. (1) using quantum mechanics. Show that the problem can be solved exactly, and find the ground state energy of the particle and the ground state wave-function, in terms of the ground state $\phi_0(x)$ of the harmonic oscillator which you are not required to write down explicitly.
5. Calculate the average value of the position operator $\langle X \rangle$ on the ground state and find the quantum mechanical expression of the electric susceptibility. Compare with the classical expression and comment on the fact that χ does not depend on the Planck constant h.
6. Let's assume now that the electric field causes only a small perturbation on the harmonic oscillator. Using stationary perturbation theory, find the perturbed ground state wavefunction to first order and use it to calculate the average value of the position operator on this state. Calculate the electric susceptibility of the system in this approximate way, compare with the exact value and comment the result.

Hints: The X operator can be written in terms of creation and destruction operators as $X = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$ where, for the wavefunctions of the harmonic oscillator $|\phi_n\rangle$, we have $\langle \phi_{n'}|a|\phi_n\rangle = \sqrt{n}\delta_{n',n-1}$ $\langle \phi_{n'}|a^\dagger|\phi_n\rangle = \sqrt{n+1}\delta_{n',n+1}$.

Problem 4. Interaction between two distant neutral atoms.

Consider two far-apart "charged oscillators" as depicted in the Figure below.
The Hamiltonian describing the system is taken to be:



$$H = \left[\left(\frac{\mathbf{p}_1^2}{2m} + \frac{1}{2} m\omega^2 \mathbf{r}_1^2 \right) + \left(\frac{\mathbf{p}_2^2}{2m} + \frac{1}{2} m\omega^2 \mathbf{r}_2^2 \right) \right] + \left[\frac{e^2}{R^3} \left(x_1 x_2 + y_1 y_2 - 2 z_1 z_2 \right) \right] = H_0 + V \qquad (2)$$

where R is the distance between the two positive charges, which we imagine to be fixed at their position, and aligned along the z-direction. This is a rough model for two far-apart neutral atoms, with fixed (positive) nuclei, the basic approximation being that the Coulomb attraction between the electron and the corresponding nucleus has been replaced by a spring of frequency ω, to simplify the calculation. The interaction potential $V = (e^2/R^3)(x_1 x_2 + y_1 y_2 - 2z_1 z_2)$ is, instead, the correct expression for the dipole-dipole interaction of the two neutral objects. We are interested in the quantum mechanics of this system, neglecting the spin of the two particles.

1. By neglecting V at first, classify the first three low-lying states of the two independent three-dimensional harmonic oscillators (i.e., ground state, first and second excited states), including the degeneracy of each level, its energy E_α^0, and the associated unperturbed wave-functions (in terms of the single oscillator wavefunctions $\phi_n(x)$, which you do not need to write down explicitly).

2. Consider now the changes in the *ground state energy* induced by the presence of the dipole-dipole term V. Calculate the shift of the ground state energy from the unperturbed value, $\Delta E_{gs} = E_{gs} - E_{gs}^0$ to *first order* in V.

3. Perform now the calculation of the shift ΔE_{gs} *up to second order* in V, and plot how the resulting ground state energy $E_{gs}(R)$ depends on R for large separations R.

   Hint: Use the fact that, for a single one-dimensional harmonic oscillator, the only relevant non-vanishing matrix element of the operator x, if ϕ_n denotes the nth eigenstate and ϕ_0 the ground state, is:

   $$\langle \phi_n | x | \phi_0 \rangle = \sqrt{\hbar/(2m\omega)}\,\delta_{n,1} \ .$$