ICFP M2 2021/2022

Condensed Matter Theory

Homework

by Benjamin Lenz (benjamin.lenz@sorbonne-universite.fr)
and Indranil Paul (indranil.paul@univ-paris-diderot.fr)

Please note:

This homework is due in the first exercise group (TD) after the break, i.e. on 25 November 2021. Please hand in your solutions of parts A , B and C of this homework on separate sheets of paper in order to facilitate grading: Mark the sheets by the letter corresponding to that part (A, B, or C) in a well-visible manner, and do not forget to write your name on all sheets.

A. Stoner theory of ferromagnetism in metals

Consider the Hubbard model on a lattice $\mathcal{H} = \sum_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}} - \mu)c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$, with interaction $U > 0$. Here $\mathbf{k}$ denotes wavevector, i denotes a lattice site, $\epsilon_{\mathbf{k}}$ is the electron dispersion, μ is the chemical potential, and $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the density operator at site i for spin $\sigma = (\uparrow, \downarrow)$.

(a) Argue that $n^2_{i\sigma} = n_{i\sigma}$ for electrons. Use this property to show that the interaction can be expressed as $-(U/2)\sum_i(n_{i\uparrow} - n_{i\downarrow})^2$ plus a constant. This constant can be ignored in the rest of the calculation.

(b) We will treat the interaction using mean field approximation

$$(n_{i\uparrow} - n_{i\downarrow})^2 \approx (n_{i\uparrow} - n_{i\downarrow})\langle(n_{i\uparrow} - n_{i\downarrow})\rangle + \langle(n_{i\uparrow} - n_{i\downarrow})\rangle(n_{i\uparrow} - n_{i\downarrow}) - \langle(n_{i\uparrow} - n_{i\downarrow})\rangle^2.$$

Consider the mean field ansatz $\langle n_{i\uparrow} - n_{i\downarrow}\rangle = (m/\mu_B) \equiv \tilde{m}$, where μ_B is the Bohr magneton, and $\tilde{m}$ is the dimensionless magnetization taken to be uniform over all the sites. Following these steps, show that the free energy per unit volume can be written as

$$F(T, \tilde{m}) = U/(2v)\tilde{m}^2 - (k_BT/\Omega_0)\sum_{\mathbf{k}\sigma}\log[1 + e^{-\xi_{\mathbf{k}\sigma}/(k_BT)}],$$

where v is the volume of a unit cell, k_B is Boltzmann constant, T is temperature, $\xi_{\mathbf{k}\uparrow} = \epsilon_{\mathbf{k}} - \mu - U\tilde{m}$, and $\xi_{\mathbf{k}\downarrow} = \epsilon_{\mathbf{k}} - \mu + U\tilde{m}$, and Ω_0 is volume of the system. Hint: Remember the free energy per unit volume is defined as $F = -k_BT\log(\mathcal{Z})/\Omega_0$, where $\mathcal{Z} \equiv \mathrm{Tr}\left[e^{-\mathcal{H}/(k_BT)}\right]$ is the partition function. Set the unit cell volume $v = 1$ for the rest of the calculations.

(c) Expand the free energy as $F(T, \tilde{m}) = F(T,0) + (a/2)\tilde{m}^2 + (b/4)\tilde{m}^4 + \cdots$. It will be useful to replace $(2/\Omega_0)\sum_{\mathbf{k}} \to \int d\epsilon\rho(\epsilon)$, where $\rho(\epsilon)$ is the density of states. Also useful will be the formula for Sommerfeld expansion. Express a and b in terms of U, k_BT, density of states at Fermi energy $\rho(\epsilon_F)$, and its first two derivatives with respect to energy $\rho'(\epsilon_F)$ and $\rho''(\epsilon_F)$. In the Sommerfeld expansion ignore terms involving the third and higher derivatives.

(d) Assume $b > 0$ in the rest of the calculations. Until now $\tilde{m}$ is an unknown mean field parameter. The value of it is fixed by minimizing the free energy with respect to $\tilde{m}$. Find $\tilde{m}$ for the case $a > 0$, and for the case $a < 0$. Interpret these two cases in terms of two phases of the system.

