Exchange and ordering

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2011 School - Time-dependent phenomena in magnetism
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Part 2

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Outline

1. Spin waves
2. Frustration
3. Phase transitions
4. Magnetism and metals

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Outline

1. Spin waves
2. Frustration
3. Phase transitions
4. Magnetism and metals

3

$$\hat{\mathcal{H}} = A\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$$

Two spins

$\uparrow\uparrow$ ferromagnetic

$\downarrow\downarrow$ ferromagnetic

$\uparrow\downarrow$ antiferromagnetic

$\downarrow\uparrow$ antiferromagnetic

If $A > 0$, the antiferromagnetic state has lowest energy

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$$\frac{1}{2} + \frac{1}{2} = 0, 1$$

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$$\frac{1}{2} + \frac{1}{2} = 0, 1$$

$$D^{(\frac{1}{2})} \otimes D^{(\frac{1}{2})} = D^{(0)} \oplus D^{(1)}$$

2^2 = 1 + 3

singlet triplet

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$\hat{\mathcal{H}} = A\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$

Two spins

$\uparrow\uparrow$ ferromagnetic

$\downarrow\downarrow$ ferromagnetic

$\uparrow\downarrow$ antiferromagnetic

$\downarrow\uparrow$ antiferromagnetic

If $A > 0$, the antiferromagnetic state has lowest energy

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$\hat{\mathcal{H}} = A\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$ $\qquad \hat{\mathbf{S}}^{\text{tot}} = \hat{\mathbf{S}}^a + \hat{\mathbf{S}}^b$

$$\Longrightarrow (\hat{\mathbf{S}}^{\text{tot}})^2 = (\hat{\mathbf{S}}^a)^2 + (\hat{\mathbf{S}}^b)^2 + 2\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$$

$$\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b = \begin{cases} \frac{1}{4} & \text{if} \quad s = 1 \\ -\frac{3}{4} & \text{if} \quad s = 0. \end{cases}$$

	Eigenstate	m_s	s	$\hat{\mathbf{S}}^a \cdot \hat{\mathbf{S}}^b$
Triplet: $E = A/4$	$\lvert\uparrow\uparrow\rangle$	1	1	$\frac{1}{4}$
	$\frac{\lvert\uparrow\downarrow\rangle + \lvert\downarrow\uparrow\rangle}{\sqrt{2}}$	0	1	$\frac{1}{4}$
	$\lvert\downarrow\downarrow\rangle$	−1	1	$\frac{1}{4}$
Singlet: $E = -3A/4$	$\frac{\lvert\uparrow\downarrow\rangle - \lvert\downarrow\uparrow\rangle}{\sqrt{2}}$	0	0	$-\frac{3}{4}$

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Spin waves

$$\mathcal{H} = -2\mathcal{J}\sum_i \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}$$

(Heisenberg ferromagnet J>0)

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Spin waves

$$\mathcal{H} = -2\mathcal{J}\sum_i \left[\hat{S}_i^x \hat{S}_{i+1}^x + \hat{S}_i^y \hat{S}_{i+1}^y + \hat{S}_i^z \hat{S}_{i+1}^z\right]$$

(Heisenberg ferromagnet J>0)

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Spin waves

$$\hat{\mathcal{H}} = -2\mathcal{J}\sum_i \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)\right]$$

(Heisenberg ferromagnet J>0)

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Spin waves

$$\hat{\mathcal{H}} = -2\mathcal{J}\sum_i \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)\right]$$

Ground state $|\Phi\rangle$ $\quad \uparrow$

(Heisenberg ferromagnet J>0)

$$\hat{\mathcal{H}}|\Phi\rangle = -2NS^2\mathcal{J}|\Phi\rangle$$

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Spin waves

$$\hat{\mathcal{H}} = -2\mathcal{J}\sum_i \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)\right]$$

