§ Magnetism in metals:

§ Electron gas — Bloch's criterion
Herring's "
Variational wave fns for spin waves
Stoner continuum vs spin waves
Ceperly's m.c. results

§ L.D.A. - results and a critique

§ Hubbard model - Stoner MFT
Eqn of State
Kanamori's criterion for f.m.

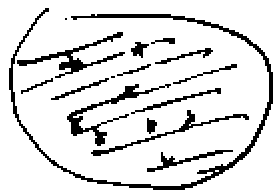
Nagaoka's theorem:

§ e^--gas - Bloch FM

$$H = \sum \epsilon_k c^+_{k\sigma} c_{k\sigma} + \frac{1}{2} \sum_{q\neq 0}{}' V_q\, c^+_{k+q\sigma_1} c^+_{p-q\sigma_2} c_{p\sigma_2} c_{k\sigma_1}$$

$$\epsilon_k = \frac{\hbar^2 k^2}{2m} \; ; \quad V_q = \frac{4\pi e^2}{q^2 \Omega},$$

Jellium: smeared +ve charges.



$$N = 2 \sum_{k<k_F} 1 = \Omega \frac{k_F^3}{3\pi^2}$$

$$\therefore \rho = k_F^3 / 3\pi^2 \; , \quad k_F = \{3\pi^2 \rho\}^{1/3}$$

Dimensional scaling of H

$$E_{kin} = 2 \sum_{k<k_F} \epsilon_k \sim \Omega \frac{\hbar^2 k_F^5}{m}$$

{ Dropping constants

$$\therefore E_{kin} \sim N \frac{\hbar^2 k_F^2}{m}$$

Energy unit in Atomic units $\quad \mathcal{E}_{at} = \dfrac{e^2}{a_0}, \quad a_0 = \dfrac{\hbar^2}{me^2} \sim .52 A^0$

$\sim 27.2\,eV$

$$\boxed{\overline{E}_{kin} \sim \frac{N}{r_s^2} \sim \Omega \rho^{5/3} \sim \int d^3r\, \rho(r)^{5/3}}$$

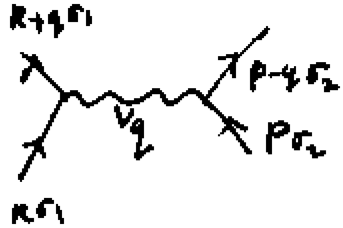
r_s : mean e^- spacing (dimensionless)

$$a_0^3 \frac{4\pi}{3} r_s^3 = \frac{\Omega}{N} = \frac{3\pi^2}{k_F^3}$$

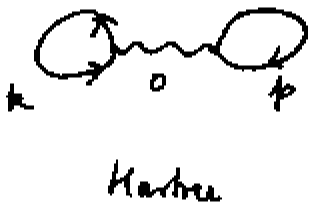
$$\therefore a_0 r_s = \frac{1}{\alpha k_F} \qquad \alpha = \left(\frac{4}{9\pi}\right)^{1/3} \sim .521$$

$V_q \, c^{\dagger}_{k+q\sigma_1} \, c^{\dagger}_{p-q\sigma_2} \, c_{p\sigma_2} \, c_{k\sigma_1}$

Potential energy:



HF $\qquad \langle F | \hat{V} | F \rangle$



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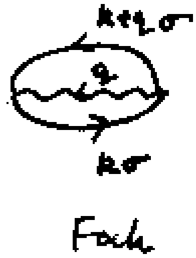


$$E_{ex} = E_{Fock} = -\frac{1}{2} \sum_{k_1, k_2} \frac{f_{k_1\sigma} f_{k_2\sigma}}{|k_1 - k_2|^2} (4\pi e^2)$$

$$\left. \begin{aligned} f_{k\sigma} &= 1 \quad \text{occ} \\ &= 0 \quad \text{unocc} \end{aligned} \right\}$$

