

Homework 1

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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

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

The relation between the magnetic moment and the spin is

$$\mathbf{m} = -g\mu_B \mathbf{S}, \quad (2)$$

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

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

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 $a \sim 1 \text{ \AA}$, we find $H_{\text{dipole-dipole}} \sim 5 \times 10^{-5} \text{ eV}$.

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 \mathbf{M} and \mathbf{H} when there is no interaction: we label this “free” susceptibility as χ_0 . We then

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

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 ($\mathbf{S}_i \cdot \mathbf{S}_j$ or $\mathbf{D} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$), this formalism is *exact*: \mathbf{M} is essentially

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

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 δ_{ij} factor in the single electron propagator), and each ring equals the electron occupation because $n_i^2 = n_i$, 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

$$\mathbf{M} = \chi_0 \mathbf{H} + \lambda_M \chi_0 \mathbf{H} + \lambda_M \chi_0 \lambda_M \chi_0 \mathbf{H} + \dots,$$

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

$$\chi_0 = \frac{C}{T}, \quad C = \frac{\mu_0 n}{3k_B} \mu_B^2 g^2 j(j+1), \quad (5)$$

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 \mathbf{m}_j can be approximated by \mathbf{M}/n , ignoring all thermal and quantum fluctuation of \mathbf{m}_j . Therefore, from the single-site Hamiltonian in the Heisenberg model (z is the number of nearest neighbors of each site)

$$H = -2zJS_i \cdot S_j = -\frac{2zJ}{g^2\mu_B^2} \mathbf{m}_i \cdot \frac{\mathbf{M}}{n}, \quad (6)$$

and therefore we get

$$\mathbf{B}_M = \frac{2zJ}{ng^2\mu_B^2} \mathbf{M}, \quad \mathbf{H}_M = \underbrace{\frac{2zJ}{n\mu_0g^2\mu_B^2}}_{\lambda_M} \mathbf{M}. \quad (7)$$

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

$$\mathbf{M} = \frac{C}{T - T_c} \mathbf{H}, \quad T_c = C\lambda_M = \frac{2zJ}{3k_B}(j+1)j. \quad (8)$$

So now we can estimate J from T_c by

$$J = \frac{3}{2} \frac{k_B T_c}{zj(j+1)}. \quad (9)$$

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 $J = 8.4 \times 10^{-3}$ 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

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

and the total magnetic moment is

$$\boldsymbol{\mu} = -g_J \mu_B \mathbf{J}, \quad (11)$$

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

The electron configuration of Cr^{3+} is $[\text{Ar}]3d^3$. 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 $2/5 \cdot \mu_B \cdot 3/2 = 3/5 \mu_B$. 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 $3\mu_B$, exactly what is measured experimentally.

The electron configuration of Fe^{3+} is $[\text{Ar}]3d^5$, 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 $2\mu_B \cdot 5/2 = 5\mu_B$, which agrees with the experimental value.

The electron configuration of Gd^{3+} is $[\text{Xe}]4f^7$, 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 $2\mu_B \cdot 7/2 = 7\mu_B$, 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- \uparrow band and the spin- \downarrow band. Since the Fermi energy in the two bands is the same, when, say, the magnetic field is upward, we have less spin- \uparrow electrons than spin- \downarrow 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. (Although the electrons are “constrained” in circular motion in the xy plane, the \mathbf{x} and \mathbf{p} degrees of freedom play an important role in Landau diamagnetism instead of being totally frozen, so we still classify Landau diamagnetism as an itinerant mechanism.) In an external magnetic field (say, in the z direction), the k_x and k_y variables are no longer good quantum numbers, and the Hamiltonian becomes an “oscillator” in the xy plane plus a free-electron term in the z direction and reads

$$E = \left(n + \frac{1}{2}\right) \hbar \omega_c + \frac{\hbar^2 k_z^2}{2m}, \quad (12)$$

where

$$\omega_c = \frac{eB}{m}. \quad (13)$$

So we find

$$E = - \underbrace{\left(-\frac{e}{m} \hbar \left(n + \frac{1}{2}\right)\right)}_{\mu} \cdot B + \frac{\hbar^2 k_z^2}{2m},$$

and we find the magnetic moment is less than zero, and therefore we get a paramagnetic response.

