

PHYSICS 232

Homework 2

Due in class, Wednesday February 8

1. In this problem you will evaluate the diamagnetic susceptibility of the free electron gas. The case of a three-dimensional gas is described in several of the books, *e.g.* Peierls, "Quantum Theory of Solids". Here we will do the case of two-dimensions, which is a shade simpler, and is also of current interest because of recent work on the quantum Hall effect. Neglect the interaction of the magnetic field with the spin.

- (a) Show that, in the absence of a magnetic field, the density of states, $\rho(\epsilon)$, of a two-dimensional electron gas is a constant and evaluate it. Assume a rectangular sample of area $S = L_x \times L_y$.
- (b) Write down the Hamiltonian including a magnetic field, B , perpendicular to the plane containing the electrons. It is convenient (but not essential) to use the gauge

$$A_x = 0 ; \quad A_y = Bx .$$

- (c) Show that, in the gauge of part (b), an energy eigenfunction can be written as the product of a plane wave in the y -direction and a simple harmonic oscillator wave function which describes the x dependence.

- (d) Hence show that the energy levels are

$$E = (n + \frac{1}{2})\hbar\omega_c,$$

where $n = 0, 1, 2, \dots$, and ω_c , called the cyclotron frequency, is given by $\omega_c = eB/mc$. (*n.b.* The level splitting, $\hbar\omega_c$, is just $2\mu_B B$, where $\mu_B \equiv e\hbar/2mc$ is the Bohr magneton.)

- (e) Show that a *classical* particle in a magnetic field moves in *closed* orbits at a frequency ω_c .
- (f) Determine the degeneracy of the levels in part (d) and hence show that the total number of states in a range of energy $\hbar\omega_c$ is the same both with and without the field.
- (g) Show that the thermodynamic potential $\Omega \equiv F - \mu N$, where F is the free energy and μ the chemical potential, can be written as

$$\Omega = - \int_{-\infty}^{\infty} Q(\epsilon) f(\epsilon) d\epsilon,$$

where $Q(\epsilon) \equiv \int_{-\infty}^{\epsilon} d\epsilon' \rho(\epsilon')$ is the cumulative density of states, and $f(\epsilon)$ is the Fermi function.

- (h) Consider fields which are not too large and which therefore satisfy the condition $\hbar\omega_c \ll k_B T$ ($\ll \epsilon_F$). (Remember that $\hbar\omega_c = 2\mu_B B$.) Evaluate the difference in F (which is the same as the energy U in this limit) between the case of finite B and the case of $B = 0$, to lowest order in B .

Note: because of the result of part (f) this difference involves the *derivative* of $f(\epsilon)$ and hence only involves states close to the Fermi surface. Note also that one can neglect the change in μ to this order. Note finally that in the opposite limit, $\mu_B B \gg k_B T$, the diamagnetic susceptibility oscillates as a function of B as the Landau levels go through the Fermi surface. This is called the de-Haas Van Alphen effect, see *e.g.* Peierls and Ashcroft and Mermin, and is useful in determining the form of the Fermi surface (which is not a sphere in real metals because of the periodic potential due to the ions).

- (j) From the difference in (free) energy obtained in (h) write down the diamagnetic susceptibility. By what factor does it differ from the paramagnetic spin susceptibility?

2. Show that if $k_B T \ll \epsilon_F$, the temperature-dependent correction to the Pauli paramagnetic spin susceptibility is given by

$$\chi(T) = \chi(0) \left(1 - \frac{\pi^2}{6} (k_B T)^2 \left[\left(\frac{\rho'}{\rho} \right)^2 - \frac{\rho''}{\rho} \right] \right),$$

where ρ , ρ' and ρ'' are the density of states at the Fermi energy and its derivatives. Show that for free electrons this reduces to

$$\chi(T) = \chi(0) \left(1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right).$$

