

## 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  $\omega_c$ , 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  $\omega_c$ .

(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  $\mu$  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  $\mu$  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  $\rho$ ,  $\rho'$  and  $\rho''$  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

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

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.