

Midterm

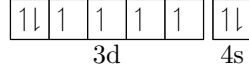
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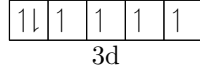
1 Problem 1

1.1

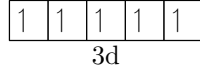
The electron configuration of Fe is $[\text{Ar}]3d^64s^2$, and according to Hund's rule, the spins are



The electron configuration of Fe^{2+} is $[\text{Ar}]3d^6$, and according to Hund's rule, the spins are



Fe^{3+} is obtained by reducing one electron and the spins are



For an iron atom, we only need to work on the 3d orbital because the 4s orbital is full. the total spin quantum number is $S = 2$, and the total orbital angular momentum quantum number is $L = 2$. Therefore

$$g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} = \frac{3}{2}. \quad (1)$$

Since the 3d shell is more than half filled, we have $J = L + S = 4$, and the total magnetic moment should be

$$\mu = \mu_B g_J J = 6\mu_B. \quad (2)$$

1.2

The experimentally observed atomic magnetic moment is $2.22\mu_B$, which doesn't agree with the aforementioned prediction. If somehow the orbital angular momentum is quenched, then $S = J = 2$, and $g_J = 2$. So the total angular momentum is 2, which is close to 2.22, but g_J should be multiplied to the former and the result $4\mu_B$ is no longer close to $2.22\mu_B$. The predicted $4\mu_B$ magnetic moment however agrees well with the $4.4\mu_B$ magnetic moment of Fe^{2+} [8], which should have the same magnetic moment with Fe atom because in both of them, only the 3d orbital is open.

1.3

α -Fe has a bcc structure; and the lattice constant is 2.86 \AA (this can be found with Material-Project). So there are 8 nearest atoms for each iron atom. The distance between two nearest neighbor iron atoms is

$$2.86 \text{ \AA} \cdot \frac{\sqrt{3}}{2} = 2.48 \text{ \AA}.$$

1.4

We work in Hartree atomic units. Since the exact many-body wave function of a iron atom is hard to obtain, as an estimation of magnitude, we place only one electron on each iron atom, the wave function of which is

$$\varphi(\mathbf{r}) = Ar^2 e^{-r/2}. \quad (3)$$

The wave function is normalized as

$$A^2 \cdot 4\pi \cdot \int_0^\infty r^2 dr r^4 e^{-r} = 1 \Rightarrow A = \frac{1}{24\sqrt{5\pi}}. \quad (4)$$

Suppose a is the distance between two iron atoms. We have

$$\begin{aligned} J &= \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \varphi_2^*(\mathbf{r}_1) \varphi_1(\mathbf{r}_1) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \varphi_1^*(\mathbf{r}_2) \varphi_2(\mathbf{r}_2) \\ &= \int d^3\mathbf{r}_1 \int d^3\mathbf{r}_2 \varphi(\mathbf{r}_1 - a\hat{\mathbf{x}}/2) \varphi(\mathbf{r}_1 + a\hat{\mathbf{x}}/2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \varphi(\mathbf{r}_2 + a\hat{\mathbf{x}}/2) \varphi(\mathbf{r}_2 - a\hat{\mathbf{x}}/2), \end{aligned} \quad (5)$$

where

$$\varphi_2(\mathbf{r}) = \varphi(\mathbf{r} - a\hat{\mathbf{x}}/2), \quad \varphi_1(\mathbf{r}) = \varphi(\mathbf{r} + a\hat{\mathbf{x}}/2) \quad (6)$$

are single-electron wave functions localized around two nearest iron atoms. In Hartree atomic units, 2.48 \AA is 4.69 au .

`overlap-integral.jl` is a naive code to calculate this integral; the convergence is poor though; if we increase the density of the real space mesh, J decreases; when the mesh is a $30 \times 30 \times 30$ one we have $J = 0.027 \text{ Hartree}$; but that's of course not reliable ...

