# Outline

- Exchange interaction: singlect and triplet wave functions, intra- and inter-atomic exchange in solids
- Self-consistent mean field theory for the ferromagnetic Heisenberg model
- Spin wave excitations of a ferromagnet

# Two-particle wave functions

Two-particle wave functions: $\Psi(\xi_1, \xi_2)$, where $\xi \equiv \{\mathbf{r}, \sigma\}$ .

Indistinguishability requires that $|\Psi(\xi_1, \xi_2)|^2 = |\Psi(\xi_2, \xi_1)|^2$ .

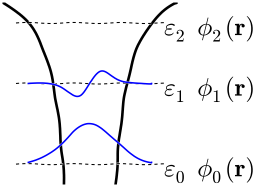
$$\Psi(\xi_1, \xi_2) = \Psi(\xi_2, \xi_1) \qquad \text{(bosons)}$$
$$\Psi(\xi_1, \xi_2) = -\Psi(\xi_2, \xi_1) \qquad \text{(fermions)}$$

Pauli repulsion: for two indistinguishable fermions

$$\Psi(\xi_1 = \xi, \xi_2 = \xi) = 0$$

Q: For non-interacting particles, how do we construct the two-body wave functions?

# Singlet and triplet wave functions, I




For spinless particles, the lowest energy state is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{\phi_0(\mathbf{r}_1)\phi_1(\mathbf{r}_2) - \phi_0(\mathbf{r}_2)\phi_1(\mathbf{r}_1)}{\sqrt{2}}$$

It's energy is $\varepsilon_0 + \varepsilon_1$

Spin-1/2 particle in a non-degenerate level: $\phi_0(\mathbf{r})|\uparrow\rangle$ and $\phi_0(\mathbf{r})|\downarrow\rangle$

Spin-singlet wave function

$$\Psi_S(\xi_1, \xi_2) = \phi_0(\mathbf{r}_1)\phi_0(\mathbf{r}_2)\frac{|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}$$

Its energy is $E_S = 2\varepsilon_0$, and total spin $= 0$.

| | | |
|---|---|---|
| For singlet wave functions: | coordinate part is | symmetric |
| | spin part is | antisymmetric |

# Singlet and triplet wave functions, II

Suppose the lowest single-particle energy level is doubly degenerate: $\phi_a(\mathbf{r})$ and $\phi_b(\mathbf{r})$ both have energy $\varepsilon_0$.

For two fermions, there are four degenerate wave functions:

$$\phi_a(\mathbf{r})|\uparrow\rangle\ , \phi_a(\mathbf{r})|\downarrow\rangle\ , \phi_b(\mathbf{r})|\uparrow\rangle\ , \phi_b(\mathbf{r})|\downarrow\rangle$$

$$\Phi(\mathbf{r}_1,\mathbf{r}_2) = \frac{\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)}{\sqrt{2}} = -\Phi(\mathbf{r}_2,\mathbf{r}_1)$$

Triplet wave functions: energy $= 2\varepsilon_0$, total spin $=1$.

$$\begin{aligned}
\Psi_T^{\Uparrow}(\xi_1,\xi_2) &= \Phi(\mathbf{r}_1,\mathbf{r}_2)|\uparrow_1\rangle|\uparrow_2\rangle \\
\Psi_T^{\Downarrow}(\xi_1,\xi_2) &= \Phi(\mathbf{r}_1,\mathbf{r}_2)|\downarrow_1\rangle|\downarrow_2\rangle \\
\Psi_T^{\otimes}(\xi_1,\xi_2) &= \Phi(\mathbf{r}_1,\mathbf{r}_2)\frac{|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle}{\sqrt{2}}
\end{aligned}$$

# Singlet and triplet wave functions, III

| | *singlet* | *triplet* |
|---|---|---|
| energy | $2\varepsilon_0$ | $2\varepsilon_0$ |
| total spin | 0 | 1 |
| coordinate part | symmetric | antisymmetric |
| spin part | antisymmetric | symmetric |
| | $\Phi(\mathbf{r}_1 = \mathbf{r}_2) \neq 0$ | $\Phi(\mathbf{r}_1 = \mathbf{r}_2) = 0$ |

For non-interacting particles, singlet and triplet states have the same energy. This changes once we take interactions into account:

$$\begin{aligned} \widehat{H} &= \frac{\widehat{\mathbf{p}}_1^2}{2m} + U(\mathbf{r}_1) && \text{yields } \varepsilon_0 \\ &+ \frac{\widehat{\mathbf{p}}_2^2}{2m} + U(\mathbf{r}_2) && \text{yields } \varepsilon_0 \\ &+ \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} |\Phi(\mathbf{r}_1, \mathbf{r}_2)|^2 && \text{favours triplets!} \end{aligned}$$