(e) Consider the case $a > 0$, and introduce a small external magnetic field h. The free energy is now given by $F(T, \tilde{m}, h) = F(T, \tilde{m}) - \mu_B \tilde{m} h$. Minimize the free energy and find $\tilde{m}$ to lowest order in h. Then calculate the spin susceptibility $\chi_s \equiv (\partial m/\partial h)_{h\to 0}$. How does the spin susceptibility behave as $a \to 0$?

(f) If the so-called *Stoner criterion* $a < 0$ is not satisfied, then spontaneous ferromagnetism will not occur. But even then, the magnetic susceptibility may be altered. We introduce the *Stoner enhancement factor* S at zero temperature via $\chi = S \cdot \chi_P$, where χ_P denotes the Pauli paramagnetic susceptibility (see exercise sheet 4).
Relate S to the parameter a and explain with the densities of states (DOS) shown in Fig. 1 why Pd and Pt are said to be on the verge of ferromagnetism.

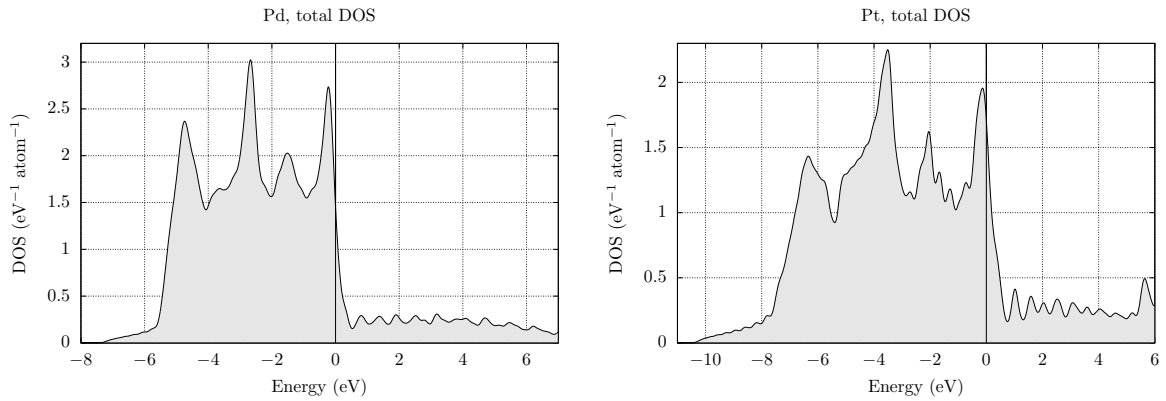

Figure 1: Density of states of Pd (left) and Pt (right), calculated by density functional theory. The Fermi energy is set at $E = 0$.

(g) Use the DOS of Pd and Pt to calculate the Pauli paramagnetic susceptibility χ_P. Compare your calculation to the measured magnetic susceptibilities of Fig. 2 to estimate the Stoner enhancement factor S.
Hint: *cgs* units are often a mess - you can use that the molar susceptibility is given in *cgs* units by $\chi_{P,\rho}^{cgs} = \mu_B^2 \cdot N_A \cdot \rho(\epsilon_F)$, where $\mu_B^2 \cdot N_A = 3.23 \cdot 10^{-5} \frac{\text{emu} \cdot \text{eV}}{\text{mol}}$.

