Phys 726 – lecture 9

Origin of magnetism

* In the classical picture, magnetism is characterized by a conventional vector in real space (or possibly a vector field over a sample)

→ e.g. a local moment $\vec{\mu} = (\mu_x, \mu_y, \mu_z)$ orders with respect to other moments because of a direct magnetic coupling

$$E \sim -J \vec{\mu}_1 \cdot \vec{\mu}_2$$

(here $J>0$ favours ferromagnetic alignment

→ e.g. a ~~dipl~~ dipole $\vec{d}_1$ interacting with another dipole $\vec{d}_2$ separated by $\vec{r} = r\hat{r}$

$$E \sim \frac{\vec{d}_1 \cdot \vec{d}_2 - (\hat{r}\cdot\vec{d}_1)(\hat{r}\cdot\vec{d}_2)}{r^3}$$

* At the microscopic level, we can justify magnetism without resorting to any direct interaction between the electron spins

$$\rightarrow \hat{H} = \sum_{\alpha} \int d^3r \, \hat{\psi}^{\dagger}_{\alpha}(\vec{r}) \, T \, \hat{\psi}_{\alpha}(\vec{r})$$

$$+ \frac{1}{2} \sum_{\alpha\beta} \int d^3r \int d^3r' \, \hat{\psi}^{\dagger}_{\alpha}(\vec{r}) \hat{\psi}^{\dagger}_{\beta}(\vec{r}') V(\vec{r},\vec{r}') \hat{\psi}_{\beta}(\vec{r}') \hat{\psi}_{\alpha}(\vec{r})$$

kinetic energy T and interaction coupling V are typically independent of spin (i.e. they don't carry indices α, β ranging over $\uparrow$ and $\downarrow$)

$\rightarrow$ the necessary ingredients are

(i) Pauli exclusion (true for all fermions)

(ii) particle-particle repulsion (e.g. Coulomb repulsion of particles carrying like charge)

* Consider particles subject to a contact potential $g\delta(\vec{r}-\vec{r}')$

→ for spinless fermions

$$\hat{\psi}^\dagger(\vec{r})\hat{\psi}^\dagger(\vec{r}')|vac\rangle \to 0 \quad \text{as } \vec{r}\to\vec{r}'$$

since $(\hat{\psi}^\dagger(\vec{r}))^2=0$; hence, these particles can ~~we~~ never feel a short-range repulsion

→ for spinful fermions, there's now an additional quantum number, and the states

$$\hat{\psi}_\uparrow(\vec{r})^\dagger \hat{\psi}_\uparrow(\vec{r}')^\dagger |vac\rangle$$

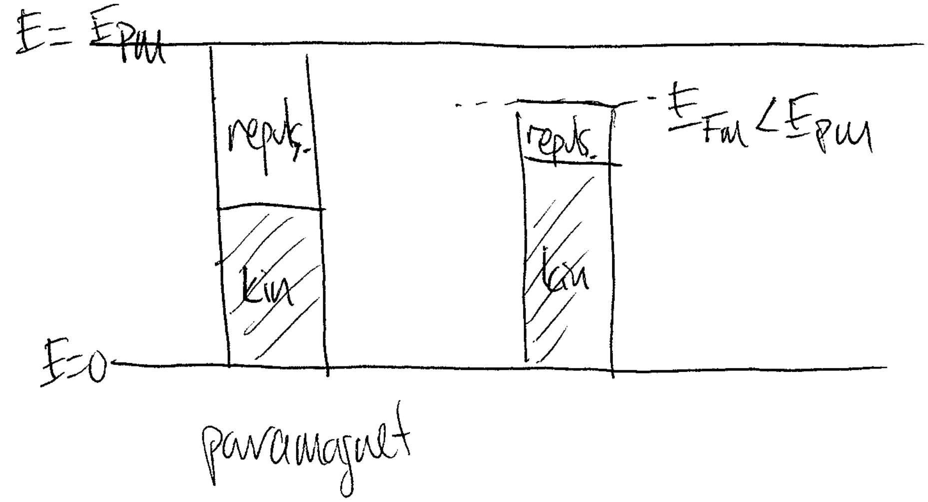
and $\hat{\psi}_\downarrow(\vec{r})^\dagger \hat{\psi}_\downarrow(\vec{r}')^\dagger |vac\rangle$

are lower in energy (by an amount $\sim g$) than

$$\hat{\psi}_\uparrow^\dagger(\vec{r})\hat{\psi}_\downarrow^\dagger(\vec{r}')|vac\rangle$$

→ gives us a path to itinerant ferromagnetism

* Ferromagnetic alignment will raise the ~~...~~ kinetic energy but may lower the overall energy if the repulsive contribution decreases enough:



<u>EXAMPLE</u>: Spin-S fermions (generalization of spin $S=1/2$ electrons) subject to a contact potential.