Flipped spin $|j\rangle$ ↑↑↑↑↑↑↑↓↑↑↑↑↑↑↑↑↑↑↑↑

$$|j\rangle = \hat{S}_j^- |\Phi\rangle$$

$$\hat{\mathcal{H}}|j\rangle = 2\left[(-NS^2\mathcal{J} + 2S\mathcal{J})|j\rangle - S\mathcal{J}|j+1\rangle - S\mathcal{J}|j-1\rangle\right]$$

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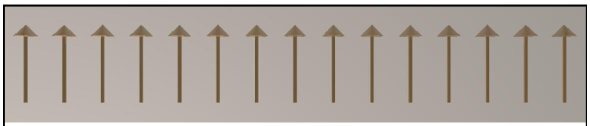

- Start with a ferromagnetic chain of spins

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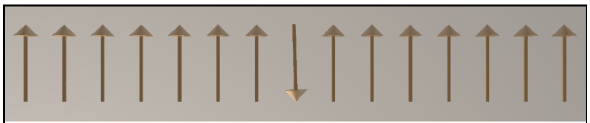

- Start with a ferromagnetic chain of spins
- Then reverse one spin

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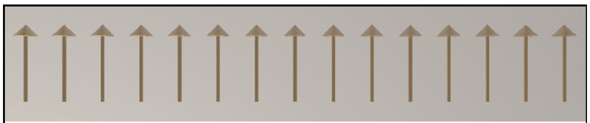
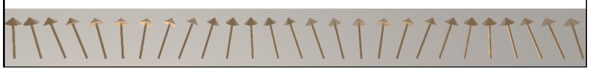


- Start with a ferromagnetic chain of spins
- Then reverse one spin
- The spins are exchange coupled and so the excitation becomes quickly delocalised on a time scale which scales with ħ/J



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Spin waves

$$\hat{\mathcal{H}} = -2\mathcal{J}\sum_i \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)\right]$$

Flipped spin $|j\rangle$ ↑↑↑↑↑↑↑↓↑↑↑↑↑↑↑↑↑↑↑↑

$$|j\rangle = \hat{S}_j^- |\Phi\rangle$$

$$\hat{\mathcal{H}}|j\rangle = 2\left[(-NS^2\mathcal{J} + 2S\mathcal{J})|j\rangle - S\mathcal{J}|j+1\rangle - S\mathcal{J}|j-1\rangle\right]$$

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Spin waves

$$\hat{\mathcal{H}} = -2\mathcal{J}\sum_i \left[\hat{S}_i^z \hat{S}_{i+1}^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+)\right]$$

Flipped spin $|j\rangle$ ↑↑↑↑↑↑↑↓↑↑↑↑↑↑↑↑↑↑↑↑

$$|j\rangle = \hat{S}_j^- |\Phi\rangle$$

$$\hat{\mathcal{H}}|j\rangle = 2\left[(-NS^2\mathcal{J} + 2S\mathcal{J})|j\rangle - S\mathcal{J}|j+1\rangle - S\mathcal{J}|j-1\rangle\right]$$

q-state $|q\rangle$ ↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑↑

smeared out single flipped spin

$$|q\rangle = \frac{1}{\sqrt{N}}\sum_j e^{iqR_j}|j\rangle$$

$$\hat{\mathcal{H}}|q\rangle = E(q)|q\rangle$$

$$E(q) = -2NS^2\mathcal{J} + 4\mathcal{J}S(1 - \cos qa)$$

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Number of thermally excited spin waves:

$$n_{\text{magnon}} = \int_0^\infty \frac{g(\omega)\,\mathrm{d}\omega}{\mathrm{e}^{\hbar\omega/k_\mathrm{B}T} - 1}$$

In three dimensions: $g(\omega) \propto \omega^{1/2}$

$$n_{\text{magnon}} \propto T^{3/2}$$

In one or two dimensions, the integral diverges.
Magnetism not stable in Heisenberg model in 1D or 2D
(Mermin-Wagner-Berenzinskii theorem,
due to also to Coleman)

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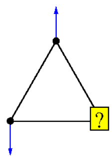
Triangle of spins



AF interactions for n.n.

