Lecture XII: Metallic magnetism and quantum critical phenomena

▷ References:

E. C. Stoner, *Ferromagnetism*, Rep. Prog. Phys. **11**, 43 (1947).

J. A. Hertz, *Quantum critical phenomena*, Phys. Rev. B **14**, 1165 (1976).

Although we have seen that effects of weak interaction in an electron gas can be largely benign, we know that strong interaction can lead to the development of magnetic correlations in the ground state.

Consider, e.g., the lattice Hubbard model: $\hat{H} = \hat{H}_0 + \hat{H}_U$

$$\hat{H}_0 = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} c^\dagger_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma}, \qquad \hat{H}_U = U \sum_i^N \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ and $\sum$-convention on spin

Dispersion $\epsilon_{\mathbf{p}}$ (a function of the lattice geometry) is, for the present, left unspecified

Phase diagram of $\hat{H}$ is rich, exhibiting a range of correlated ground states depending sensitively on density and strength of interaction

In lattice system, commensurability effects can trigger transition to charge or spin density wave state...

while, at large U, the electron system can 'freeze' into an insulating antiferromagnetic Mott-Hubbard phase

Aim: here we will show that, at low densities the system may adopt an itinerant (i.e. mobile) spin polarised phase, the Stoner ferromagnet.

▷ Physical argument: Capacity of interacting electron system to form a ferromagnetic phase reflects competition between the k.e. and p.e. Being forbidden by Pauli exclusion to occupy the same site, electrons of the same spin can escape the local Hubbard interaction. However, the same exclusion principle requires the system to occupy higher lying single-particle states raising their k.e. When total reduction in p.e. outweighs increase in k.e. a transition to a spin polarised or ferromagnetic phase is induced.

Operationally, it is useful to separate interaction into channels sensitive to charge and spin densities,

$$\hat{H}_U = \frac{U}{4}\sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 - \frac{U}{4}\sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2.$$

Since fluctuations in charge density have little effect on thermodynamics of low density system, neglect their influence setting $\hat{H}_U \simeq -U\sum_i (\hat{S}^z_i)^2$, where $\hat{S}^z_i = (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})/2$.

Exercise: how would you rewrite interaction in a spin-rotationally invariant manner?

Cast as coherent state PI:

$$\mathcal{Z} = \int D(\bar{\psi},\psi) \exp\left\{-\int_0^\beta d\tau \left[\sum_{\mathbf{p}} \bar{\psi}_{\mathbf{p}\sigma}(\partial_\tau + \xi_{\mathbf{p}})\psi_{\mathbf{p}\sigma} - \frac{U}{4}\sum_i (\sum_\sigma \bar{\psi}_{i\sigma}\sigma\psi_{i\sigma})^2\right]\right\}$$

$$\xi_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \mu$$

Hubbard-Stratonovich decoupling:

$$\mathcal{Z} = \int Dm \int D(\bar{\psi},\psi) \exp\left\{-\int d\tau \left(\frac{U}{4}\sum_i m_i^2(\tau) + \sum_{\mathbf{p}} \bar{\psi}_{\mathbf{p}\sigma}(\partial_\tau + \xi_{\mathbf{p}}\psi_{\mathbf{p}\sigma} + \frac{U}{2}\sum_{i\sigma} \bar{\psi}_{i\sigma}\sigma m_i\,\psi_{i\sigma}\right)\right\}$$

where m_i is local magnetisation density

Gaussian integration over Grassmann degrees of freedom:

$$\mathcal{Z} = \mathcal{Z}_0 \int Dm \exp\left\{-\frac{U}{4}\int_0^\beta d\tau \sum_i m_i^2(\tau) + \sum_\sigma \mathrm{tr}\ln\left(1 - \frac{U}{2}\sigma\hat{m}\,\hat{G}_0\right)\right\}$$

where $\hat{G}_0 = (i\epsilon_n - \xi_{\hat{\mathbf{p}}})^{-1}$ and $\hat{m} = \{m_i(\tau)\,\delta_{ij}\delta(\tau-\tau')\}$

▷ From here, one can proceed in one of two ways:

(1) Vary action on m and find saddle-point magnetisation
$\rightsquigarrow$ self-consistent BCS-like equation for magnetisation