3. Show that the ground state energy of the four spin antiferromagnetic nearest-neighbor Heisenberg chain (with periodic boundary conditions)

$$\mathcal{H} = J (\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_4 \cdot \mathbf{S}_1),$$

is

$$E = -4JS^2 \left[1 + \frac{1}{2S} \right].$$

Hint: Write the Hamiltonian in the form

$$\mathcal{H} = \frac{1}{2}J \left[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2 - (\mathbf{S}_1 + \mathbf{S}_3)^2 - (\mathbf{S}_2 + \mathbf{S}_4)^2 \right].$$

4. (a) Starting from the statistical mechanics expression for $\langle m \rangle$, where m is the magnetization, show that the paramagnetic susceptibility, $\chi = \partial \langle m \rangle / \partial h$, of an atom with Hamiltonian \mathcal{H}_{atom} is given, in the limit of zero field h , by

$$\chi = \int_0^\beta \langle e^{\tau \mathcal{H}_{atom}} J_z e^{-\tau \mathcal{H}_{atom}} J_z \rangle d\tau,$$

where the average is taken over \mathcal{H}_{atom} . Forget about units and take the magnetic moment to be simply J_z . You must note that, in general, J_z does not commute with \mathcal{H}_{atom} .

- (b) Show that in the classical limit (where J_z *does* commute with \mathcal{H}_{atom}), then the susceptibility is given by

$$\chi = \frac{1}{k_B T} \langle J_z J_z \rangle,$$

i.e. the susceptibility is proportional to the mean square fluctuation in the magnetic moment.

- (c) Derive this last result *directly* from classical statistical mechanics.

5. Consider a $J = 2$ ion in a uniaxial crystal field. Give symmetry arguments showing that, to lowest order in the angular momentum operators, the crystal field Hamiltonian can be written

$$\mathcal{H}_{CF} = A (3J_z^2 - J(J+1)),$$

for some constant A . Sketch the level splittings if A is positive and compute the paramagnetic susceptibility of the atom for this case, (a) with the field in the x -direction, and (b) with the field in the z -direction. Without doing any further calculation, what is the susceptibility if the field is in the y -direction? Explain your answer.

6. Prove that the self-energy of a complex charge density, $\rho(\mathbf{r})$, defined by

$$\int d^3r \int d^3r' \frac{\rho^*(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$

is always positive.

7. *This question is important. Please make sure that you make a serious effort at it.*

Consider the one-band Hubbard model with two sites. There is a single orbital on each site and they are assumed to be orthogonal to each other. The Hamiltonian is given (in second quantized notation) by

$$\mathcal{H} = -t \sum_{\sigma} (c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}) + U(n_{1\uparrow}n_{1\downarrow} + n_{2\uparrow}n_{2\downarrow}).$$

The first term describes the kinetic energy of the electrons in the tight binding approximation, $\sigma = \uparrow$ or \downarrow is the spin and t is the hopping matrix element which takes an electron from site 1 to site 2 or vice-versa. The second term involving U is the Coulomb repulsion which results if two electrons (inevitably with opposite spin) are on the same site. ($n_{1\uparrow}$ is the occupation of up-spin electrons on site 1 etc.)

- (a) Find the energy eigenvalues and eigenstates for the case of two electrons.

Hint: Work out what the basis states are and diagonalize separately the states with parallel and with antiparallel spins. The parallel spin case is trivial, the antiparallel case needs a bit of work.

- (b) Show that when $U \gg t$ the lowest levels can be described by a spin Hamiltonian with *antiferromagnetic* coupling

$$H = J \mathbf{S}_1 \cdot \mathbf{S}_2,$$

where $J = 4t^2/U$.

Note: This antiferromagnetic coupling is observed in high temperature superconductors and *may* be responsible for superconducting pairing. Anderson argues that this interaction, which he calls *Kinetic Exchange*, generally dominates other possible mechanisms for exchange interactions in insulators, and is therefore responsible for the majority of magnetic insulators being antiferromagnetic rather than ferromagnetic.