1.5

We suppose that the magnetic moment at one iron atom is $2.22\mu_B$, no matter what this non-integer value means. The effective j , if we assume $g_J = 2$ (see above), is 1.11 . We use $J = 7.5 \text{ meV}$ for the Heisenberg interaction between the magnetic moments between two nearest atoms. Then we have

$$T_c = \frac{2zJ}{3k_B} j(j+1) = \frac{2zJ}{3k_B} j(j+1) = 1087 \text{ K}. \quad (7)$$

This has the same order of magnitude of the observed temperature 1043 K .

1.6

If the iron atoms are arranged into a 1D chain and the lattice constant is the same as the iron-iron distance in $\alpha\text{-Fe}$, the Heisenberg interaction strength J won't change. So we can put J directly into the 1D magnon dispersion relation

$$\hbar\omega_k = 4JS(1 - \cos ka). \quad (8)$$

Here S should be replaced by $j = 1.11$. The speed is

$$\frac{d\omega_k}{dk} = \frac{4JSa}{\hbar} \sin ka. \quad (9)$$

When $k = 10\% \cdot 2\pi/a$, we have

$$v = \frac{4JSa}{\hbar} \sin \frac{\pi}{5} = 6.6 \times 10^3 \text{ m/s}. \quad (10)$$

2 Problem 2

2.1

A material is **metamagnetic** if when the external magnetic field passes a finite value H_c , the magnetic configuration changes all of a sudden. This is a phenomenological term and may

be driven by various physical mechanisms. The material $\text{Sr}_3\text{Ru}_2\text{O}_7$ is metamagnetic, because experiments have observed that around $\mu_0 H = 7.9 \text{ T}$, a sharp peak can be seen in magnetic susceptibility [3], and therefore there is indeed a sudden change in the magnetization.

The low-field phase is paramagnetic, and the high-field phase is itinerantly ferromagnetic: the material shows “a rapid change from a paramagnetic state at low fields to a more highly polarized state” [7]. (On the other hand, some other metamagnetic materials undergo an antiferromagnetism-to-ferromagnetism transition; this is not the case for $\text{Sr}_3\text{Ru}_2\text{O}_7$.)

The boundary between the two phases was once thought to be a quantum critical point: above the phase boundary between the low-field phase and the high-field phase, the resistance doesn’t have typical Fermi-liquid behaviors [7]; the phase boundary between the two phases is a first-order phase transition line with a terminating end point, and this critical point is pushed to $T = 0$ when the external magnetic field is pointed towards the c direction, creating a quantum critical point [2]. Further investigations however have found that there are actually *two* peaks in susceptibility near $\mu_0 H = 7.9 \text{ T}$, and this “quantum critical point” is surrounded by two first-order phase transitions [5, 3]. The exotic temperature-resistance curve likely comes from an SDW order on top of the ferromagnetic moment formed between the two aforementioned first-order phase transition, which also gives rise to anisotropic resistance (or in other words, electronic nematic) which isn’t induced by the crystal structure and can’t be seen away from $\mu_0 H = 7.9 \text{ T}$ [6, 1].

2.2

$\text{Sr}_3\text{Ru}_2\text{O}_7$ is an itinerant magnetic material and the metamagnetic transition is likely due to Fermi surface instability. This is explained in [4] with a toy model. The effect or the coupling between the electron magnetic moment and the external magnetic field is to modify the chemical potential differently for spin-up and spin-down electrons. Suppose the magnetic field is along $-\hat{z}$, and thus the energy of spin-down electrons is lifted and the energy of spin-up electrons is pushed downwards. So the Fermi surface of the latter expands, while the Fermi surface of the former shrinks. When the spin-up Fermi surface is large enough and exceeds a von Hove singularity, it becomes unstable and undergoes a symmetry breaking process and becomes connected to the boundaries of the first Brillouin zone on one direction (either x or y). So now the translational symmetry of the electronic transportation behavior is broken (see Fig. 2(b) in [4]), and we get an electronic nematic state, and since the shapes of the spin-up/down Fermi surfaces have radical differences, we are now in an itinerant ferromagnetic phase. This is just the metamagnetic transition.