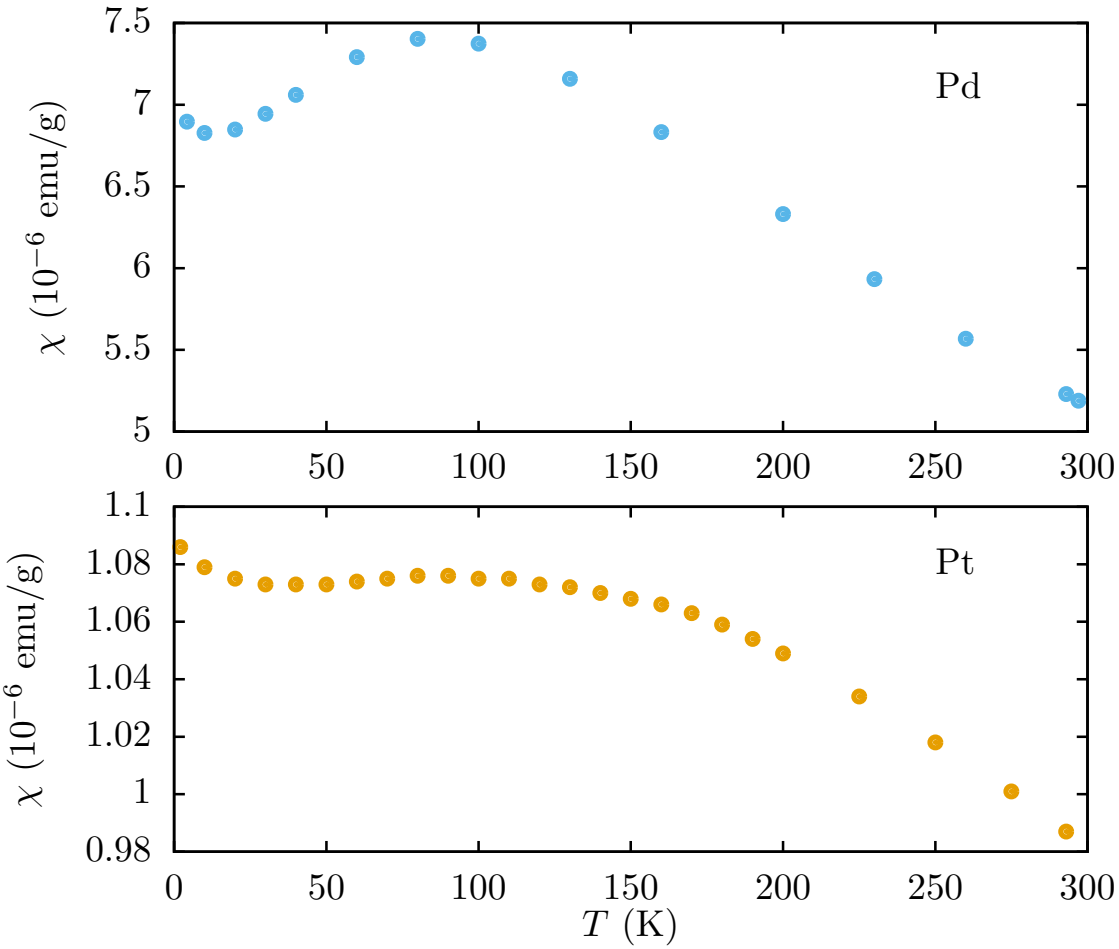

Figure 2: Magnetic susceptibility of Pd and Pt measured as a function of temperature. Data taken from *Jamieson & Manchester*, J. Phys. F: Met. Phys. **2**, 323 (1972) and from *van Dam, Gubbens & van den Berg*, Physica **70**, 520 (1973).

Remember:

Please hand in your solutions of parts A , B and C of this homework on separate sheets of paper in order to facilitate grading: Mark the sheets by the letter corresponding to that part (A, B, or C) in a well-visible manner, and do not forget to write your name on all sheets.

B. Stoner theory revisited

In this exercise, we will revisit the mean-field approximation of the Hubbard model, the so-called *Stoner model*, and investigate it in a slightly different way by means of Green's functions. Before resorting to approximations, we start this time with the equation of motion of the single-particle Green's function of the Hubbard model on a lattice, $\mathcal{H} = \sum_{ij\sigma}(t_{ij} - \mu\delta_{ij})c^\dagger_{i\sigma}c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$.