Curie paramagnetism comes from the coupling between the spin and the external magnetic field of localized electrons. Here we no longer have band structures and no \mathbf{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

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} \quad (14)$$

into the partition function.

Van Vleck paramagnetism comes from the second order perturbation of (14). It has the same order of magnitude with **Larmor (or Langenvin) diamagnetism**, which comes from the B^2 term

$$H_{\text{Larmor}} = \mu_0^2 \frac{e^2}{8m_e} r_{\perp}^2 H^2 \quad (15)$$

in the electromagnetic coupling Hamiltonian.

Now we estimate the magnitudes of the mechanisms for copper. From an existing QuantumESPRESSO calculation (see [Electron density of states for fcc copper](#)), we know that around the Fermi surface, the density of states is $2.48 \times 10^{28} \text{ eV}^{-1} \cdot \text{m}^{-3}$, and we have

$$\chi_{\text{Pauli}} = 2\mu_0 \mu_B^2 \rho_0(\varepsilon_F) = 3.2 \times 10^{-5}, \quad \chi_{\text{Landau}} = -\frac{1}{3} \chi_{\text{Pauli}} = -1.1 \times 10^{-5}. \quad (16)$$

It should be noted that the second equation only works when the free electron approximation works well enough, and is just an estimation of magnitude. But anyway, Pauli paramagnetism and Landau diamagnetism have comparable orders of magnitude.

2.2 Strength of Cu's magnetic response

[1] gives the magnetic susceptibility of cooper:

$$\chi = \left(-0.083 + \frac{0.023}{T} \right) \times 10^{-6} \text{ cgs unit.} \quad (17)$$

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 $M = \chi H = -8.29 \times 10^{-7} \text{ cgs unit}$. The expected magnetic moment is $5 \times 10^{-8} \text{ emu}$, 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 g/cm^3 , so we need 0.54 g cooper.

3 Mean-field solution of 1D Ising model

3.1 Mean-field approximation

The Ising model

$$H = -J \sum_{\langle i, j \rangle} s_i s_j - h \sum_i s_i \quad (18)$$

is defined on a lattice, each site of which has q nearest neighbors. Assuming the spins have minimal fluctuation, and we have $\langle s_i \rangle = m$, we have

$$s_i s_j \approx \langle s_i \rangle s_j + s_i \langle s_j \rangle - \langle s_i \rangle \langle s_j \rangle = m(s_i + s_j) - m^2,$$

and therefore (the $1/2$ factor comes from the fact that a site is counted twice if we go over all bonds)

$$\begin{aligned} H &= -Jmq \sum_i s_i + \frac{Nq}{2} \cdot Jm^2 - h \sum_i s_i \\ &= -\underbrace{(h + Jmq)}_{h_{\text{eff}}} \sum_i s_i + \frac{NqJm^2}{2}. \end{aligned} \quad (19)$$

This essentially is the Weiss molecular field approximation. The m^2 term is absent in (6), but this doesn't matter: when calculating $\langle s_i \rangle$, m is a constant and is not summed over, so the m^2 term can be seen as a constant and we have

$$H \simeq -\underbrace{(h + Jmq)}_{h_{\text{eff}}} \sum_i s_i,$$

which is just (6). The only difference is that in Section 1.1, we have taken the high temperature limit, while here we do not.

(Another way to get this approximation is by integrate out microscopic s_i degrees of freedom, and get a theory $f(m)$ about $\sum_i s_i/N$, and then find the m that minimizes $f(m)$. This last method can in principle be systematically improved because we can include more fluctuation around this minimum.)