Note: Exchange favours ‖ spins

§ Dimensional analysis

$$E_{ex} \sim -\Omega e^2 k_F^4 \simeq -N e^2 k_F$$

$$\therefore \overline{E}_{ex} \sim -N \frac{1}{r_s}$$

$$\therefore \frac{\overline{E}}{N} = \left\{ \frac{2.21}{r_s^2} - \frac{.916}{r_s} + E_{correlation} \right\}$$

$$= \frac{1}{r_s^2} \left\{ 2.21 - .916\, r_s + r_s^2 \log(r_s c) + r_s^3 \ldots \right\}$$

High density $\Rightarrow$ r_s small $\therefore$ less interacting

Low " $\Rightarrow$ r_s large $\therefore$ more interacting

metals: Alkalis ~ $r_s \sim 2 \to 4$

Cs has larger r_s - larger atom as well!

• Bloch $E_{ex} \propto -\Omega \sum_\sigma k_{F_\sigma}^{4/3}$ { since each spin species is a fermi gas! }

$$N_\uparrow = \frac{N}{2}(1+\zeta) \qquad N_\downarrow = \frac{N}{2}(1-\zeta) \qquad \zeta = \frac{N_\uparrow - N_\downarrow}{N}$$

$$k_{F_\pm} = k_F (1 \pm \zeta)^{1/3}$$

$$\frac{\bar{E}[\zeta]}{N} = \left[\frac{2.21}{r_s^2} \frac{(1+\zeta)^{5/3} + (1-\zeta)^{5/3}}{2} - \frac{.916}{r_s} \frac{(1+\zeta)^{4/3} + (1-\zeta)^{4/3}}{2} + \cdots \right]$$

$$\left.\begin{array}{ll} \zeta = 0 & \text{for } r_s < 5.4531 \\ = 1 & \ " \ r_s > 5.4531 \end{array}\right\} \text{Bloch's criterion.}$$

• Conyers Herring: spin waves à la Herring-Kittel

$$|F\rangle = \prod_{|q| < k_{F_\uparrow}} C_{q\uparrow}^{+} |vac\rangle$$ say a fully saturated FM

$$|\Psi_q\rangle_{\text{variational}} = \sum_k \psi_k \, c^\dagger_{k+q\downarrow} c_{k\uparrow} |F\rangle$$ — state with momentum "q"

$c_{k\uparrow}$ creates a hole $|k|<k_F$

$c^\dagger_{k+q\downarrow}$ creates a ↓ particle $|k|>k_F$, ψ_k decides the best combination of k's

Variational Procedure.

$$\frac{\langle\Psi_q|H|\Psi_q\rangle}{\langle\Psi_q|\Psi_q\rangle} = E_{var} = E_0 + \epsilon_q$$ minimize w.r.t. ψ_q

Alternately: think of $|\Psi_q\rangle = A_q^\dagger |F\rangle$

$$A_q^\dagger = \sum \psi_k \, c^\dagger_{k+q\downarrow} c_{k\uparrow}$$

Think of "restricted" eigenvalue problem

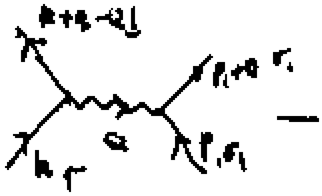
$$[H, A_q^\dagger]|F\rangle = \epsilon_q A_q^\dagger |F\rangle$$

{Exercise: Prove equivalence to Variational procedure}

$\langle F| c_{p\uparrow} c^\dagger_{p+q\downarrow}$ projects linear eqn for ψ_p

$$[T, A_q^\dagger] = \sum \psi_k (\epsilon_{k+q} - \epsilon_k) \, c^\dagger_{k+q\downarrow} c_{k\uparrow}$$

$$[V, A_q^\dagger] = \frac{1}{2} \sum V_Q \Big\{ c^\dagger_{p_1+Q\sigma_1} c_{p_1\sigma_1} c^\dagger_{k+q-Q\downarrow} c_{k\uparrow} - c^\dagger_{k+q\downarrow} c^\dagger_{p_1+Q\sigma_1} c_{p_1\sigma_1} c_{k+Q\uparrow} \Big\}$$