Magnetic frustration

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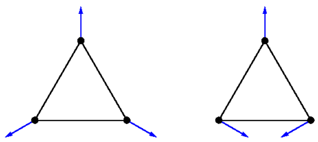
Triangle of spins

Classical Heisenberg spins
120° state



Two different chiralities

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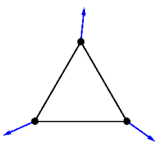
Triangle of spins

Classical Heisenberg spins
120° state



Two different chiralities

...and rotational symmetry

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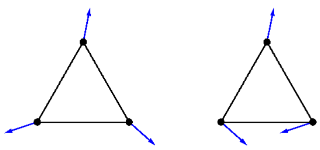
Triangle of spins

Classical Heisenberg spins
120° state



Two different chiralities

...and rotational symmetry

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$$\frac{1}{2}+\frac{1}{2}=0,1$$

$$\frac{1}{2}+\frac{1}{2}+\frac{1}{2}=\frac{1}{2},\frac{1}{2},\frac{3}{2}$$

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$$\frac{1}{2}+\frac{1}{2}=0,1$$

$$D^{(\frac{1}{2})}\otimes D^{(\frac{1}{2})}=D^{(0)}\oplus D^{(1)}$$

2^2 = 1 + 3

$$\frac{1}{2}+\frac{1}{2}+\frac{1}{2}=\frac{1}{2},\frac{1}{2},\frac{3}{2}$$

$$D^{(\frac{1}{2})}\otimes D^{(\frac{1}{2})}\otimes D^{(\frac{1}{2})}=2D^{(\frac{1}{2})}\oplus D^{(\frac{3}{2})}$$

2^3 = 2 + 2 + 4

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Triangle of spins

$$\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=\frac{1}{2}\left(S_{\rm tot}(S_{\rm tot}+1)-3s(s+1)\right)$$

$$S_{\rm tot}=\frac{3}{2}\implies\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=+\frac{3}{4}$$ quartet

$$S_{\rm tot}=\frac{1}{2}\implies\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=-\frac{3}{4}$$ 2 doublets

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Triangle of spins

$$|\Psi_{M=3/2}\rangle=|\uparrow\uparrow\uparrow\rangle$$

$$|\Psi^{(k)}_{M=1/2}\rangle=\frac{1}{\sqrt{3}}\sum_{j=0}^{2}e^{2\pi ijk/3}C_3^j|\downarrow\uparrow\uparrow\rangle$$

$$|\Psi^{(k)}_{M=-1/2}\rangle=\frac{1}{\sqrt{3}}\sum_{j=0}^{2}e^{2\pi ijk/3}C_3^j|\uparrow\downarrow\downarrow\rangle$$

$$|\Psi_{M=-3/2}\rangle=|\downarrow\downarrow\downarrow\rangle$$

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Triangle of spins

$$|\Psi_{M=3/2}\rangle=|\uparrow\uparrow\uparrow\rangle$$ $S=\frac{3}{2}$ $C_z|\Psi_{M=3/2}\rangle=0$

$$|\Psi^{(k)}_{M=1/2}\rangle=\frac{1}{\sqrt{3}}\sum_{j=0}^{2}e^{2\pi ijk/3}C_3^j|\downarrow\uparrow\uparrow\rangle$$

$k=0$ $S=\frac{3}{2}$ $C_z|\Psi^{(0)}_{M=1/2}\rangle=0$

$k=1$ $S=\frac{1}{2}$ $C_z|\Psi^{(1)}_{M=1/2}\rangle=|\Psi^{(1)}_{M=1/2}\rangle$

$k=2$ $C_z|\Psi^{(2)}_{M=1/2}\rangle=-|\Psi^{(2)}_{M=1/2}\rangle$

Chirality $$C_z=\frac{1}{4\sqrt{3}}\mathbf{S}_1\cdot(\mathbf{S}_2\times\mathbf{S}_3)$$

see M. Trif et al. PRB **82**, 045429 (2010)