→ $\hat{\psi}^{\dagger}_{\alpha}(\vec{r}) = \sum_{k} \phi^{*}_{k}(\vec{r})\, c^{\dagger}_{k\alpha}$ creates a particle

with spin projection $\alpha = -S, \ldots, S$

→ In a paramagnet, the $(2S+1)$ values are all equally likely

$$\hat{H} = \sum_\alpha \int d^3r\, \hat{\psi}^\dagger_\alpha(\vec{r}) T \hat{\psi}(r) + \frac{1}{2} \sum_{\alpha\beta} \int d^3r\, d^3r'\, \hat{\psi}^\dagger_\alpha(\vec{r})\, \hat{\psi}^\dagger_\beta(\vec{r}')$$

$$\times\, g\,\delta(\vec{r}-\vec{r}')\, \hat{\psi}_\beta(\vec{r}')\, \hat{\psi}_\alpha(\vec{r})$$

$$= \sum_\alpha \int d^3r\, \hat{\psi}^\dagger T \psi + \frac{1}{2} \sum_{\alpha\beta} \int d^3r\, \hat{\psi}^\dagger_\alpha(\vec{r})\, \psi^\dagger_\beta(\vec{r})\, g\, \hat{\psi}_\beta(\vec{r})\, \hat{\psi}_\alpha(\vec{r})$$

$$\frac{1}{2} \sum_{\alpha\beta} (1-\delta_{\alpha\beta}) = \frac{1}{2} \sum_{\alpha \neq \beta} = \sum_{\alpha < \beta}$$

$\alpha = \beta$ term forbidden since $\psi^\dagger_\alpha(\vec{r})\, \hat{\psi}^\dagger_\alpha(\vec{r}) = 0$

$$= \sum_\alpha \int d^3r\, \hat{\psi}^\dagger T \psi + g \sum_{\alpha<\beta} \int d^3r\, \hat{\psi}^\dagger_\alpha\, \hat{\psi}^\dagger_\beta\, \hat{\psi}_\beta\, \hat{\psi}_\alpha$$

→ If the particles are mutually interacting but otherwise free, then $T = -\frac{\hbar^2}{2m} \vec{\nabla}^2$ and $\phi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$ is a plane wave state

The kinetic term is

$$\sum_\alpha \int d^3r \left(\sum_k \frac{1}{\sqrt{V}} e^{-i\vec{k}\cdot\vec{r}} c_{k\alpha}^\dagger\right)\left(\frac{-\hbar^2\nabla^2}{2m}\right)\left(\sum_{k'} \frac{1}{\sqrt{V}} e^{+i\vec{k}'\cdot\vec{r}} c_{k'\alpha}\right)$$

$$= \sum_\alpha \sum_{kk'} \underbrace{\frac{1}{V}\int d^3r\, e^{i(\vec{k}'-\vec{k})\cdot\vec{r}}}_{\delta_{kk'}} \frac{\hbar^2 k^2}{2m} c_{k\alpha}^\dagger c_{k'\alpha}$$

$$= \sum_\alpha \sum_k \frac{\hbar^2 k^2}{2m} c_{k\alpha}^\dagger c_{k\alpha}$$

Its ground state is a Fermi sea with $2S+1$ fermions per $\vec{k}$ state filled up to the wavevector k_F that accommodates N particles

$$N = \sum_\alpha \sum_k \theta(k_F - k) = (2S+1)V \int \frac{d^3k}{(2\pi)^3} \theta(k_F - k)$$

$$= \frac{(2S+1)}{8\pi^3} V \cdot \int_0^{k_F} 4\pi k^2 dk = \frac{(2S+1)V}{2\pi^2} \cdot \frac{1}{3} k_F^3$$

i.e. $$k_F = \left(\frac{6\pi^2 N}{(2S+1)V}\right)^{1/3} = \left(\frac{6\pi^2}{(2S+1)} n\right)^{1/3}$$

$$E_0 = \sum_\alpha \sum_k \frac{\hbar^2 k^2}{2m}\theta(k_F-k) = \frac{(2S+1)}{8\pi^3}\frac{\hbar^2}{2m} V\int_0^{k_F} 4\pi k^2 dk \cdot k^2$$