3.2 The partition function

As is said in the last section, we can just ignore the m^2 term, and the partition function is

$$\begin{aligned} Z &= \sum_{\{s_i\}} e^{\beta h_{\text{eff}} \sum_i s_i} \\ &= \prod_i \sum_{s_i = \pm 1} e^{\beta h_{\text{eff}} s_i} = \prod_i 2 \cosh(\beta h_{\text{eff}}) \\ &= 2^N \cosh^N(\beta h_{\text{eff}}). \end{aligned} \quad (20)$$

3.3 Find the total magnetization

The total magnetic moment can be obtained using

$$\sum_i \langle s_i \rangle = \frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial h}, \quad (21)$$

which, in our case, is

$$\begin{aligned} \sum_i \langle s_i \rangle &= \frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial h_{\text{eff}}} \\ &= \frac{1}{\beta} \frac{1}{2^N \cosh^N(\beta h_{\text{eff}})} 2^N N \cosh^{N-1}(\beta h_{\text{eff}}) \cdot \beta \sinh(\beta h_{\text{eff}}) \\ &= N \tanh(\beta h_{\text{eff}}), \end{aligned}$$

and therefore

$$m = \frac{1}{N} \sum_i \langle s_i \rangle = \tanh(\beta h_{\text{eff}}),$$

and we eventually get the self-consistent equation

$$m = \tanh\left(\frac{h + Jqm}{k_B T}\right). \quad (22)$$

3.4 The critical temperature

In the $T \rightarrow \infty$ limit, we have the Curie-Weiss law

$$m = \frac{h + Jqm}{k_B T} \Rightarrow m = \frac{h/k_B}{T - T_c}, \quad T_c = \frac{Jq}{k_B}. \quad (23)$$

This estimation of T_c is actually accurate in the level of (22): the condition to have non-zero solution of (22) is that the slope of \tanh is larger than 1 (the LHS of (22)), so that when $T \rightarrow 0$, the RHS of (22) goes to a constant, and a cross point occurs between the two parts of (22). When $h = 0$, the slope of \tanh is one, if and only if

$$m = \frac{Jqm}{k_B T} \Rightarrow T = \frac{Jq}{k_B},$$

which is just T_c in (23).

3.5 Critical exponent of m

When $h = 0$ and T is near T_c , m is small, but the first-order Taylor expansion in (23) can't give the relation between m and T when $h = 0$, so we need to take the next term into consideration. We have

$$m = \frac{Jqm}{k_B T} - \frac{1}{3} \left(\frac{Jqm}{k_B T} \right)^3 + \dots,$$

or in other words

$$m \approx \frac{T_c}{T} m - \frac{1}{3} \left(\frac{T_c}{T} m \right)^3,$$

and we find

$$m \approx \pm \sqrt{\frac{3T^2(T_c - T)}{T_c^3}} \approx \pm \sqrt{\frac{3(T_c - T)}{T_c}}. \quad (24)$$

So we find $m \propto (T_c - T)^{1/2}$, and therefore the critical exponent $\beta = 1/2$.

The mean-field level Landau theory gives exactly the same prediction, because as is said in Section 3.1, finding the m that minimizes the free energy is equivalent to the mean-field approximation done above, and the former is just the mean-field level Landau theory. But after more fluctuation is taken into account (i.e. we do a Ginzburg-Landau theory instead of a mean-field Landau theory), we find β deviates from the mean-field value and has dimension dependence. When $d = 2$, $\beta = 1/8$, and when $d = 3$, $\beta = 0.326$.