(h) We set $\hbar = 1$ and recall the equation of motion (e.o.m.) of the single-particle Green's function (see also exercise (i) of exercise sheet 5)

$$EG^R_{A,B}(E) = \langle [A,B]_\zeta \rangle + G^R_{[A,\mathcal{H}],B}(E)$$

Use the higher-order Green's function

$$\Gamma^R_{ilm;j\sigma}(E) = G^R_{c^\dagger_{i,-\sigma}c_{l,-\sigma}c_{m,\sigma}\ ,\ c^\dagger_{j,\sigma}}(E)$$

to derive an expression for the e.o.m. of the Hubbard model. Here, $-\sigma$ denotes the opposite spin direction of σ.

(i) Use the mean-field decoupling (in this case also known as *Hartree-Fock approximation*) of exercise (b), namely

$$AB \xrightarrow{MF} A\langle B\rangle + \langle A\rangle B - \underbrace{\langle A\rangle\langle B\rangle}_{\text{const.}},$$

but this time for the operators $A \equiv c_{i\sigma}$, $B \equiv n_{i,-\sigma}$ to derive a simpler (Hartree-Fock) expression for the higher-order Green's function $\Gamma^R_{iii;j\sigma}(E)$.

(j) Insert the Hartree-Fock expression of $\Gamma^R_{iii;j\sigma}(E)$ into the e.o.m. of the Green's function and solve for $G_{\mathbf{k}\sigma}(E)$ by Fourier transformation into k-space. Compare the poles of the Green's function with the quasiparticle energies of exercise (b).

(k) In order to solve the Green's function, we still need to determine the expectation value $\langle n_{-\sigma}\rangle$. Here, we will make use of the spectral theorem (see also ex. 6 of exercise sheet 5): Use the Cauchy principal value relation, $\lim_{\eta\to 0^+}\frac{1}{x-x_0+i\eta} = \mathcal{P}\frac{1}{x-x_0} - i\pi\delta(x-x_0)$, to calculate the spin-dependent spectral function $A_{\mathbf{k}\sigma}(E)$ of the system. Then, make use of the sum rule $\langle n_\sigma\rangle = \frac{1}{N}\sum_k \int_{-\infty}^{\infty} d\omega\ n_F(\omega)A_{\mathbf{k}\sigma}(\omega-\mu)$ to derive an expression for the expectation value $\langle n_{-\sigma}\rangle$. N denotes here the number of discrete $\mathbf{k}$ values and $n_F(\omega)$ is the Fermi function.

(l) With the expression for average particle numbers $\langle n_{-\sigma}\rangle$, the magnetization m can be recast in the form $m = \frac{1}{2N}\sinh(\beta U m)\sum_k \left(\cosh(\beta U m) + \cosh(\beta(\epsilon_k - \mu + \frac{Un}{2}))\right)^{-1}$.
Use the density of states of the non-interacting system, $\rho_0(E) = \frac{1}{N}\sum_{\mathbf{k}}\delta(E-\epsilon_{\mathbf{k}})$, to transform the k-summation into an integral over energy.

(m) Calculate the magnetization for $T \to \infty$. Remember that the hyperbolic functions can be developed for small argument x ($\sinh(x) = x + \frac{x^3}{6} + \dots$ and $\cosh(x) = 1 + \frac{x^2}{2} + \dots$).

(n) *Excitation spectrum.* Under specific conditions, the magnetization can be non-zero. In this case, the energies of electrons with up- and down-spin differ by an exchange splitting $\Delta E_{ex} = 2Um$, which is $\mathbf{k}$-independent. Interpret the quasiparticle energies $\xi_{\mathbf{k}\sigma}$ of the single-electron Green's function as the energy cost to add an electron with ($\mathbf{k}$,σ) to the N-particle system. Sketch the excitation energy of the system $\Delta E_{\sigma\sigma'}(\mathbf{k},\mathbf{q}) \equiv E_{\sigma'}(\mathbf{k}+\mathbf{q}) - E_{\sigma}(\mathbf{k})$ assuming quasi-free electrons, i.e. $\epsilon_{\mathbf{k}} = k^2/(2m^*)$, for (1) excitations without spin-flip, $\Delta E_{\sigma\sigma}$ and (2) excitations with spin-flip, $\Delta E_{\uparrow\downarrow}$. In the latter case, how do the excitation spectra differ for $2Um > \epsilon_F$ from $2Um < \epsilon_F$?