When the external magnetic field is stronger, the spin-up Fermi surface keeps expanding, and finally it’s connected to all the four boundaries of the 1BZ, and now the previously lost translational symmetry is restored (see Fig. 2(c) in [4]). This explains why nematic electron fluid is only observed near the so-called quantum critical point $\mu_0 H = 7.9 \text{ T}$: when the magnetic field grows larger, the restored translational symmetry kills the nematic phase. Since now the shape of the two Fermi surfaces are still drastically different, we are still in an itinerant ferromagnetic phase.

3 Problem 3

3.1

The model Hamiltonian is

$$\begin{aligned}
H = & \sum_k \varepsilon_k^\sigma c_k^\dagger c_k + \sum_k \varepsilon_k^\nu f_k^\dagger f_k + \sum_q \hbar \omega_q b_q^\dagger b_q \\
& + \frac{1}{L} \sum_{k, k', q} V_q c_{k+q}^\dagger f_{k'-q}^\dagger f_{k'} c_k \\
& + \frac{1}{\sqrt{L}} \sum_{k, q} g_{kq} c_{k+q}^\dagger b_q f_k + \text{h.c.} \\
& - \mu N,
\end{aligned} \tag{11}$$

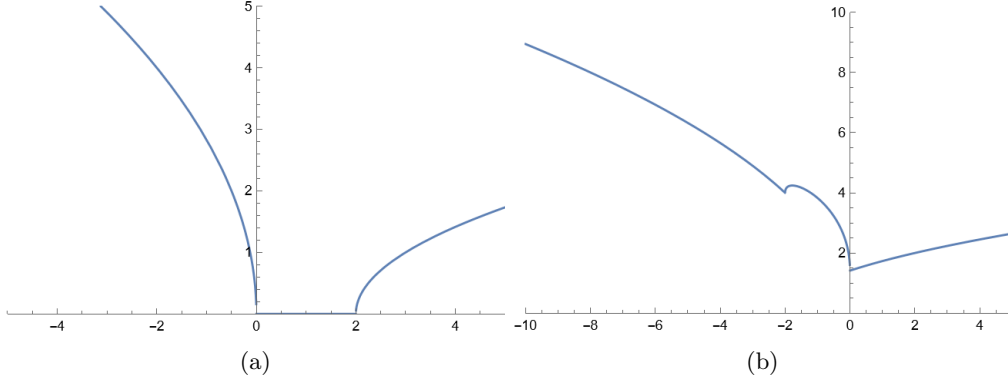


Figure 1: Density of state plots (a) Insulator (b) Metal

where L is the length of the sample and the last term is the chemical potential. Here the $1/2V$ factor before the Coulomb interaction term is replaced by $1/V$ because otherwise we have a $f^\dagger c^\dagger c f$ term; in the electron-phonon scattering term, we only have the $c^\dagger f b$ channel, because the conduction band is energetically higher than the valence band and therefore hopping from the latter to the former needs the additional energy from an existing phonon.

3.2

When the conduction and valence bands are upward and downward dispersing parabolas centered around Γ , the evolution of the DOS when we close the gap can be seen in Fig. 1. In the insulating phase, there is a period where the DOS is exactly zero; in the metal phase, there is a bump in the DOS curve corresponding to the overlap between the two bands.

In the insulating phase there is no conductivity, because there is no active carrier: the conduction band is completely empty; the valence band contains no hole. In the metallic phase we have

$$\sigma = \frac{n_e e^2 \tau_e}{m_e} + \frac{n_h e^2 \tau_h}{m_h}. \quad (12)$$

3.3

We consider a case in which phonons are “frozen” into a mean field, and the \mathbf{q} of that mean field is small compared with the momenta of electrons. We have

$$X_i = \frac{1}{\sqrt{N}} \sum_q e^{iqaj} X_q, \quad X_q = \sqrt{\frac{\hbar}{2M\omega_q}} (b_q + b_{-q}^\dagger). \quad (13)$$

Since q involved here is small, in the system we have a lattice displacement field of a macroscopic wave length, and the displacement field is almost constant in the eyes of electrons in a small region. So if we use X to refer to the displacement field in a small region, then we have

$$X = \frac{1}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_0}} (b + b^*), \quad (14)$$

where now b is the (complex) mean field representing the phonon mean field. Since X is an intensive property, it can be seen that $b \propto \sqrt{N}$.

