Lecture 8: Quantum magnetism – spin wave theory

§1. Direct exchange interacting: (ferro-magnetic Heisenberg model)

The exchange interaction is from the Coulomb interaction between d-electrons on neighbours sites.

$$H_{Coulomb} = \frac{1}{2}\int dr_1 dr_2 \; \hat{\psi}^*_{\sigma}(r_1)\, \hat{\psi}^*_{\sigma'}(r_2)\, \frac{e^2}{r_{12}}\, \psi_{\sigma'}(r_2)\, \psi_{\sigma}(r_2)$$

Expand it in the Wannier basis (local atomic orbit), you will find it contains a spin-spin interaction term which was found by Heisenberg

$$H = -2J \sum_{\langle ij \rangle} \left[\vec{S}_i \cdot \vec{S}_j + \frac{1}{4} n_i n_j\right],$$ where $\vec{S}_i$, n_i are spin and charge on each site.

J is the exchange integral $J = \int \phi^*_i(r_1)\, \phi^*_j(r_2)\, \frac{e^2}{r_{12}}\, \phi_i(r_2)\, \phi_j(r_1)\, dr_1 dr_2$.

ϕ_i and ϕ_j has significant overlap

if electrons i, and j are with total spin singlet, then their orbital wavefunction must be symmetric, which Contribution a positive exchange energy $E_x = J$

if "i" and "j" are total spin triplet, their orbit wavefunction is anti-symmetric, $\rightarrow$ $E_{ex} = -J$

Singlet $\vec{S}_i \cdot \vec{S}_j = \frac{1}{2}(\vec{S}_i + \vec{S}_j) - \frac{3}{4} = -\frac{3}{4}$

triplet $\rightarrow \frac{1}{4}$

which agrees with above Heisenberg model,

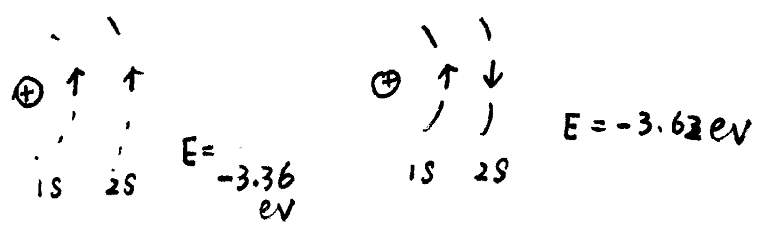
Direct exchange: FM to save interaction energy

If we neglect the Kinetic energy, and other terms in interaction energy and set each site with one electron, we arrive at the celebrated Heisenberg ferromagnetic model. There is an inconsistency for this model, because usually FM occurs in metal where electrons are itinerant. Heisenberg model describes the local moment, but it indeed grasps many interesting features of FM.

Itinerant v.s. local moments is a subtle issue / open issue.

C.f. He-atom in the excited state 1S 2S. $\longrightarrow$ triplet energy is lower.

$\Delta E = 0.3\,eV$.



§ Ferromagnetic Heisenberg model

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j = -J \sum_{\langle ij \rangle} \left\{ \frac{1}{2} \left(S_i^+ \cdot S_j^- + S_i^- \cdot S_j^+ \right) + S_i^z \cdot S_j^z \right\}$$

$$[S_i^x , S_j^y] = i \delta_{ij} S_i^z$$

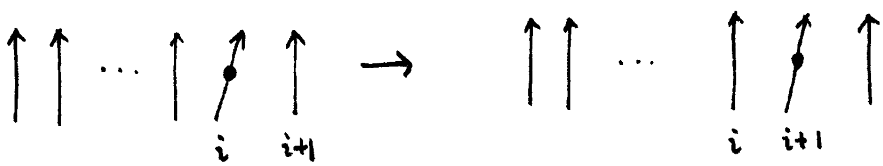
FM Heisenberg model's ground state is known

$$|\Omega\rangle = |S\rangle_1 \otimes |S\rangle_2 \otimes \cdots |S\rangle_N$$

$$H|\Omega\rangle = -J \sum_{ij} S_i^z S_j^z |\Omega\rangle - \frac{1}{2} J \sum_{\langle ij \rangle} \underbrace{\left(S_i^+ \cdot S_j^- + S_i^- \cdot S_j^+ \right) |\Omega\rangle}_{0} = -JNzS^2 |\Omega\rangle.$$

The fully polarized state with total spin NS. with degeneracy $NS(NS+1)$.