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Tetrahedron of spins

$$D^{(1/2)}\otimes D^{(1/2)}\otimes D^{(1/2)}\otimes D^{(1/2)}=2D^{(0)}\oplus 3D^{(1)}\oplus D^{(2)}$$

$$\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=\frac{1}{2}\left(S_{\rm tot}(S_{\rm tot}+1)-4s(s+1)\right)$$

$$S_{\rm tot}=2\implies\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=+\frac{3}{2}$$ pentet

$$S_{\rm tot}=1\implies\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=-\frac{1}{2}$$ 3 triplets

$$S_{\rm tot}=0\implies\sum_{\langle i,j\rangle}\hat{\mathbf{S}}_i\cdot\hat{\mathbf{S}}_j=-\frac{3}{2}$$ 2 singlets

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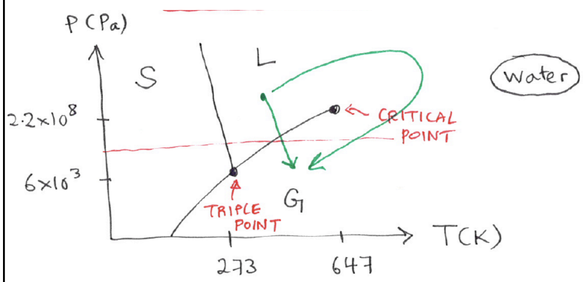
Phase transitions and magnetism



- Liquid-gas phase transition – can avoid the phase transition. Not so for liquid-solid.

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- Simplest model to illustrate symmetry breaking comes from Landau theory.
- Guess a form for the Helmholtz function (per m^3):

$$F(M) = F_0 + a(T)M^2 + bM^4 + \cdots$$

- Can exclude odd powers because of the symmetry:

$$F(M) = F(-M)$$

- Choose the constants such that

$$a(T) = a_0(T - T_C)$$
$$b > 0$$

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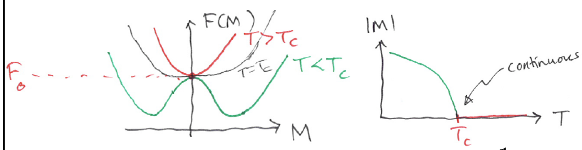
- Find the minimum by differentiating:

$$\partial F/\partial M = 0$$
$$2M[a_0(T - T_C) + 2bM^2] = 0$$
$$M = 0 \text{ or } M = \pm\left(\frac{a_0}{2b}(T_C - T)\right)^{1/2}$$



$$T < T_C, \quad M \propto (T_C - T)^\beta \quad \beta = \frac{1}{2}$$

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- Now add a magnetic field

$$F(M,H) = F(M) - \mu_0 MH$$

- Set μ_0=1 for ease of notation. Differentiating gives:

$$\frac{\partial F(M,H)}{\partial M} = \frac{\partial F(M)}{\partial M} - H$$
$$\frac{\partial F(M)}{\partial M} = H$$
$$\frac{\partial H}{\partial M} = \frac{\partial^2 F(M)}{\partial M^2}$$
$$\chi = \frac{\partial M}{\partial H} = \left(\frac{\partial^2 F(M)}{\partial M^2}\right)^{-1}$$

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$$2M[a_0(T - T_C + 2bM^2] = H$$
$$\text{At } T_C,\ M^3 \propto H \implies M \propto H^{1/3}$$
$$T = T_C, \qquad M \propto H^{1/\delta}, \qquad \delta = 3$$

$$2a_0(T - T_C) + 6bM^2 = \frac{\partial H}{\partial M} = \chi^{-1}$$
$$\chi = \begin{cases} \frac{1}{2a_0(T - T_C)} & T > T_C \\ \frac{1}{4a_0(T_C - T)} & T < T_C \end{cases}$$
$$\chi \propto |T - T_C|^{-\gamma}, \quad \gamma = 1$$