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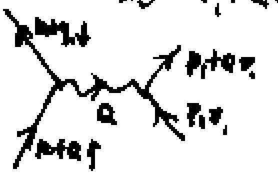
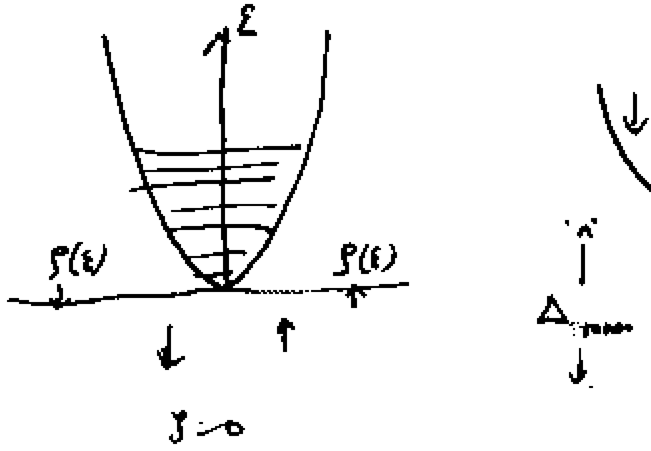


"Contracting" with $\langle F | c^{\dagger}_{k\uparrow} c_{k+q\downarrow}$ gives

$$\left(\omega_q - \tilde{\epsilon}_{k+q\downarrow} - \tilde{\epsilon}_{k\uparrow}\right)\psi_k = \sum V_{k-k'}\, \psi_{k'} \left(f_{k'\uparrow} - f_{k'+q\downarrow}\right)$$

$$\left.\begin{aligned} \tilde{\epsilon}_{k\uparrow} &= \epsilon_k - \sum V_{k-k'} f_{k'\uparrow} \\ \tilde{\epsilon}_{k\downarrow} &= \epsilon_k - \sum V_{k-k'} f_{k'\downarrow} \end{aligned}\right\}$$

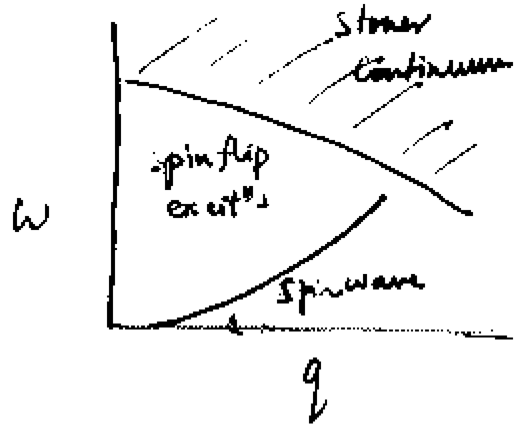
self energies are spin dependent



Δ_{ex} - Exchange splitting or Stoner Gap.

$$\omega^{\text{stoner}}_{q,k} = \tilde{\epsilon}_{k+q\downarrow} - \tilde{\epsilon}_{k\uparrow} \geq 0 \text{ for } \forall q, k \quad \underline{\text{For stability}}$$

These are 1 particle excitations:



Spinwave collective mode obtained from (integral) eqn

$$\left(\omega_q - \tilde{\epsilon}_{k+q\downarrow} - \tilde{\epsilon}_{k\uparrow}\right)\psi_k = \int \frac{4\pi e^2}{(k-k')^2}\,\psi_{k'}\left(f_{k'\downarrow} - f_{k'+q\uparrow}\right)$$

Eigenvalue problem:

C. Herring ΦR (1956)

A. K. Rajagopal ΦR (1967)

$$\omega = D q^2 \qquad D \cdot \left(1 - \frac{5.48}{r_s}\right) \qquad \left.\begin{array}{l} D > 0 \text{ for } r_s > 5.48 \\ < 0 \quad r_s < 5.48 \end{array}\right\}$$

$q \to 0$

$$\left.\begin{array}{ll} \text{Bloch} & 5.45 \\ \text{Herring} & 5.48 \end{array}\right\}$$

3A

§ Hubbard model Stoner M.F.T.