low energy excitations



method 1: equation of motion

$$\dot{S}_{i,x} = \frac{J}{i\hbar}[S_{i,x}, H] = \frac{J}{i\hbar}\sum_{\vec{\delta}} i[S_{i,z}\, S_{i+\vec{\delta},y} - S_{i,y}\cdot S_{i+\vec{\delta},z}]$$

or $$\dot{\vec{S}}_i = \frac{-J}{\hbar}\sum_{\vec{\delta}} \vec{S}_i \times \vec{S}_{i+\delta}$$

$$\frac{d}{dt}[S_i^-] = J\frac{i}{\hbar}\sum_{\vec{\delta}}\left[S_i^z\cdot S_{i+\delta}^- - S_i^-\cdot S_i^z\right].$$ set $\langle S_i^z\rangle \to S$

$$\to \frac{i}{\hbar} S \sum_{\vec{\delta}} [S_{i+\delta}^- - S_i^-],$$ do Fourier transform $S_i^- = S^- e^{i(kr-\omega t)}$

$$\Rightarrow \hbar\omega = (-J\sum_{\delta}[e^{i\vec{k}\vec{\delta}} - 1] = 2J\sum_{\delta=\hat{x},\hat{y},\hat{z}}(1-\cos\vec{k}\cdot\vec{\delta})$$

at $k\to 0 \Rightarrow \omega_k = 2\cdot\frac{J}{2}(ka)^2 = J\cdot(ka)^2$.

§ Holstein- Primakov transformation

$$S^z = S - a^+a, \quad S^+ = \sqrt{2S-a^+a}\; a \qquad S^- = a^+\sqrt{2S-a^+a}$$

a^+a describes the derivation from the Classic background. ($[a, a^+] = 1$).

but $a^+a = 0, 1, \cdots S$.

$$[S^+, S^z] = -S^+, \quad [S^-, S^z] = S^-, \quad [S^+, S^-] = 2S^z$$

ex: check H-P representation satisfies the commutation relation.

For state $|m\rangle$, $a^+a|m\rangle = (S-m)|m\rangle$.

plug in the H-P representation, and keep to quadrtic level

$$S^z = S - a^\dagger a, \quad S^+ = \sqrt{2S}\, a, \quad S^- = a^\dagger \sqrt{2S}$$

$$\Rightarrow H = -J \sum_{i,j} \left[(S - a_i^\dagger a_i)(S - a_j^\dagger a_j) + \frac{1}{2}(2S)(a_i^\dagger a_j + a_j^\dagger a_i) \right]$$

$$= -\frac{N}{2} z J S^2 + zJS \sum_l a_l^\dagger a_l - JS \sum_{i,\delta} (a_i^\dagger a_{i+\delta} + h.c.)$$

$\rightarrow$ Fourier transform $\Rightarrow$ $a_k = \frac{1}{\sqrt{N}} \sum_i e^{-ikR_i} a_k$

$$\Rightarrow H = -NzJS^2 + \sum_k \omega_k a_k^\dagger a_k, \quad \omega_k = 2JS\sum_{\delta = \hat{x},\hat{y},\hat{z}}(1 - \cos \vec{k}\cdot\vec{\delta}) \xrightarrow{k \to 0} JS(ka)^2$$

- Bloch's law

the $-M(T) + M(0) = g\mu_B \sum_l a_l^\dagger a_l = g\mu_B N \int \frac{d^3k}{(2\pi)^3} \cdot \frac{1}{e^{\hbar\omega_k/kT} - 1}$

$$\frac{M(0) - M(T)}{g\mu_B N} \approx \int_0^\Lambda \frac{k^2 dk}{(2\pi)^3} \frac{1}{e^{JSk^2/k_BT} - 1}$$

set $x = \frac{JSk^2a^2}{k_BT}$ $\Rightarrow k \propto (xT)^{1/2}$

$$\propto \int_0^{\Lambda^2/T} dx^{1/2} \frac{dx}{e^x - 1} (T)^{3/2} \rightarrow T^{3/2} \int_0^{+\infty} dx \frac{x^{1/2}}{e^x - 1}$$

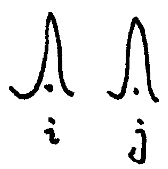
$$\boxed{\Delta M \propto T^{3/2}}$$

c.f. Curie-Weiss result $\Delta M(T) = \frac{1}{S} e^{-\frac{3T_c}{(S+1)T}}$, which doesn't consider the collective effect.

