Homework 1

Jinyuan Wu

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1 Hund's rule and magnetic exchange as a result of Coulomb interactions

1.1 Why Coulomb interaction is stronger than magnetic dipole coupling?

The magnetic dipole-dipole interaction Hamiltonian is

$$H = -\frac{\mu_0}{4\pi |\boldsymbol{r}|^3} \left[3 \left(\boldsymbol{m}_1 \cdot \hat{\boldsymbol{r}} \right) \left(\boldsymbol{m}_2 \cdot \hat{\boldsymbol{r}} \right) - \boldsymbol{m}_1 \cdot \boldsymbol{m}_2 \right] - \mu_0 \frac{2}{3} \boldsymbol{m}_1 \cdot \boldsymbol{m}_2 \delta(\boldsymbol{r}). \tag{1}$$

The relation between the magnetic moment and the spin is

$$\boldsymbol{m} = -g \mu_{\mathrm{B}} \boldsymbol{S}, \tag{2}$$

where $\hbar \boldsymbol{S}$ the spin angular momentum (and $\boldsymbol{S}$ has no dimension in it). So we have

$$\begin{aligned} H &= -\frac{\mu_0 \mu_{\mathrm{B}}^2}{4\pi |\boldsymbol{r}|^3} (3 (\boldsymbol{S}_1 \cdot \hat{\boldsymbol{r}}) (\boldsymbol{S}_2 \cdot \hat{\boldsymbol{r}}) - \boldsymbol{S}_1 \cdot \boldsymbol{S}_2) - \frac{2}{3} \mu_0 \mu_{\mathrm{B}}^2 \boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \delta(\boldsymbol{r}) \\ &\sim -\frac{\mu_0 g_1 g_2 \mu_{\mathrm{B}}^2}{4\pi a^3} \sim -\frac{\mu_0 \mu_{\mathrm{B}}^2}{4\pi a^3}, \end{aligned} \tag{3}$$

where a is the characteristic length scale about the distances between atoms, and may be estimated by the lattice constant, while g_1, g_2 are dimensionless and usually not large. Taking $a \sim 1\,\text{Å}$, we find $H_{\text{dipole-dipole}} \sim 5 \times 10^{-5}\,\mathrm{eV}$.

The exchange interaction depends more strongly on the distance between atoms, because it involves wave function overlapping. We can derive T_{c} from the Weiss mean field theory using J and then infer the magnitude of J from experimentally observed T_{c}. Suppose we already find the relation between $\boldsymbol{M}$ and $\boldsymbol{H}$ when there is no interaction: we label this "free" susceptibility as χ_0. We then

$$\boldsymbol{M} = \chi_0 \boldsymbol{H}_{\text{total}} = \chi_0 (\boldsymbol{H} + \boldsymbol{H}_M) = \chi_0 (\boldsymbol{H} + \lambda_M \boldsymbol{M}). \tag{4}$$

Note that when the electrons are completely localized, the coupling between the external field and magnetic moments is linear, and the interaction between spins is two-body ($\boldsymbol{S}_{\boldsymbol{i}} \cdot \boldsymbol{S}_{\boldsymbol{j}}$ or $\boldsymbol{D} \cdot (\boldsymbol{S}_{\boldsymbol{i}} \times \boldsymbol{S}_{\boldsymbol{j}})$), this formalism is *exact*: $\boldsymbol{M}$ is essentially

$$\frac{1}{V} \sum_{\boldsymbol{i}, \sigma_1, \sigma_2} \frac{\hbar}{2} \left\langle c^\dagger_{\boldsymbol{i}\sigma_1} \boldsymbol{\sigma}_{\sigma_1 \sigma_2} c_{\boldsymbol{i}\sigma_2} \right\rangle,$$

and can be obtained using Now since the interaction is highly localized, the ring diagram approximation in the real space is exact (other diagrams all vanish because of the $\delta_{\boldsymbol{ij}}$ factor in the single electron propagator), and each ring equals the electron occupation because $n_{\boldsymbol{i}}^2 = n_{\boldsymbol{i}}$, and in this way, letting λ_M to be the ratio between the magnetic field generated by a ring diagram and the ring diagram itself, we have

$$\boldsymbol{M} = \chi_0 \boldsymbol{H} + \lambda_M \chi_0 \boldsymbol{H} + \lambda_M \chi_0 \lambda_M \chi_0 \boldsymbol{H} + \cdots,$$

which is just (4). Then we introduce the high-temperature approximation, and we get Curie's law

$$\chi_0 = \frac{C}{T}, \quad C = \frac{\mu_0 n}{3 k_{\mathrm{B}}} \mu_{\mathrm{B}}^2 g^2 j(j+1), \tag{5}$$

where n is the number of atoms per volume, g the Landé g factor, j the total angular momentum.