N_s = # sites
N_e = # electrons
$n = N_e/N_s$

$$H = \sum \epsilon_k n_{k\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$

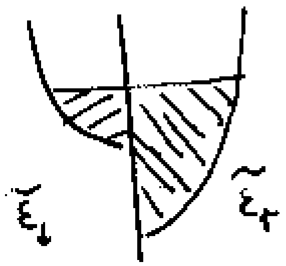
$$n_{i\uparrow} n_{i\downarrow} \sim n_{i\uparrow} \overline{n_{i\downarrow}} + n_{i\downarrow} \overline{n_{i\uparrow}} - \overline{n_{i\uparrow}}\, \overline{n_{i\downarrow}}$$

$$\overline{n_{i\uparrow}} = \frac{n+m}{2} \qquad \overline{n_{i\downarrow}} = \frac{n-m}{2}$$

$$H = \sum \tilde{\epsilon}_{k\sigma} n_{k\sigma} - U\frac{m}{2} \sum \sigma n_{i\sigma} + U\frac{n}{2} N_e + \frac{U}{4} N_s (m^2 - n^2)$$

$$\boxed{\tilde{\epsilon}_{k\sigma} = \epsilon_k - U\frac{m}{2}\sigma}$$

Minimize wrt m.



Partial polarization m - in general

$$U \rho(\epsilon_F) > 1 \quad \text{for F.M}$$

$\underline{T > T_c}$

$$\chi(Q) = 2\mu_B^2 \frac{\chi_0(Q)}{1 - U\chi_0(Q)}$$ susceptibility/site

$$\chi_0(Q) = \frac{1}{N_s} \sum_k \frac{f_k - f_{k+Q}}{\epsilon_{k+Q} - \epsilon_k}$$

$$Q \to 0 \qquad \chi_0(\omega) \to \rho(\epsilon_F)\left\{1 - \frac{T^2}{T_F^2}\right\} : \quad \chi = \frac{4\mu_B^2 \rho(\epsilon_F)}{1 - U\rho(\epsilon_F)\left\{1 - \frac{T^2}{T_F^2}\right\}}$$

$$T_F = \frac{6}{\pi k_F}\left[\left(\frac{\rho'(\epsilon_F)}{\rho(\epsilon_F)}\right)^2 - \frac{\rho''(\epsilon_F)}{\rho(\epsilon_F)}\right]^{-1/2}$$

~ 1eV ~10,000°K

Problem with observed Curie law in T_c, N_s

$$\chi \sim \frac{1}{(T - T_{SF})} \qquad T_{SF} \ll T_F$$

$$= T_F \left(1 - U\rho(\epsilon_F)\right)^{1/2}$$

Weak itinerant ferromagnets Ni_3Al, $ZrZn_2$, Sc_3In

Paramagnon theories . . .

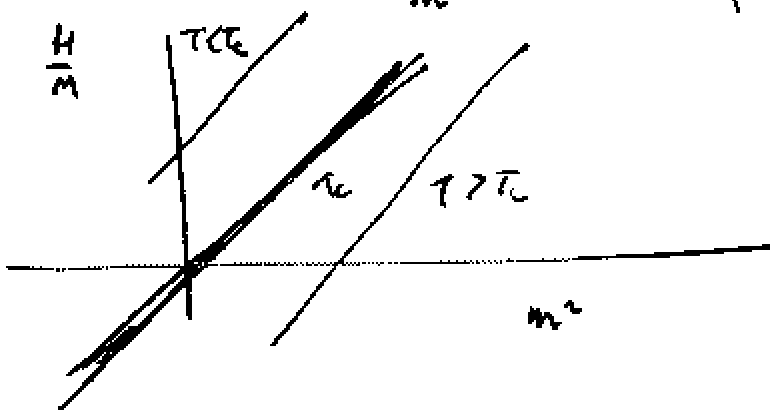
p_0 = zero Temp moment
p_{eff} = $T \gg T_c$ $\Big\}$ $\frac{p_{eff}}{p_0} \gg 1$