specific heat: $E = \int_0^\Lambda \frac{k^2 dk}{(2\pi)^3} \frac{JSk^2/\rho}{e^{JSk^2/k_BT} - 1} \approx \int_0^{+\infty} dx^{1/2} \frac{x^2}{e^x - 1} (T)^{5/2}$

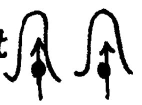
$$\Rightarrow \boxed{C_v = \frac{dE}{dT} \propto T^{3/2}}$$

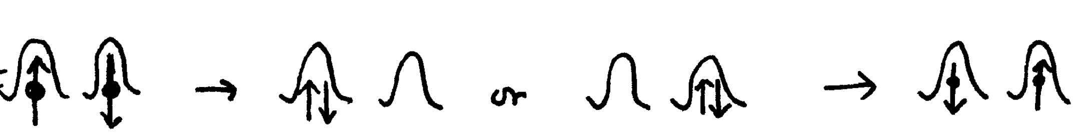
§: Super-exchange and anti-ferro Heisenberg model



The wavefunction overlap ϕ_i and ϕ_j is negligible, thus no direct exchange, but super-exchange can occur through virtual hopping process.

$$H = H_0 + H_{int} \; ; \quad H_0 = -t\,(C^{\dagger}_{i\sigma} C_{j\sigma} + h.c.), \quad H_{int} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

triplet  $\rightarrow$ no exchange : forbidden by Pauli's exclusion principle.

Singlet  $\Delta E = -\dfrac{4t^2}{U}$

super-exchange reduce kinetic energy $\Delta H = \dfrac{\langle f|H_0|m\rangle\langle m|H_0|i\rangle}{E_0 - E_m}$

$$H = J \sum_{\langle ij\rangle} \{ \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \}, \quad J = \frac{4t^2}{U}$$

FM : metal, direct exchange, spin polarize to reduce Coulomb interaction.

AFM : insulator, super-exchange. to reduce kinetic energy.

important feature: on a even bipartite, the Classic Neel state is NOT the ground state. Classicly, FM & AFM Heisenberg models are the same by doing $\vec{S} \rightarrow -\vec{S}$ on one sublattice. But quantum mechanically, $-\vec{S}$ does not obey the commutation relation of spin, thus AFM and FM are not the same.

Let us start from the classic Neel state $\underset{i}{\uparrow}\underset{i+1}{\downarrow}\uparrow\downarrow\uparrow\downarrow\cdots$

The $\vec{S}_i\cdot\vec{S}_{i+1} = S_{iz}\cdot S_{i+1,z} + \frac{1}{2}(S_{i+}\cdot S_{i+1,-} + S_{i-}\cdot S_{i+1,+})$

$$\vec{S}_i\cdot\vec{S}_{i+1}|\cdots \underset{i}{\downarrow}\underset{i+1}{\uparrow}\cdots\rangle = -\frac{1}{4}|\cdots\underset{i}{\downarrow}\underset{i+1}{\uparrow}\cdots\rangle + \frac{1}{2}|\cdots\underset{i}{\uparrow}\underset{i+1}{\downarrow}\cdots\rangle, \Rightarrow$$

Neel state isnot even the eigenstate.

§ Modified - HP boson method / Bogoliubov transformation

On sublattice A, we define $S_{A+} = \sqrt{2S-a^\dagger a}\; a$, $S_{A-} = a^\dagger\sqrt{2S-a^\dagger a}$, $S_z = S - a^\dagger a$

B, we define $S_{B-} = \sqrt{2S-b^\dagger b}\; b$, $S_{B+} = b^\dagger\sqrt{2S-b^\dagger b}$, $S_z = b^\dagger b - S$.

i.e. $a^\dagger a$ and $b^\dagger b$ describle the deviation from the Neel config.

plug in the AF Heisenberg model, and keep to quadrtic level, ⇒

$$H = -\frac{NZJS^2}{2} + ZSJ\left(\sum_i a_i^\dagger a_i + \sum_j b_j^\dagger b_j\right) + JS\sum_{\langle ij\rangle}(a_i^\dagger b_j^\dagger + a_i b_j)$$

where a and b are defined on the two sublattices, respectively.