Until now no information concerning magnetic interaction is used. Now the next step is to use the magnetic interaction to find λ_M. Here we introduce the mean-field approximation and assume that $\boldsymbol{m}_j$ can be approximated by $\boldsymbol{M}/n$, ignoring all thermal and quantum fluctuation of $\boldsymbol{m}_j$. Therefore, from the single-site Hamiltonian in the Heisenberg model (z is the number of nearest neighbors of each site)

$$H = -2zJ\boldsymbol{S_i}\cdot\boldsymbol{S_j} = -\frac{2zJ}{g^2\mu_\mathrm{B}^2}\boldsymbol{m}_i\cdot\frac{\boldsymbol{M}}{n}, \tag{6}$$

and therefore we get

$$\boldsymbol{B}_M = \frac{2zJ}{ng^2\mu_\mathrm{B}^2}\boldsymbol{M}, \quad \boldsymbol{H}_M = \underbrace{\frac{2zJ}{n\mu_0 g^2\mu_\mathrm{B}^2}}_{\lambda_M}\boldsymbol{M}. \tag{7}$$

Putting (7) and (5) into (4), we get

$$\boldsymbol{M} = \frac{C}{T-T_\mathrm{c}}\boldsymbol{H}, \quad T_\mathrm{c} = C\lambda_M = \frac{2zJ}{3k_\mathrm{B}}(j+1)j. \tag{8}$$

So now we can estimate J from T_c by

$$J = \frac{3}{2}\frac{k_\mathrm{B}T_\mathrm{c}}{zj(j+1)}. \tag{9}$$

For iron, the bcc structure means $z=8$, and we can take $j=1$, and the experimentally measured T_c is 1043 K, and we find $J = 8.4\times10^{-3}\,\mathrm{eV}$.

So we find $H_\text{exchange}/H_\text{magnetic dipole-dipole}\sim 160$, and therefore the order of magnitude of the exchange interaction is much larger than the magnetic dipole-dipole interaction, and that's why the exchange interaction is the dominant effect.

1.2 The atomic ground state configuration of Cr^{3+}, Fe^{3+} and Gd^{3+}

The Hund's rules have their root in L-S coupling. After the occupation of each electron shell is determined, we apply the following rules one by one:

1. For each electron shell, make the total spin as large as possible.
2. After the total spin is determined, make the total orbital angular momentum as large as possible.
3. When S and L are already determined, if the shell is not yet half-filled, take $J=|L-S|$; otherwise $J=L+S$.
4. Now S, L, and J are all decided, and the Landé g-factor is

$$g_J = \frac{3}{2}+\frac{S(S+1)-L(L+1)}{2J(J+1)}, \tag{10}$$

and the total magnetic momentum is

$$\boldsymbol{\mu} = -g_J\mu_\mathrm{B}\boldsymbol{J}, \tag{11}$$

where $\hbar\boldsymbol{J}$ is the total angular momentum.

The electron configuration of Cr^{3+} is $[Ar]3d^3$. To maximize L, we want the $l=0,1,2$ orbitals to be filled, so $L=3$; the maximal total spin momentum available is $S=3/2$. Since the d orbitals are not yet half-filled, we have $J=|L-S|=3/2$, and therefore $g=2/5$, and the total magnetic moment is $2/5\cdot\mu_\mathrm{B}\cdot 3/2 = 3/5\mu_\mathrm{B}$. This deviates far from the experimentally measured value. One explanation is here is angular momentum quenching happens, and the total magnetic moment is essentially the total spin magnetic moment, which is $3\mu_\mathrm{B}$, exactly what is measured experimentally.

The electron configuration of Fe^{3+} is $[Ar]3d^5$, so the 3d shell is half-filled, and each orbital therefore only contains one electron, and the spins of all electrons are aligned to each other. So in this shell we have $L=0$, $S=5/2$, and therefore $J=5/2$. We have $g=2$, so the magnitude of the magnetic moment is $2\mu_\mathrm{B}\cdot 5/2 = 5\mu_\mathrm{B}$, which agrees with the experimental value.

The electron configuration of Gd^{3+} is $[Xe]4f^7$, so the 4f shell is half-filled, and therefore $L=0$, $S=7/2$, and therefore $J=7/2$. We have $g=2$, so the magnitude of the magnetic moment is $2\mu_\mathrm{B}\cdot 7/2 = 7\mu_\mathrm{B}$, which agrees with the experimental result.

1.3 Other magnetic mechanism from Coulomb interaction

Apart from the direct exchange interaction, we also have superexchange, double exchange, the Dzyaloshinskii-Moriya interaction, and the RKKY interaction.

