Midterm

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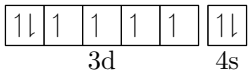
1 Problem 1

1.1

The electron configuration of Fe is $[\mathrm{Ar}]3\mathrm{d}^6 4\mathrm{s}^2$, and according to Hund's rule, the spins are



The electron configuration of Fe^{2+} is $[\mathrm{Ar}]3\mathrm{d}^6$, 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

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

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

$$\mu = \mu_{\mathrm{B}} g_J J = 6\mu_{\mathrm{B}}. \tag{2}$$

1.2

The experimentally observed atomic magnetic moment is $2.22\mu_{\mathrm{B}}$, 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 $4\mu_{\mathrm{B}}$ is no longer close to $2.22\mu_{\mathrm{B}}$. The predicted $4\mu_{\mathrm{B}}$ magnetic moment however agrees well with the $4.4\mu_{\mathrm{B}}$ 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 Å (this can be found with MaterialProject). So there are nearest atoms for each iron atom. The distance between two nearest neighbor iron atoms is

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

1.4

1.5

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 $Sr_3Ru_2O_7$ is metamagnetic, because experiments have observed that around $\mu_0 H = 7.9\,\mathrm{T}$, 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 $Sr_3Ru_2O_7$.)

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 phrase 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 $\mu_0 H = 7.9\,\mathrm{T}$, 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 $\mu_0 H = 7.9\,\mathrm{T}$ [6, 1].

2.2

$Sr_3Ru_2O_7$ 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 modifying the chemical potential for

This also explains why nematic electron fluid is only observed near the so-called quantum critical point $\mu_0 H = 7.9\,\mathrm{T}$: because when the external magnetic field is stronger, the

3 Problem 3

3.1

The model Hamiltonian is

$$\begin{aligned} H = &\sum_k \varepsilon_k^{\mathrm{c}} c_k^\dagger c_k + \sum_k \varepsilon_k^{\mathrm{v}} f_k^\dagger f_k + \sum_q \hbar\omega_q b_q^\dagger b_q \\ &+ \frac{1}{L}\sum_{k,k',q} V_q c_{k+q}^\dagger f_{k'-q}^\dagger f_{k'} c_k \\ &+ \frac{1}{\sqrt{L}}\sum_{k,q} g_{kq} c_{k+q}^\dagger b_q f_k + \mathrm{h.c.} \\ &- \mu N, \end{aligned} \tag{3}$$

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

3.3

We consider a case in which phonons are "frozen" into a mean field, and the $\boldsymbol{q}$ of that mean field is small compared wit the momenta of electrons. We have

$$X_i = \frac{1}{\sqrt{N}} \sum_q \mathrm{e}^{\mathrm{i}qaj} X_q, \quad X_q = \sqrt{\frac{\hbar}{2M\omega_q}} (b_q + b_{-q}^\dagger). \tag{4}$$

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

$$X = \frac{1}{\sqrt{N}} \sqrt{\frac{\hbar}{2M\omega_0}} (b + b^*), \tag{5}$$

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)

$$\begin{aligned} H &= \sum_k \varepsilon_k^{\mathrm{c}} c_k^\dagger c_k + \sum_k \varepsilon_k^{\mathrm{v}} f_k^\dagger f_k + \frac{g_0}{\sqrt{L}} \sum_k (b c_k^\dagger f_k + b^* f_k^\dagger c_k) \\ &= \sum_k \begin{pmatrix} c_k^\dagger & f_k^\dagger \end{pmatrix} \begin{pmatrix} \varepsilon_k^{\mathrm{c}} & \frac{g_0}{\sqrt{L}} b \\ \frac{g_0}{\sqrt{L}} b^* & \varepsilon_k^{\mathrm{v}} \end{pmatrix} \begin{pmatrix} c_k \\ f_k \end{pmatrix}. \end{aligned} \tag{6}$$

Diagonalization of this Hamiltonian gives

$$\varepsilon_k^{\mathrm{c}',\mathrm{v}'} = \frac{\varepsilon_k^{\mathrm{c}} + \varepsilon_k^{\mathrm{v}} \pm \sqrt{(\varepsilon_k^{\mathrm{c}} - \varepsilon_k^{\mathrm{v}})^2 + \frac{4g_0^2}{L} |b|^2}}{2}. \tag{7}$$