Remember:

Please hand in your solutions of parts A , B and C of this homework on separate sheets of paper in order to facilitate grading: Mark the sheets by the letter corresponding to that part (A, B, or C) in a well-visible manner, and do not forget to write your name on all sheets.

C. Van-Hove singularities

In Fig. 1 we observed spikes in the density of states. Crystalline solids often have singularities in the density of states, so-called van-Hove singularities[1]. They occur at energies E_c, for which the energy dispersion $E_i(\mathbf{k})$ of certain bands i has a horizontal tangent, i.e. $\nabla_{\mathbf{k}} E_i(\mathbf{k}) = 0$. Formally we can see this when rewriting the density of states as a surface integral over the surface of constant energy, $S(E)$:

$$\rho(E) = \frac{V}{N} \sum_i \frac{1}{(2\pi)^d} \int_{S(E)} \frac{\mathrm{d}s}{|\nabla_{\mathbf{k}} E_i(\mathbf{k})|}$$

Here $\mathrm{d}s$ denotes a surface element on the constant-energy surface $S(E)$, d is the dimension and i runs over all bands of the dispersion. Around an energy E_c with $\nabla_{\mathbf{k}} E_i(\mathbf{k}) = 0$ we can perform a principal axis transformation[2] to rewrite the dispersion as

$$E \approx E_c + \sum_{i=1}^{d} \epsilon_i \kappa_i^2$$

Here, κ_i is the wave vector component and ϵ_i the diagonal element of the Hessian matrix along the principal axis i.

(o) Analyze the type of singularity in $d = 3$ dimensions by assuming that the dispersion has (i) a minimum, (ii) a maximum, or (iii) a saddle point at $\mathbf{k}_c$: How does the density of states

$$\rho(E) = \frac{V}{N} \sum_i \int_{BZ} \frac{\mathrm{d}^d k}{(2\pi)^d} \delta(E - E_i(\mathbf{k}))$$

behave close to $\mathbf{k}_c$?

(p) Repeat the calculation for $d = 2$ dimensions and check your result for the nearest-neighbor tight-binding model on a 2D square lattice (see exercise sheet 1): Where are the minima, maxima and saddle points of the dispersion? Which type of singularity in the density of states do they correspond to?
Hints: (1) To perform the integral in case of a saddle point of the dispersion, use that

$$\int \frac{\mathrm{d}x}{\sqrt{a + x^2}} = \frac{1}{2} \left(\log\left(1 + \frac{x}{\sqrt{a + x^2}}\right) - \log\left(1 - \frac{x}{\sqrt{a + x^2}}\right) \right)$$

(2) To plot the density of states of the 2D square lattice you can use the following expression in terms of the complete elliptic integral of first kind[3]:

$$\rho_{\text{sq.lat.}}(E) = \begin{cases} \frac{1}{2\pi^2 |t|} K\left(\sqrt{1 - \frac{E^2}{16t^2}}\right), & \text{for } |E| < 4|t| \\ 0 & \text{else} \end{cases}$$

(q) Relate your findings of exercises (o) and (p) to the Stoner criterion. What are the consequences of having Van-Hove singularities of different type right at the Fermi energy?

[1] First discussed by L. Van Hove in the context of phonon dispersions: *Van Hove*, Phys. Rev. **89**, 1189 (1953).

[2] This amounts to a diagonalization of the symmetric $d \times d$ Hessian matrix of E at $\mathbf{k}_c$: $\frac{\partial^2}{\partial k_i \partial k_j} E(\mathbf{k})|_{\mathbf{k}_c}$.

[3] The complete elliptic integral of first kind is defined by $K(x) = \int_0^{\pi/2} \frac{\mathrm{d}\theta}{\sqrt{1 - x^2 \sin^2 \theta}}$ and is tabulated in most modern plotting tools, e.g. in gnuplot (function *EllipticK*) and python (scipy library → *scipy.special.ellipk*).