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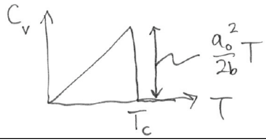
- Effect on Helmholtz function:

$$F = \begin{cases} F_0 & T > T_C \\ F_0 - \frac{a^2}{4b} & T < T_C \end{cases}$$

- Heat capacity:

$$C_V = -T\frac{d^2F}{dT^2} = \begin{cases} 0 & T > T_C \\ -\frac{a_0^2 T}{2b} & T < T_C \end{cases}$$



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- If M varies in space, have to generalize:

$$F_{tot} = \int d^dx\,\left[F(M) + \tfrac{1}{2}c\,[\nabla M(x)]^2\right]$$

$$\chi^{-1}_{ij} = \frac{\delta^2 F_{tot}}{\delta M_i(x)\,\delta M_j(x')}$$

$$= (2a + 4bM^2 - c\nabla^2)\,\delta(x-x')$$

$$\chi(q) = \frac{1}{2a + 4bM^2 + cq^2} \propto \frac{1}{1+q^2\xi^2}$$

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- Hence the correlation length behaves as follows:

$$\xi = \sqrt{\frac{c}{2a+4bM^2}} = \begin{cases} (\frac{c}{2a})^{1/2} & T > T_C \\ (\frac{c}{-4a})^{1/2} & T < T_C \end{cases}$$

$$\xi \propto |T - T_C|^{-\nu}, \quad \nu = \frac{1}{2}$$

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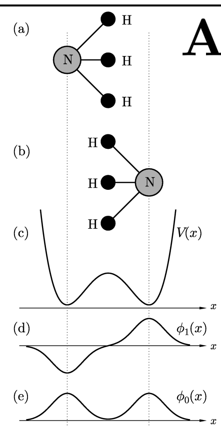
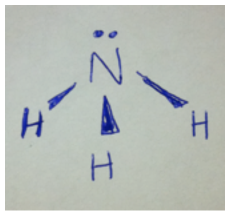
Ammonia NH_3





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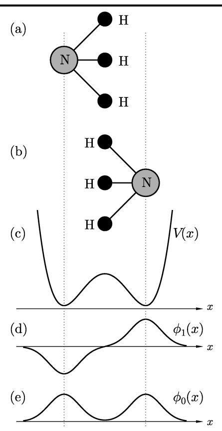

$$|\text{Left}\rangle = \frac{\phi_0 - \phi_1}{\sqrt{2}}$$

$$|\text{Right}\rangle = \frac{\phi_0 + \phi_1}{\sqrt{2}}$$

$$\frac{E_1 - E_0}{h} = 24\,\text{GHz}$$

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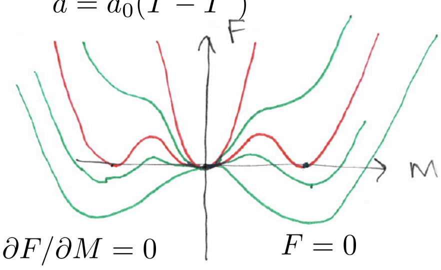
- First-order phase transition – extend the Landau model to a sixth order term

$$F = F_0 + aM^2 + bM^4 + cM^6$$

$$c > 0$$

$$a = a_0(T - T^*)$$



$\partial F/\partial M = 0$ $\quad F = 0$

solve simultaneously

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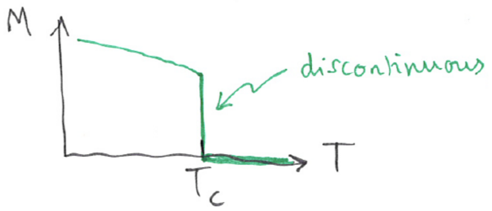
$$M^2 = -2a/b$$
$$a = a_0(T - T^*) = b^2/4c$$