$$= \frac{(2S+1)}{2\pi^2}\frac{\hbar^2}{2m}\cdot V\cdot \frac{1}{5}k_F^5$$

$$= (2S+1)\frac{\hbar^2}{4\pi^2 m} V\cdot\frac{1}{5}\left(\frac{6\pi^2}{(2S+1)}\frac{N}{V}\right)^{5/3}$$

$$= \cancel{(2S+1)}\cdot\frac{\hbar^2}{20\pi^2 m}\cancel{V}\,(6\pi^2)^{5/3}\cdot\left(\frac{N}{V}\right)^{2/3}\cdot\frac{N}{\cancel{V}}\cdot\frac{1}{\cancel{(2S+1)}}\cdot\frac{1}{(2S+1)^{2/3}}$$

$$= N\cdot\frac{\hbar^2}{20\pi^2 m}\frac{(6\pi^2)^{5/3}}{(2S+1)^{2/3}}\cdot n^{2/3}$$

$$= N\cdot\frac{\hbar^2\cdot 6\pi^2}{20\pi^2 m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3}$$

$$= N\cdot\frac{3\hbar^2}{10m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3}$$

Energy per particle

$$\frac{E_0}{N} = \frac{3\hbar^2}{10m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3}$$

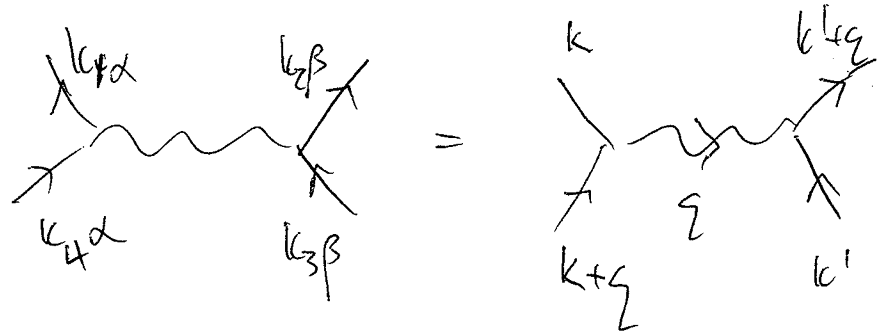
The interaction term is

$$g \sum_{\alpha<\beta} \int d^3r\, \psi^\dagger_\alpha(\vec{r})\, \psi^\dagger_\beta(\vec{r})\, \psi_\beta(\vec{r})\, \psi_\alpha(\vec{r})$$

$$= g \sum_{\alpha<\beta} \int d^3r \left(\frac{1}{\sqrt{V}} \sum_{k_1} e^{-i\vec{k}_1\cdot\vec{r}} c^\dagger_{k_1\alpha}\right)\left(\frac{1}{\sqrt{V}} \sum_{k_2} e^{-i\vec{k}_2\cdot\vec{r}} c^\dagger_{k_2\beta}\right)$$

$$\cdot \left(\frac{1}{\sqrt{V}} \sum_{k_3} e^{+i\vec{k}_3\cdot r} c_{k_3\beta}\right)\left(\frac{1}{\sqrt{V}} \sum_{k_4} e^{+i\vec{k}_4\cdot\vec{r}} c_{k_4\alpha}\right)$$

$$= \frac{g}{V} \sum_{\alpha<\beta} \sum_{k_1 \cdots k_4} \underbrace{\frac{1}{V} \int d^3r\, e^{i(k_3+k_4-k_1-k_2)\cdot\vec{r}}}_{\delta_{k_1+k_2,\, k_3+k_4}} c^\dagger_{k_1\alpha} c^\dagger_{k_2\beta} c_{k_3\beta} c_{k_4\alpha}$$



$$= \frac{g}{V} \sum_{\alpha<\beta} \sum_{kk'q} c^\dagger_{k\alpha} c^\dagger_{k'+q\,\beta} c_{k'\beta} c_{k+q\,\alpha}$$