2 Landau diamagnetism and Pauli paramagnetism

2.1 The physical origins of various magnetic responses in a solid

Pauli paramagnetism comes from the spin-magnetic field coupling of itinerant electrons: the external magnetic field splits the spin-↑ band and the spin-↓ band. Since the Fermi energy in the two bands is the same, when, say, the magnetic field is upward, we have less spin-↑ electrons than spin-↓ electrons, and we have an overall downward spin and therefore an overall upward magnetic moment, so there is a paramagnetic response.

Landau diamagnetism comes from the coupling between orbital angular momentum and the external magnetic field of itinerant electrons. In an external magnetic field (say, in the z direction), TODO: intuitive explanation

Curie paramagnetism comes from the coupling between the spin and the external magnetic field of localized electrons. Here we no longer hand band structures and no $\boldsymbol{k}$ variable, and the degrees of freedom are n, l, m and the spin m_s, and Curie's $1/T$ law can be derived by putting the first-order perturbation of

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} \tag{12}$$

into the partition function.

Van Vleck paramagnetism comes from the second order perturbation of (12). It has the same order of magnitude with **Larmor (or Langenvin) diamagnetism**, which comes from the B^2 term

$$H_{\text{Larmor}} = \mu_0^2 \frac{e^2}{8m_{\text{e}}} r_\perp^2 H^2 \tag{13}$$

in the electromagnetic coupling Hamiltonian.

2.2 Strength of Cu's magnetic response

[1] gives the magnetic susceptibility of cooper:

$$\chi = \left(-0.083 + \frac{0.023}{T} \right) \times 10^{-6} \text{cgs unit.} \tag{14}$$

Suppose the lab is in room temperature, and we set $T = 300\,\text{K}$. (Although SQUID requires cooling of the superconducting probe, this doesn't mean the sample should also be cooled. Indeed, [2] shows some cases where SQUID is used to measure neural activities in the brain.) Since χ doesn't have H dependence, the relation between M and H is linear, and with $H = 10\,\text{Oe}$, we have $M = \chi H = -8.29 \times 10^{-7}$ cgs unit. The expected magnetic moment is 5×10^{-8} emu, and therefore the volume needed is (note that we are working with cgs units)

$$\frac{5 \times 10^{-8}}{8.29 \times 10^{-7}} \text{cm}^3 = 0.06\,\text{cm}^3,$$

and the density of Cu is $8.96\,\text{g}/\text{cm}^3$, so we need $0.54\,\text{g}$ cooper.

3 Spin waves

3.1 Spin wave with staggering Heisenberg coefficients

So now we have two sublattices, denoted by A and B, and the Hamiltonian is

$$H = -2J_1 \sum_i \boldsymbol{S}_{i\text{A}} \cdot \boldsymbol{S}_{i\text{B}} - 2J_2 \sum_i \boldsymbol{S}_{i\text{B}} \cdot \boldsymbol{S}_{i+1,\text{A}}. \tag{15}$$

We have

$$[\boldsymbol{S}_i, \boldsymbol{S}_i \cdot \boldsymbol{S}_j] = -\mathrm{i}\boldsymbol{S}_i \times \boldsymbol{S}_j,$$

so

$$\begin{aligned}\frac{\mathrm{d}\boldsymbol{S}_{i\mathrm{A}}}{\mathrm{d}t} &= \frac{1}{\mathrm{i}\hbar}[\boldsymbol{S}_{i\mathrm{A}}, H] = \frac{1}{\mathrm{i}\hbar}[\boldsymbol{S}_{i\mathrm{A}}, -2J_2\boldsymbol{S}_{i-1,\mathrm{B}} \cdot \boldsymbol{S}_{i\mathrm{A}} - 2J_1\boldsymbol{S}_{i\mathrm{A}} \cdot \boldsymbol{S}_{i\mathrm{B}}] \\ &= \frac{2}{\hbar}\boldsymbol{S}_{i\mathrm{A}} \times (J_2\boldsymbol{S}_{i-1,\mathrm{B}} + J_1\boldsymbol{S}_{i\mathrm{B}}),\end{aligned} \tag{16}$$

and similarly

$$\frac{\mathrm{d}\boldsymbol{S}_{i\mathrm{B}}}{\mathrm{d}t} = \frac{2}{\hbar}\boldsymbol{S}_{i\mathrm{B}} \times (J_1\boldsymbol{S}_{i\mathrm{A}} + J_2\boldsymbol{S}_{i+1,\mathrm{A}}). \tag{17}$$