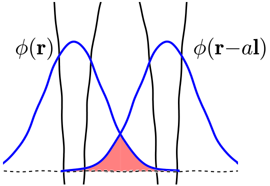
# Singlet and triplet states for electrons. Intra-atomic exchange

Exchange energy:

$$\begin{aligned} J_{\mathrm{ex}} &= E_S - E_T \\ &= \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \left[ |\Phi_S(\mathbf{r}_1, \mathbf{r}_2)|^2 - |\Phi_T(\mathbf{r}_1, \mathbf{r}_2)|^2 \right] \\ &= \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_1)\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_2) \end{aligned}$$

Intra-atomic exchange: $J_{\mathrm{ex}}^{\mathrm{intra}} \sim e^2/a_B \sim \mathrm{eV}$

Hund's rules: Electrons in incomplete atomic shells tend to maximize the total spin.
NB: This is why $d$- and $f$-shells of transitional elements and rare-earths carry large spins ($\Rightarrow$ large magnetic moments).




Neighbouring lattice sites, equal energy levels, $s$-shell electrons (for simplicity)

$$\phi_a(\mathbf{r}) \equiv \phi(\mathbf{r}) \qquad \phi_b(\mathbf{r}) \equiv \phi(\mathbf{r} - a\mathbf{l})$$

$$\begin{aligned} J_{\mathrm{ex}} &= E_S - E_T \\ &= \int \mathrm{d}\mathbf{r}_1 \mathrm{d}\mathbf{r}_2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \phi(\mathbf{r}_1)\phi(\mathbf{r}_1 - a\mathbf{l})\phi(\mathbf{r}_2)\phi(\mathbf{r}_2 - a\mathbf{l}) \\ &\sim \frac{e^2}{a_B} \Big[ \underbrace{\int \mathrm{d}\mathbf{r}\, \phi(\mathbf{r})\phi(\mathbf{r} - a\mathbf{l})}_{\text{overlap}} \Big]^2 \sim \frac{e^2}{a_B} e^{-a/a_B} \\ &\sim 1 - 100\,\mathrm{meV} \end{aligned}$$

and can have either sign

# Interatomic exchange in solids II

For two localized spins, exchange energy $E = -J_{\mathrm{ex}} \mathbf{s}_1 \cdot \mathbf{s}_2$

Indeed, $\widehat{\mathbf{S}} = \widehat{\mathbf{s}}_1 + \widehat{\mathbf{s}}_2 \quad \Rightarrow \quad \mathbf{S}^2 = \mathbf{s}_1^2 + \mathbf{s}_2^2 + 2\mathbf{s}_1 \cdot \mathbf{s}_2$, and $\mathbf{S}^2 = S(S+1)$.

$$\mathbf{s}_1 \cdot \mathbf{s}_2 = \frac{S(S+1) - s_1(s_1+1) - s_2(s_2+1)}{2}$$

For spins-$1/2$:

$$\text{singlet: } S = 0 \qquad \mathbf{s}_1 \cdot \mathbf{s}_2 = -\frac{3}{4}$$

$$\text{triplet: } S = 1 \qquad \mathbf{s}_1 \cdot \mathbf{s}_2 = \frac{1}{2}\left(1 \cdot 2 - \frac{3}{4} - \frac{3}{4}\right) = \frac{1}{4}$$

So that $E_S - E_T = J_{\mathrm{ex}}$

# Interatomic exchange in solids III: Heisenberg model

$$\widehat{H} = -J \sum_{i=1}^{N} \sum_{\alpha=1}^{z} \widehat{\mathbf{S}}_i \cdot \widehat{\mathbf{S}}_{i+\alpha}$$

Where

$\sum_i$ runs over the lattice sites

$\sum_\alpha$ runs over the nearest neighbours of site $i$

At low $T$-s:

$\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$

$J > 0$: ferromagnetic order

$\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$

$J < 0$: antiferromagnetic order

# Self-consistent mean-field approximation for the FM Heisenberg model I

$$\widehat{H} = -J \sum_{i\alpha} \widehat{\mathbf{S}}_i \widehat{\mathbf{S}}_{i+\alpha} - \mu \mathbf{B} \sum_i \widehat{\mathbf{S}}_i$$

*Assume* total magnetization $\mathbf{M} = \mu \left\langle \sum_i \widehat{\mathbf{S}}_i \right\rangle / N \equiv \mu \langle \mathbf{S} \rangle \neq 0$

$$\underbrace{\left(\widehat{\mathbf{S}}_i - \langle \mathbf{S} \rangle\right)\left(\widehat{\mathbf{S}}_j - \langle \mathbf{S} \rangle\right)}_{\text{“fluctuations”}} = \widehat{\mathbf{S}}_i \widehat{\mathbf{S}}_j - \left(\widehat{\mathbf{S}}_i + \widehat{\mathbf{S}}_j\right) \langle \mathbf{S} \rangle + \underbrace{\langle \mathbf{S} \rangle^2}_{\text{const}}$$