$$a = a_0(T - T^*) = \begin{cases} 0 & b > 0 \\ b^2/4c & b < 0 \end{cases}$$

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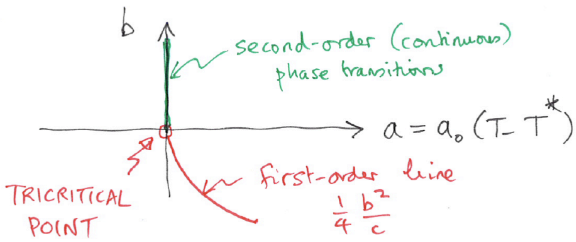
- Generalized model has a *tricritical point*



$$a = a_0(T - T^*) = \begin{cases} 0 & b > 0 \\ b^2/4c & b < 0 \end{cases}$$

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Magnetism and metals

a) Some revision

$$g(k)\,dk = \frac{2 \times 4\pi k^2\,dk}{(2\pi)^3} \quad \text{(2: spin)}$$

$$n = \frac{N}{V} = \int_0^{k_F} g(k)\,dk = \frac{k_F^3}{3\pi^2}$$

$$\Rightarrow k_F^3 = 3\pi^2 n \qquad E_F = \frac{\hbar^2 k_F^2}{2m}$$

$$n \propto E_F^{3/2}$$

$$\frac{dn}{n} = \frac{3}{2}\frac{dE_F}{E_F} \qquad g(E_F) = \frac{dn}{dE}\Big)_{E_F} = \frac{3}{2}\frac{n}{E_F}$$

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b) Pauli paramagnetism

$$n_\pm = \frac{1}{2}\int_0^\infty g(E \pm \mu_B B)\, f(E)\, dE, \qquad f(E) = \frac{1}{e^{\beta(E-\mu)}+1}$$

$\updownarrow 2\mu_B B$

$$n_\pm \simeq \frac{1}{2}\int_0^\infty \left[g(E) \pm \mu_B B \frac{\partial g}{\partial E} \right] f(E)\, dE$$

$$M = \mu_B (n_+ - n_-)$$

$$\simeq \mu_B^2 B \int_0^\infty \frac{dg}{dE} f(E)\, dE$$

$$\left[g(E) f(E)\right]_0^\infty - \int_0^\infty \frac{df}{dE} g(E)\, dE$$

$$\left[g(E) f(E)\right]_0^\infty = 0 \quad \because g(0) = f(\infty) = 0$$

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$$M = \mu_B^2 B \int_0^\infty \left(-\frac{\partial f}{\partial E}\right) g(E)\, dE$$

$$n = \int_0^\infty f(E)\, g(E)\, dE$$

Two cases

(i) degenerate limit $(T=0)$

$$-\frac{df}{dE} = \delta(E - E_F)$$

$$M = \mu_B^2 B\, g(E_F)$$

$$\therefore \chi = \frac{\mu_0 M}{B} = \mu_0 \mu_B^2\, g(E_F) \quad \text{(T-independent)}$$

using $g(E_F) = \frac{3}{2}\frac{n}{E_F}$ $\therefore$ $\chi = \dfrac{n\mu_0\mu_B^2}{\frac{2}{3} k_B T_F}$

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(ii) non-degenerate limit

$$f(E) \simeq e^{-(E-\mu)/k_BT}$$

$$-\frac{df}{dE} = \frac{f}{k_BT}$$

$$M = \frac{\mu_B^2 B}{k_BT}\underbrace{\int_0^\infty f(E)\,g(E)\,dE}_{n} = \frac{n\mu_B^2 B}{k_BT}$$

$$\chi = \frac{\mu_0 M}{B} = \frac{n\mu_0\mu_B^2}{k_BT} \qquad \text{Curie-like} \propto 1/T$$

Can show that for Pauli sus.

$$\chi(T) = \frac{n\mu_0\mu_B^2}{\frac{2}{3}k_BT_F}\left(1 - \frac{\pi^2}{12}\left(\frac{T}{T_F}\right)^2 + \dots\right)$$

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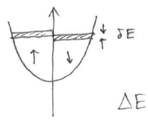
c Spontaneous FM in absence of B?