§ Equation of state – Arrott Plots

$$F = \frac{\alpha}{2}(T - T_c) m^2 + \beta_4 m^4 - mH$$

$$\frac{\partial F}{\partial m} = 0 \Rightarrow \qquad H = \alpha(T - T_c)m + \beta m^3$$

$$\frac{H}{m} = \alpha(T - T_c) + \beta m^2$$



§ KANAMORI CRITERION for FM

More stringent conditions than $U\rho(\epsilon_F) > 1$ needed.

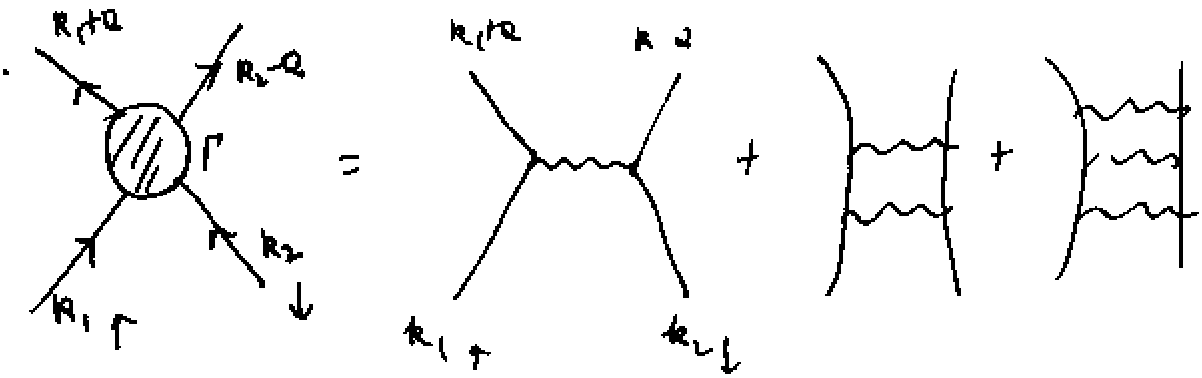
Ni e.g. has E_F in close proximity of a peak in DOS & has low hole density.

Low density large U ($\to\infty$) is Brueckner type limit à la Nuclear Matter
Galitskii - Migdal - rigorous low density expansion possible (Yang-Lee too)

Goldstone series

maximizes # of ↑ lines is dominant at low density

since
$$\left.\begin{aligned} k\uparrow &\to (1-f_k) \\ k\downarrow &\to f_k \end{aligned}\right\}$$



$$\Gamma = U_{eff}(k_1, k_2) = \frac{U}{1 + \frac{U}{N_s} \sum_Q \frac{(1-f_{k_1+Q})(1-f_{k_2-Q}) + ff}{\epsilon_{k_1+Q} + \epsilon_{k_2-Q} - \epsilon_{k_1} - \epsilon_{k_2}}}$$

As $U \to \infty$

$$\Gamma \to \frac{1}{\frac{1}{N_s}\sum \cdots} \quad \text{finite number}$$

we can estimate by setting $k_1 = k_2 = 0$

$$\Gamma \sim \frac{1}{\int_{\epsilon_F}^{W} \frac{\rho(\epsilon)\,d\epsilon}{2\epsilon}}$$

$\therefore$ FM occurs when

$$\rho(\epsilon_F) > \langle \rho(\epsilon) \rangle_{av} = \int_{\epsilon_F}^{W} \rho(\epsilon) \frac{d\epsilon}{2\epsilon}$$

$\therefore$ Peaks at D.O.S. help rather than a flat (but large) DOS!