*MF approximation:* neglect the fluctuations $\Rightarrow$

$$\widehat{\mathbf{S}}_i \widehat{\mathbf{S}}_j \longrightarrow \left(\widehat{\mathbf{S}}_i + \widehat{\mathbf{S}}_j\right) \langle \mathbf{S} \rangle$$

$$\widehat{H} \longrightarrow \widehat{H}_{\mathrm{MF}}$$

# SC MFA for the FM Heisenberg model II

($z$ is the coordination number of the lattice.)

$$\widehat{H}_{\mathrm{MF}} = \underbrace{-J\sum_i z\langle\mathbf{S}\rangle\cdot\widehat{\mathbf{S}}_i}_{\text{molecular field: } \mu\mathbf{B}^{\mathrm{eff}} = zJ\langle\mathbf{S}\rangle} - \mu\mathbf{B}\sum_i\widehat{\mathbf{S}}_i = -\Big(zJ\langle\mathbf{S}\rangle + \mu\mathbf{B}\Big)\sum_i\widehat{\mathbf{S}}_i$$

*Self-consistency:* calculate $\langle\mathbf{S}\rangle$ using $\widehat{H}_{\mathrm{MF}}$ .

$\langle\ldots\rangle$ = QM expectation value + thermal average .

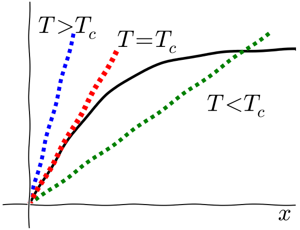
Recall lecture 3.

# SC MFA for the FM Heisenberg model III

Take $\mathbf{B} = 0$ — *spontaneous* magnetization is what we are after.
(For simplicity also take $S = 1/2$ .)

$$\langle S \rangle = \frac{1}{2} \tanh \frac{zJ}{2k_B T} \langle S \rangle$$

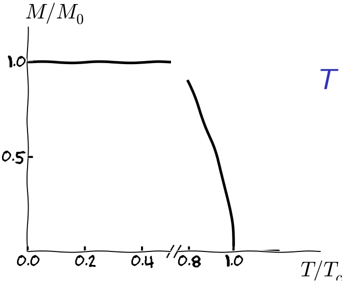
$$\text{define } x = \frac{zJ}{2k_B T} \langle S \rangle \quad \Rightarrow \quad \frac{4k_B T}{zJ} x = \tanh x$$




$$\tanh(x \ll 1) \approx x$$

$$\Rightarrow \frac{4k_B T_c}{zJ} = 1$$

# SC MFA for the FM Heisenberg model IV




$T \to T_c^-$ $\quad M(T) \propto (1 - T/T_c)^{1/2}$

second order phase transition

$T \to 0$

$$(M_0 - M)/M_0 \propto \exp\left(-2T_c/T\right)$$

Experimentally: $\Delta M/M_0 \approx AT^{3/2}$ as $T \to 0$ .

Ni: $A = (7.5 \pm 0.2) \times 10^{-6} K^{-3/2}$,
Fe: $A = (3.4 \pm 0.2) \times 10^{-6} K^{-3/2}$

The reason for this: Spin waves aka *magnons* (next step.)

## Spin wave excitations of a ferromagnet

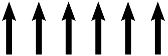
"In time of the first edition ... only a few physisists then believed in the reality of spin waves" (C Kittel)

(this was in 1953).

# Spin wave excitations of a ferromagnet

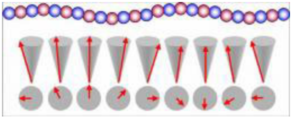
A semiclassical picture: $H = -2J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$

- Treat spins as classical angular momentum vectors of length $\hbar S$.
- One-dimensional chain with PBC



ground state

excitation



delocalized excitation has lower energy

In the ground state: $\mathbf{S}_p \cdot \mathbf{S}_{p+1} = S^2 \;\Rightarrow E_0 = -2NJS^2$
Flip a single spin: $E_1 = E_0 + 8JS^2$
Can offset some of (most of, in fact!) energy loss by delocalizing the excitation.