Evaluate as a perturbation around the noninteracting ground state

$$\Delta E = \frac{g}{V}\sum_{\alpha<\beta}\sum_{kk'q} \langle F| c^\dagger_{k\alpha} c^\dagger_{k'+q,\beta} c_{k'\beta} c_{k+q,\alpha} |F\rangle$$

$$= \frac{g}{V}\sum_{\alpha<\beta}\sum_{kk'q} \Big(\delta_{q,0}\, \theta(k_F-k)\,\theta(k_F-k') - \delta_{kk'}\,\theta(k_F-k)\,\theta(k_F-|k+q|)\,\delta_{\alpha\beta} \Big)$$

never satisfied in the sum

$$= \frac{g}{V}\sum_{\alpha<\beta}\sum_{kk'} \theta(k_F-k)\,\theta(k_F-k')$$

$$= \frac{g}{V}\sum_{\alpha<\beta}\Big(\sum_k \theta(k_F-k)\Big)\Big(\sum_{k'}\theta(k_F-k')\Big)$$

$$= \frac{g}{V}\sum_{\alpha<\beta}\left(\frac{N}{2S+1}\right)^2 = \frac{g}{V}\,\frac{(2S+1)2S}{2}\cdot\left(\frac{N}{2S+1}\right)^2 = N\cdot g\cdot\frac{S}{2S+1}\cdot\frac{N}{V}$$

Energy shift per particle is

$$\frac{\Delta E}{N} = g \cdot \frac{S}{2S+1} \cdot n$$

Total energy estimate

$$\frac{E_0 + \Delta E}{N} = \frac{3\hbar^2}{10m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3} + g\frac{S}{2S+1} \cdot n$$

* Compare with the completely polarized state in which

$$\langle F' | c^\dagger_{k\alpha} c_{k\alpha} | F' \rangle = \theta(k_F - k)\, \delta_{\alpha, S}$$

→ The Fermi wave vector is set by

$$N = \sum_\alpha \sum_k \theta(k_F - k)\, \delta_{\alpha, S} = V \int \frac{d^3k}{(2\pi)^3}\, \theta(k_F - k)$$

$$= \frac{V}{8\pi^3} \int_0^{k_F} 4\pi k^2 dk = \frac{V k_F^3}{6\pi^2} \quad \text{or} \quad k_F = \left(6\pi^2 \frac{N}{V}\right)^{1/3}$$
$$= (6\pi^2 n)^{1/3}$$

$$E_0 = \sum_{\alpha}\sum_{k} \frac{\hbar^2 k^2}{2m}\,\theta(k_F - k)\,\delta_{\alpha,s} = \frac{\hbar^2}{2m}\cdot\frac{V}{2\pi^2}\,\frac{1}{5}\,k_F^5$$

$$= \frac{\hbar^2 V}{20\pi^2 m}\left(6\pi^2 \frac{N}{V}\right)^{5/3} = \frac{\hbar^2 V}{20\pi^2 m}\,\frac{6\pi^2 N}{V}\,\left(6\pi^2 n\right)^{2/3}$$

$$= \frac{3\hbar^2 N}{10\, m}\left(6\pi^2 n\right)^{2/3}$$

Energy per particle

$$\frac{E_0}{N} = \frac{3\hbar^2}{10m}\left(6\pi^2 n\right)^{2/3}$$

But in this case the interaction term vanishes exactly

$$\Delta E = \frac{g}{V}\sum_{\alpha<\beta}\sum_{kk'q} \langle F|\, c^\dagger_{k\alpha}\, c^\dagger_{k'+q,\beta}\, c_{k'\beta}\, c_{k+q,\alpha}\, |F\rangle$$

$$= \frac{g}{V}\sum_{\alpha<\beta}\sum_{kk'q}\Big(\delta_{q,0}\,\theta(k_F-k)\,\delta_{\alpha,s}\,\theta(k_F-k')\,\delta_{\beta,s} - \delta_{kk'}\,\theta(k_F-k)\,\delta_{\alpha,s}\,\theta(k_F-|k+q|)\,\delta_{\beta,s}\,\delta_{\alpha\beta}\Big)$$

$$\equiv 0$$

Compare the PM and FM energies

$$\frac{E_{PM}}{N} = \frac{3\hbar^2}{10m}\left(\frac{6\pi^2 n}{2S+1}\right)^{2/3} + g\left(\frac{S}{2S+1}\right)n$$

and

$$\frac{E_{FM}}{N} = \frac{3\hbar^2}{10m}\left(6\pi^2 n\right)^{2/3}$$

Ferromagnetism wins out ($E_{FM} < E_{PM}$) when

$$\frac{3\hbar^2}{10m}\left(6\pi^2 n\right)^{2/3}\left(1 - \frac{1}{(2S+1)^{2/3}}\right) < g\left(\frac{S}{2S+1}\right)n$$

or

$$g > \frac{3\hbar^2}{10m}\left(6\pi^2\right)^{2/3} n^{-1/3} \underbrace{\left(\frac{2S+1}{S}\right)\left(1 - \frac{1}{(2S+1)^{2/3}}\right)}_{\text{Saturates at 2 for S increasingly large}}$$

monotonically decreasing with density