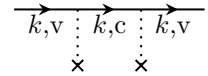
It can be easily verified that the distance between the conduction band and the valence band is increased, because when the square root in the expression is positive, it's larger than $\varepsilon_k^{\mathrm{c}} - \varepsilon_k^{\mathrm{v}}$. Note that since $b \propto \sqrt{N} \propto \sqrt{L}$, the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

The ground state total energy is then

$$\begin{aligned} E' &= \sum_k \frac{\varepsilon_k^{\mathrm{c}} + \varepsilon_k^{\mathrm{v}} - \sqrt{(\varepsilon_k^{\mathrm{c}} - \varepsilon_k^{\mathrm{v}})^2 + \frac{4g_0^2}{L} |b|^2}}{2} + \hbar\omega_0 |b|^2 \\ &\approx \underbrace{\sum_k \varepsilon_k^{\mathrm{v}}}_{E} - \sum_k \frac{g_0^2}{(\varepsilon^{\mathrm{c}} - \varepsilon_k^{\mathrm{v}}) L} |b|^2 + \hbar\omega_0 |b|^2. \end{aligned} \tag{8}$$

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

$-\mathrm{i}\Sigma_k^{\mathrm{v}}(\omega) =$ 

$$= \frac{-\mathrm{i}g_0 b}{\sqrt{L}} \cdot \frac{\mathrm{i}}{\omega - \varepsilon_k^{\mathrm{c}} + \mu} \cdot \frac{-\mathrm{i}g_0 b^*}{\sqrt{L}}, \tag{9}$$

$$\Sigma_k^{\mathrm{v}}(\omega) = \frac{g_0^2}{L} |b|^2 \frac{1}{\omega - \varepsilon_k^{\mathrm{c}}}. \tag{10}$$

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

$$\omega - \varepsilon_k^{\mathrm{v}} + \mu - \frac{g_0^2 |b|^2}{(\omega - \varepsilon_k^{\mathrm{c}} + \mu)L} = 0. \tag{11}$$

It's equivalent to (7).

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 (8). This term is to be merged with the $(T - T_{\mathrm{c}})X^2$ term. So if (8) 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 – (8) 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

[1] Rodolfo Alberto Borzi et al. "Formation of a nematic fluid at high fields in $Sr_3Ru_2O_7$". In: *Science* 315.5809 (2007), pp. 214–217.

[2] SA Grigera et al. "Angular dependence of the magnetic susceptibility in the itinerant metamagnet $Sr_3Ru_2O_7$". In: *Physical Review B* 67.21 (2003), p. 214427.

[3] SA Grigera et al. "Disorder-sensitive phase formation linked to metamagnetic quantum criticality". In: *Science* 306.5699 (2004). Fig. 2 shows the magnetic susceptibility, pp. 1154–1157.

[4] Hae-Young Kee and Yong Baek Kim. "Itinerant metamagnetism induced by electronic nematic order". In: *Physical Review B* 71.18 (2005). The model Hamiltonian is (1), and the Fermi surface configurations and the magnetization curve are displayed in Fig. 2., p. 184402.

[5] Kentaro Kitagawa et al. "Metamagnetic Quantum Criticality Revealed by ^{17}O-NMR in the Itinerant Metamagnet $Sr_3Ru_2O_7$". In: *Physical review letters* 95.12 (2005), p. 127001.

[6] C Lester et al. "Field-tunable spin-density-wave phases in $Sr_3Ru_2O_7$". In: *Nature materials* 14.4 (2015), pp. 373–378.

[7] RS Perry et al. "Metamagnetism and critical fluctuations in high quality single crystals of the bilayer ruthenate $Sr_3Ru_2O_7$". In: *Physical Review Letters* 86.12 (2001), p. 2661.

[8] Z. Ropka, R. Michalski, and R. J. Radwanski. "Electronic and magnetic properties of $FeBr_2$". In: *Phys. Rev. B* 63 (17 2001), p. 172404. DOI: 10.1103/PhysRevB.63.172404. URL: https://link.aps.org/doi/10.1103/PhysRevB.63.172404.