$$a_i = \left(\frac{2}{N}\right)^{1/2}\sum_k e^{ik\cdot R_i} a_k, \quad b_i = \left(\frac{2}{N}\right)^{1/2}\sum_k e^{ikR_i} b_k$$

$$\frac{H - H_{Neel}}{Z\cdot SJ} = \sum_k a_k^\dagger a_k + b_k^\dagger b_k + \sum_k (a_k^\dagger b_{-k}^\dagger + a_k b_{-k})\gamma_k$$

$$\gamma_k = \frac{1}{Z}\sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}} = \frac{1}{3}[\cos k_x + \cos k_y + \cos k_z] \text{ for cubic lattice}$$

$$\frac{H - H_{Neel}}{z \cdot SJ} = \sum_k (a_k^+ \; b_{-k}) \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ b_{-k}^+ \end{pmatrix} - \frac{N}{2}$$

$$\Rightarrow H = -\frac{N}{2} J \, S(S+1) + \underbrace{\sum_k}_{zJS} (a_k^+ \; b_{-k}) \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} a_k \\ b_{-k}^+ \end{pmatrix}$$

define $\begin{pmatrix} a_k \\ b_{-k}^+ \end{pmatrix} = \begin{pmatrix} ch\theta_k & -sh\theta_k \\ -sh\theta_k & ch\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_{-k}^+ \end{pmatrix}$, which keep bosons commutation relation

$$\rightarrow H_k = \sum_k (\alpha_k^+ \; \beta_{-k}) \begin{pmatrix} ch\theta_k & -sh\theta_k \\ -sh\theta_k & ch\theta_k \end{pmatrix} \begin{pmatrix} 1 & \gamma_k \\ \gamma_k & 1 \end{pmatrix} \begin{pmatrix} ch\theta_k & -sh\theta_k \\ -sh\theta_k & ch\theta_k \end{pmatrix} \begin{pmatrix} \alpha_k \\ \beta_{-k}^+ \end{pmatrix}$$

$$= \sum_k (\alpha_k^+ \; \beta_{-k}) \begin{bmatrix} ch2\theta_k - \gamma_k sh2\theta_k, & -sh2\theta_k + \gamma_k ch2\theta_k \\ -sh2\theta_k + \gamma_k ch2\theta_k, & ch2\theta_k - \gamma_k sh2\theta_k \end{bmatrix} \begin{pmatrix} \alpha_k \\ \beta_{-k}^+ \end{pmatrix}$$

set $\tanh 2\theta_k = \gamma_k \Rightarrow \quad ch2\theta_k = \frac{1}{\sqrt{1-\gamma_k^2}} \quad sh2\theta_k = \frac{\gamma_k}{\sqrt{1-\gamma_k^2}}$

$$\Rightarrow H_k = \sum_k (\alpha_k^+, \; \beta_{-k}) \begin{bmatrix} \gamma_k & \\ & \gamma_k \end{bmatrix} \begin{bmatrix} \alpha_k \\ \beta_{-k}^+ \end{bmatrix} = \sum_k \hbar \omega_k \{ (\alpha_k^+ \alpha_k + 1/2) + (\beta_k^+ \beta_k + 1/2) \}$$

$\Rightarrow \omega_k = z|J|\, S\sqrt{1-\gamma_k^2}$, in the limit of $k \to 0$

$$1 - \gamma_k^2 = 1 - \left\{ \frac{1}{3} \left[3 - \frac{1}{2}(k^2) \right] \right\}^2 = \left[1 - \left[1 - \frac{k^2}{z} \right]^2 \right] = 1 - \left(1 - \frac{2k^2}{z}\right)$$

$$= \frac{2k^2}{z}$$

$\Rightarrow \omega_k = J \cdot S\sqrt{2z}\; |k|$, which is linear.

§ low-T specific heat

$$\mathcal{U} = \int \frac{k^2 dk}{(2\pi)^3} \frac{\hbar\omega_k}{e^{\hbar\omega_k/k_BT}-1} \propto T^4 \int \frac{x^3 dx}{e^x - 1}$$

$$C_V = \frac{\partial \mathcal{U}}{\partial T} \propto T^3$$

§: zero-point motion

$$S - \langle S_A \rangle = \frac{1}{N/2} \sum_i a_i^\dagger a_i = \frac{2}{N} \sum_k{}' a_k^\dagger a_k = \frac{2}{N} \sum_k{}' \operatorname{sh}^2\theta_k \langle \beta_k \beta_k^\dagger \rangle,$$ $\sum_k{}'$ sum over half BZ.

$$= \sum_k \frac{1}{2} \left[\frac{1}{\sqrt{1-\gamma_k^2}} - 1 \right],$$