flip $\frac{1}{2}g(E_F)\,\delta E$ electrons increasing their energy by δE

$$\Delta E_{KE} = \frac{1}{2}g(E_F)(\delta E)^2 \quad ①$$

$$n_\pm = \frac{1}{2}(n \pm g(E_F)\,\delta E)$$

$$n_+ - n_- = g(E_F)\,\delta E$$

$$\Delta E_{PE} = -\frac{1}{2}U(n_+ - n_-)^2 = -\frac{1}{2}U(g(E_F)\,\delta E)^2 \quad ②$$

$$\Delta E = ① + ② - MB = \frac{1}{2}g(E_F)(\delta E)^2\left[1 - Ug(E_F)\right] - MB$$

$\mu_B g(E_F)\,\delta E$

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$$\Delta E = \frac{M^2}{2\mu_B^2 g(E_F)}\left[1 - Ug(E_F)\right] - MB$$

minimized when $\frac{M}{\mu_B^2 g(E_F)}\left[1 - Ug(E_F)\right] - B = 0$

$$\Rightarrow \chi = \frac{\mu_0 M}{B} = \frac{\chi_P}{1 - Ug(E_F)}$$

χ_P ← Pauli sus. $\mu_0\mu_B^2 g(E_F)$

$Ug(E_F) > 1$ Stoner criterion

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d Response of electron gas to $H(r) = H_q \cos q\cdot r$

$$e^{ik\cdot r} \to e^{ik\cdot r}\left[1 \pm \frac{g\mu_0\mu_B H_q}{4} \times \left(\frac{e^{iq\cdot r}}{E_{k+q} - E_k} + \frac{e^{-iq\cdot r}}{E_{k-q} - E_k}\right)\right]$$

$$M(r) = M_q \cos q\cdot r$$

$$M_q = \chi_q H_q$$

where $\chi_q = \chi_P\, f\left(\frac{q}{2k_F}\right)$

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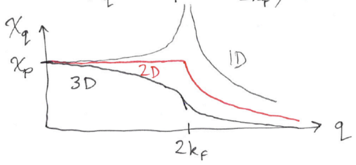
$$M_q = \chi_q H_q$$

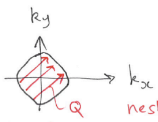
where $\chi_q = \chi_P\, f\left(\frac{q}{2k_F}\right)$



Add interactions

$$\chi_q \to \frac{\chi_q^0}{1 - \tilde{U}\chi_q^0}$$

← no interactions; ↑ dimensionless interaction



nesting instability → SDW

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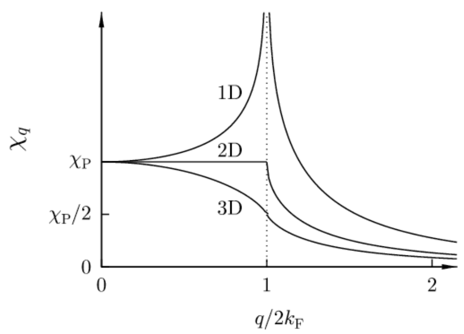
1D electron gas unstable to SDW formation



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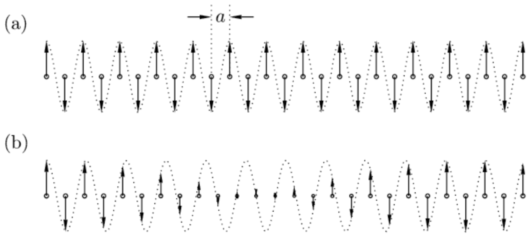
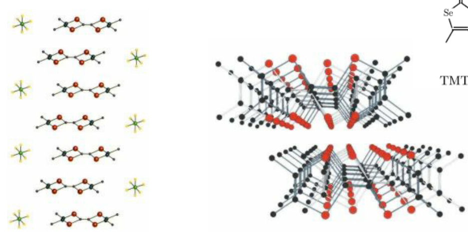
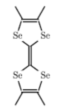
Spin-density wave