The Hamiltonian is now (since the $U(1)$ symmetry is still kept, the chemical potential term has trivial behavior in diagonalization and can be left aside)

$$\begin{aligned} H &= \sum_k \varepsilon_k^c c_k^\dagger c_k + \sum_k \varepsilon_k^v f_k^\dagger f_k + \frac{g_0}{\sqrt{L}} \sum_k (b c_k^\dagger f_k + b^* f_k^\dagger c_k) \\ &= \sum_k \begin{pmatrix} c_k^\dagger & f_k^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_k^c & \frac{g_0}{\sqrt{L}} b \\ \frac{g_0}{\sqrt{L}} b^* & \varepsilon_k^v \end{pmatrix} \begin{pmatrix} c_k \\ f_k \end{pmatrix}. \end{aligned} \quad (15)$$

Diagonalization of this Hamiltonian gives

$$\varepsilon_k^{c',v'} = \frac{\varepsilon_k^c + \varepsilon_k^v \pm \sqrt{(\varepsilon_k^c - \varepsilon_k^v)^2 + \frac{4g_0^2}{L}|b|^2}}{2}. \quad (16)$$

It can be easily verified that the distance between the conduction band and the valence band is increased, because when the square root in the expression is positive, it's larger than $\varepsilon_k^c - \varepsilon_k^v$. Note that since $b \propto \sqrt{N} \propto \sqrt{L}$, the above equation contains only intensive quantities and has no real L dependence.

The ground state total energy is then

$$\begin{aligned} E' &= \sum_k \frac{\varepsilon_k^c + \varepsilon_k^v - \sqrt{(\varepsilon_k^c - \varepsilon_k^v)^2 + \frac{4g_0^2}{L}|b|^2}}{2} + \hbar\omega_0|b|^2 \\ &\approx \underbrace{\sum_k \varepsilon_k^v}_E - \sum_k \frac{g_0^2}{(\varepsilon_k^c - \varepsilon_k^v)L} |b|^2 + \hbar\omega_0|b|^2. \end{aligned} \quad (17)$$

The second line only considers the X^2 term. So whether creating a phonon coherent state in the ground state can save energy depends on the competition between the energy saving from dressing the electron with a phonon cloud and the energy cost to create some phonons.

The above results can also be found by many-body perturbation theory. In the language of Feynman diagrams, the irreducible self-energy diagram has exactly one $f^\dagger c$ vertex and one $c^\dagger f$ vertex, and we have

$$-i\Sigma_k^v(\omega) = \begin{array}{c} \overrightarrow{k,v} \quad \overrightarrow{k,c} \quad \overrightarrow{k,v} \\ \vdots \quad \vdots \quad \vdots \\ \times \quad \times \quad \times \end{array} = \frac{-ig_0b}{\sqrt{L}} \cdot \frac{i}{\omega - \varepsilon_k^c + \mu} \cdot \frac{-ig_0b^*}{\sqrt{L}}, \quad (18)$$

$$\Sigma_k^v(\omega) = \frac{g_0^2}{L} |b|^2 \frac{1}{\omega - \varepsilon_k^c}. \quad (19)$$

Note that this self-energy is *exact*. Now the dispersion relation is given by

$$\omega - \varepsilon_k^v + \mu - \frac{g_0^2|b|^2}{(\omega - \varepsilon_k^c + \mu)L} = 0. \quad (20)$$

It's equivalent to (16).

3.4

The first correction to the free energy caused by phonons is proportional to $b^2 \sim X^2$, and it's sign depends on the competition between the two terms in (17). This term is to be merged with the $(T - T_c)X^2$ term. So if (17) saves energy in the end, T_c is higher, and therefore electron-phonon coupling enhances the existing structural instability; if the opposite case is true – (17) is greater than the old band theory ground state E – then T_c goes down and it's more difficult for the structural instability to happen.

References

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