The above equations are exact and nonlinear. Assuming each $\boldsymbol{S}$ doesn't deviate much from its ground state value, i.e. $S\hat{\boldsymbol{z}}$, we can reduce (16) and (17) into four equations about $S^{x/y}_{i,\mathrm{A/B}}$, ignoring the time evolution of z components, and replace all S^z components in these equations by S, and therefore we get

$$\begin{aligned}\frac{\mathrm{d}S^x_{i\mathrm{A}}}{\mathrm{d}t} &= \frac{2}{\hbar}(S^y_{i\mathrm{A}}(J_2S^z_{i-1,\mathrm{B}} + J_1S^z_{i\mathrm{B}}) - S^z_{i\mathrm{A}}(J_2S^y_{i-1,\mathrm{B}} + J_1S^y_{i\mathrm{B}})) \\ &= \frac{2S}{\hbar}((J_1 + J_2)S^y_{i\mathrm{A}} - J_2S^y_{i-1,\mathrm{B}} - J_1S^y_{i\mathrm{B}}),\end{aligned}$$

and similarly

$$\begin{aligned}\frac{\mathrm{d}S^y_{i\mathrm{A}}}{\mathrm{d}t} &= -\frac{2S}{\hbar}((J_1 + J_2)S^x_{i\mathrm{A}} - J_2S^x_{i-1,\mathrm{B}} - J_1S^x_{i\mathrm{B}}), \\ \frac{\mathrm{d}S^x_{i\mathrm{B}}}{\mathrm{d}t} &= \frac{2S}{\hbar}((J_1 + J_2)S^y_{i\mathrm{B}} - J_2S^y_{i+1,\mathrm{A}} - J_1S^y_{i\mathrm{A}}), \\ \frac{\mathrm{d}S^y_{i\mathrm{B}}}{\mathrm{d}t} &= -\frac{2S}{\hbar}((J_1 + J_2)S^x_{i\mathrm{B}} - J_2S^x_{i+1,\mathrm{A}} - J_1S^x_{i\mathrm{A}}).\end{aligned}$$

In the 4-momentum domain, this is equivalent to

$$\frac{2S}{\hbar}\begin{pmatrix} 0 & J_1 + J_2 & 0 & -J_1 - J_2\mathrm{e}^{-\mathrm{i}ka} \\ -(J_1 + J_2) & 0 & J_1 + J_2\mathrm{e}^{-\mathrm{i}ka} & 0 \\ 0 & -J_1 - J_2\mathrm{e}^{\mathrm{i}ka} & 0 & J_1 + J_2 \\ J_1 + J_2\mathrm{e}^{\mathrm{i}ka} & 0 & -(J_1 + J_2) & 0 \end{pmatrix}\begin{pmatrix} S^x_{i\mathrm{A}} \\ S^y_{i\mathrm{A}} \\ S^x_{i\mathrm{B}} \\ S^y_{i\mathrm{B}} \end{pmatrix} = -\mathrm{i}\omega\begin{pmatrix} S^x_{i\mathrm{A}} \\ S^y_{i\mathrm{A}} \\ S^x_{i\mathrm{B}} \\ S^y_{i\mathrm{B}} \end{pmatrix}. \tag{18}$$

The analytical form of the diagonalization of the above is too complex for human readers, but we can always plot it. The attached file contains Mathematica codes for plotting the relation between $\hbar\omega/2S$ and ka with different values of J_1 and J_2. (Just ignore the negative frequencies: since $\boldsymbol{S}_i$ is a real field, the modes with positive frequencies have already cover the whole spectrum.) It can be seen that when $J_1 = J_2$, we just get Brillouin zone folding, and when $J_1 \neq J_2$ a small gap opens at the boundary of the first Brillouin zone, quite similar to how the phonon spectrum splits into acoustic and optical branches; the $\omega \propto k^2$ relation near the Γ point is still preserved.

3.2 Distinguishing an AFM system from an FM one

The difference of the dispersion relations of FM and AFM magnons is essentially the difference of their low energy effective Hamiltonians and therefore can be reflected by measuring the specific heat capacity. For bosons, a $\omega \propto k$ dispersion relation means $C_V \propto T^3$, while a $\omega \propto k^2$ dispersion relation means $C_V \propto T^{3/2}$, so by measuring C_V we are able to know whether the material is FM or AFM.

References

[1] Raymond Bowers. "Magnetic Susceptibility of Copper Metal at Low Temperatures". In: *Phys. Rev.* 102 (6 1956), pp. 1486–1488. DOI: 10.1103/PhysRev.102.1486. URL: https://link.aps.org/doi/10.1103/PhysRev.102.1486.

[2] Sanjay P Singh. "Magnetoencephalography: basic principles". In: *Annals of Indian Academy of Neurology* 17.Suppl 1 (2014), S107.