3.6 Critical exponents for other quantities

For the free energy, we have

$$\begin{aligned} F &= -k_B T \ln Z = -k_B T N \ln 2 - N k_B T \ln \cosh(\beta h_{\text{eff}}) \\ &= -k_B T N \ln 2 - N k_B T \ln \cosh\left(\frac{h + Jqm}{k_B T}\right). \end{aligned} \quad (25)$$

The total energy is

$$U = -h_{\text{eff}} \sum_i \langle s_i \rangle = -(h + Jqm)Nm \quad (26)$$

4 Spin waves

4.1 Spin wave with staggering Heisenberg coefficients

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

$$H = -2J_1 \sum_i \mathbf{S}_{iA} \cdot \mathbf{S}_{iB} - 2J_2 \sum_i \mathbf{S}_{iB} \cdot \mathbf{S}_{i+1,A}. \quad (27)$$

We have

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

so

$$\begin{aligned} \frac{d\mathbf{S}_{iA}}{dt} &= \frac{1}{i\hbar} [\mathbf{S}_{iA}, H] = \frac{1}{i\hbar} [\mathbf{S}_{iA}, -2J_2 \mathbf{S}_{i-1,B} \cdot \mathbf{S}_{iA} - 2J_1 \mathbf{S}_{iA} \cdot \mathbf{S}_{iB}] \\ &= \frac{2}{\hbar} \mathbf{S}_{iA} \times (J_2 \mathbf{S}_{i-1,B} + J_1 \mathbf{S}_{iB}), \end{aligned} \quad (28)$$

and similarly

$$\frac{d\mathbf{S}_{iB}}{dt} = \frac{2}{\hbar} \mathbf{S}_{iB} \times (J_1 \mathbf{S}_{iA} + J_2 \mathbf{S}_{i+1,A}). \quad (29)$$

The above equations are exact and nonlinear. Assuming each \mathbf{S} doesn't deviate much from its ground state value, i.e. $S\hat{z}$, we can reduce (28) and (29) into four equations about $S_{i,A/B}^{x/y}$, ignoring the time evolution of z components, and replace all S^z components in these equations by S , and therefore we get

$$\begin{aligned} \frac{dS_{iA}^x}{dt} &= \frac{2}{\hbar} (S_{iA}^y (J_2 S_{i-1,B}^z + J_1 S_{iB}^z) - S_{iA}^z (J_2 S_{i-1,B}^y + J_1 S_{iB}^y)) \\ &= \frac{2S}{\hbar} ((J_1 + J_2) S_{iA}^y - J_2 S_{i-1,B}^y - J_1 S_{iB}^y), \end{aligned}$$

and similarly

$$\begin{aligned} \frac{dS_{iA}^y}{dt} &= -\frac{2S}{\hbar} ((J_1 + J_2) S_{iA}^x - J_2 S_{i-1,B}^x - J_1 S_{iB}^x), \\ \frac{dS_{iB}^x}{dt} &= \frac{2S}{\hbar} ((J_1 + J_2) S_{iB}^y - J_2 S_{i+1,A}^y - J_1 S_{iA}^y), \\ \frac{dS_{iB}^y}{dt} &= -\frac{2S}{\hbar} ((J_1 + J_2) S_{iB}^x - J_2 S_{i+1,A}^x - J_1 S_{iA}^x). \end{aligned}$$

In the 4-momentum domain, this is equivalent to

$$\frac{2S}{\hbar} \begin{pmatrix} 0 & J_1 + J_2 & 0 & -J_1 - J_2 e^{-ika} \\ -(J_1 + J_2) & 0 & J_1 + J_2 e^{-ika} & 0 \\ 0 & -J_1 - J_2 e^{ika} & 0 & J_1 + J_2 \\ J_1 + J_2 e^{ika} & 0 & -(J_1 + J_2) & 0 \end{pmatrix} \begin{pmatrix} S_{iA}^x \\ S_{iA}^y \\ S_{iB}^x \\ S_{iB}^y \end{pmatrix} = -i\omega \begin{pmatrix} S_{iA}^x \\ S_{iA}^y \\ S_{iB}^x \\ S_{iB}^y \end{pmatrix}. \quad (30)$$

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 \mathbf{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.

4.2 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.

4.3 Difference between a spin wave and a Bloch domain wall

The spin orientations between a Bloch domain wall are opposite, while this is not the case for a spin wave.

References

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