# Spin wave excitations of a ferromagnet

Look at the terms with the $j$-th spin: $-2J\mathbf{S}_j \cdot \underbrace{(\mathbf{S}_{j-1} + \mathbf{S}_{j+1})}_{\mathbf{B}_j^{\mathrm{eff}}}$ $\Rightarrow$ torque

Equations of motion: $\hbar \partial_t \mathbf{S}_j = 2J\mathbf{S}_j \times (\mathbf{S}_{j+1} + \mathbf{S}_{j-1})$

These equations are non-linear. Assuming small deviations from the ground state ($S_j^{x,y} \ll S$), *linearize* them: set $S_j^z = S$ and neglect terms containing $S^x S^y$ etc. Linearized equations of motion:

$$
\begin{aligned}
\hbar \partial_t S_j^x &= 2JS\left[2S_j^y - S_{j+1}^y - S_{j-1}^y\right] \\
\hbar \partial_t S_j^y &= -2JS\left[2S_j^x - S_{j+1}^x - S_{j-1}^x\right] \\
\partial_t S_j^z &= 0
\end{aligned}
$$

# Spin wave excitations of a ferromagnet

Look for travelling wave solutions:

$$S_j^x = A \exp\left[i(jka - \omega t)\right] \qquad S_j^y = B \exp\left[i(jka - \omega t)\right]$$

$$\begin{aligned} -i\hbar\omega A &= 4JS\left(1 - \cos ka\right) B \\ -i\hbar\omega B &= -4JS\left(1 - \cos ka\right) A \end{aligned}$$

The solution for $A$ and $B$ exists iff the determinant of the coefficients equals zero, which yields

$$\hbar\omega = 4JS\left(1 - \cos ka\right)$$

In the long wavelength limit $ka \ll 1$, $\cos ka \approx 1 - (ka)^2/2$, so that $\omega \propto k^2$

# Spin wave excitations of a ferromagnet

- In three dimensions, $\omega \propto k^2$ still.
- Quantum mechanical calculation gives precisely same results (see Kittel, *QTS*).

Quantized the spin waves: *magnons*, elementary excitations on top of the ferromagnetic background.

- For a mode $\mathbf{k}$ with $n_{\mathbf{k}}$ magnons, $\varepsilon_{\mathbf{k}} = \hbar\omega_{\mathbf{k}}(n_{\mathbf{k}} + 1)$.
- Excitation of a magnon $\Longleftrightarrow$ flipping of one spin.
- In a thermal equilibrium

$$n_{\mathbf{k}} = \frac{1}{\exp\left(\hbar\omega_{\mathbf{k}}/k_B T\right) - 1} \qquad \text{(Planck distribution)}$$

# Spin wave excitations of a ferromagnet

Recall that experimentally, $\Delta M/M_0 \propto T^{3/2}$ as $T \ll T_c$

Each magnon corresponds to flipping of one spin:

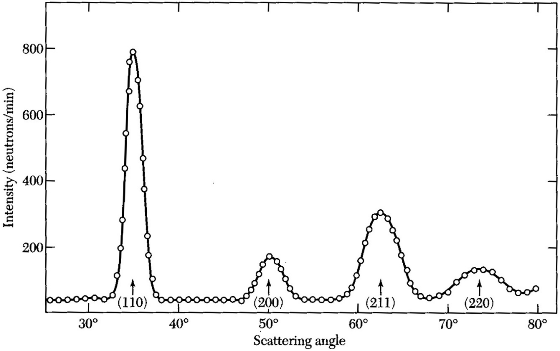
$$\Delta M \sim N_{\mathrm{magnons}} = \sum_{\mathbf{k}} n_{\mathbf{k}} = \int_0^\infty \mathrm{d}\omega\, \mathcal{D}(\omega) n_\omega$$

Recall $\mathcal{D}(\omega) \propto \omega^{1/2}$ in $d = 3$ and $\omega_{\mathbf{k}} \propto k^2$

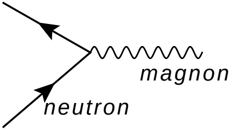
$$\begin{aligned}\Delta M &\propto \int_0^\infty \frac{\omega^{1/2}\,\mathrm{d}\omega}{\exp\left(\hbar\omega/k_B T\right) - 1} \qquad (x = \hbar\omega/k_B T)\\ &= T^{3/2} \int_0^\infty \frac{x^{1/2}\mathrm{d}x}{e^x - 1}\end{aligned}$$

# Neutron magnon scattering

Neutron scattering pattern for iron (taken from C Kittel's *ISSP*.)




$$\mathbf{q}_{\mathrm{magnon}} = \mathbf{p} - \mathbf{p}' - \mathbf{G}$$
$$\hbar\omega_{\mathbf{q}} = \mathbf{p}^2/2m - \mathbf{p}'^2/2m$$




Magnetic moment of a neutron interacts with magnetic moments in a crystal. $\Rightarrow$ diffraction of neutrons off a magnetic crystal tells us about distribution, magnitude and direction of magnetic moments.

# (THIS IS NOT A FERROMAGNET)