TMTSF salts

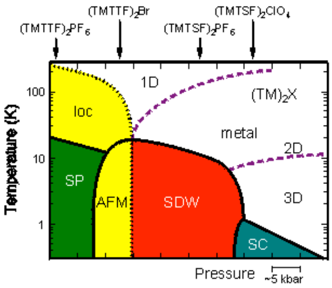




Stacks of TMTSF molecules ⇒ 1D chains

TMTSF salts

Very rich
phase diagram



e~ Real-space effects

$$\chi(r) = \frac{1}{(2\pi)^3}\int d^3q\, \chi_q\, e^{iq\cdot r}$$

$$= \frac{2k_F^3\chi_P}{\pi} F(2k_F r)$$

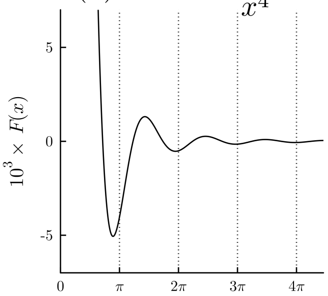
$$F(x) = -\frac{x\cos x + \sin x}{x^4}$$

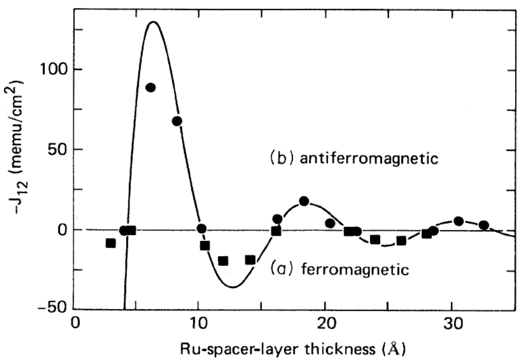
$$\sim \frac{\cos 2k_F r}{r^3}$$

RKKY coupling

$$\chi(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{q}\,\chi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{2k_F\chi_P}{\pi}F(2k_F r)$$

$$F(x) = \frac{-x\cos x + \sin x}{x^4}$$

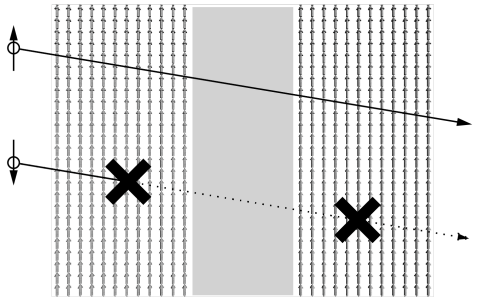




S. S. P. Parkin and D. Mauri, Phys. Rev. B **44,** 7131 (1991)

GMR = giant magnetoresistance

(a)



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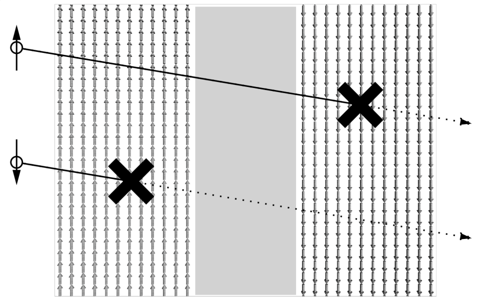
GMR = giant magnetoresistance

(b)



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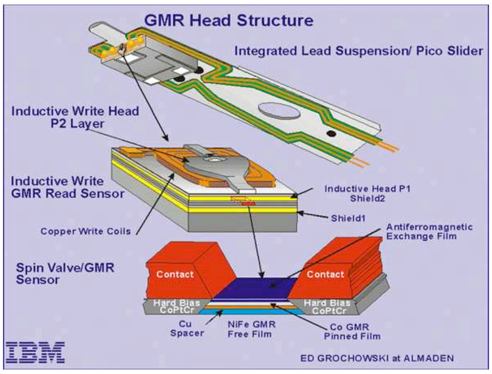

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