(2) Focusing on magnetic critical point, seek perturbative expanision in m
— mirrors closely calculation of RPA in weakly interacting electron gas

Here we follow route (2) leaving (1) as an exercise

Drawing on RPA expansion of interacting electron gas,
and noting that terms odd in powers of m vanish (N.B. symmetry $m \to -m$), obtain

$$\mathcal{Z} = \mathcal{Z}_0 \int Dm\, e^{-S[m]}$$

where, setting $q = (\omega_m, \mathbf{q})$,

$$S[m] = \frac{1}{2}\sum_q v_2(q)|m_q|^2 + \frac{1}{4N\beta}\sum_{q_i} v_4(\{q_i\})\prod_{i=1}^4 m_{q_i}\,\delta_{\sum_i q_i,0} + \dots$$

where $v_2(q) = \frac{U}{2}(1 - U\Pi(q))$ with the magnetic susceptibility $\Pi(q) = -2\chi(q)$

$$\chi(q) = \frac{2}{N\beta}\sum_k G_{0,k}G_{0,k+q} = \frac{2}{N}\sum_{\mathbf{k}} \frac{n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k+q}})}{i\omega_m + \xi_{\mathbf{k}} - \xi_{\mathbf{k+q}}}$$

i.e. susceptibility depends sensitively on dispersion $\epsilon_{\mathbf{k}}$

Static susceptibility dominated by contributions where $\xi_{\mathbf{p}} \simeq \xi_{\mathbf{p+q}}$ over a domain of the reciprocal space

i.e. regions where $\mathbf{q}$ is small
or where, for some non-zero $\mathbf{q} = \mathbf{Q}$, $\xi_{\mathbf{p}} \simeq \xi_{\mathbf{p+Q}}$ — 'nesting' condition

If we assume that the spectrum varies smoothly so that nesting symmetry is absent, the susceptibility is maximised for $\mathbf{q} = 0$

Focusing on free electron system $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m$, for $|\omega_n|/|\mathbf{q}|v_F$ small,

$$\Pi(q) \simeq \Pi_(0, \mathbf{q}) - \nu\frac{|\omega_n|}{v|\mathbf{q}|}$$

where $v = cv_F$ with c depending on dimensionality

For $\mathbf{q}$ small, $\Pi(0, \mathbf{q}) \simeq \nu[1 - \xi^2\mathbf{q}^2 + \cdots]$ where $\xi \sim 1/k_F$. Similarly

$$v_4(\{q_i\}) \mapsto v_4(0) \equiv u = \frac{2(U/2)^4}{\beta N}\sum_p [G_0(p)]^4 \sim U^4\nu'',$$

where $\nu'' = \partial_\epsilon^2|_{\epsilon=E_F}\nu(\epsilon)$

Altogether,

$$S[m] = \frac{U^2\nu}{4}\sum_q \left[r + \xi^2\mathbf{q}^2 + \frac{|\omega_n|}{v|\mathbf{q}|}\right]|m(q)|^2 + \frac{uT}{4N}\int dx\, m^4(x) + \cdots$$

where $r = 1/U\nu - 1$

▷ Finally, rescaling the magnetisation field and u, ($\int dx \equiv \int d^dx \int d\tau$)

$$S[m] = \frac{1}{2}\sum_q \left[r + \xi^2\mathbf{q}^2 + \frac{|\omega_n|}{v|\mathbf{q}|}\right]|m_q|^2 + \frac{u}{4}\int dx\, m^4(x)$$

the Hertz-Millis action

Frequency-dependent term describes damping of magnetic fluctuations due to excitation of particle/hole pairs

Restoration of spin symmetry endows magnetisation field with n-components

Action captures effects of quantum dynamical fluctuations
on Ginzburg-Landau expansion for magnetisation

▷ Mean-field theory:

$$\frac{S[m]}{\beta L^3} = \frac{r}{2}m^2 + \frac{u}{4}m^4.$$

Minimising the action with respect to m, one finds a Stoner transition
to a spin polarised ferromagnetic phase when

$$r = 0, \text{i.e.} \qquad U_c\nu = 1$$

for $U > U_c$, $m = \sqrt{-r/4u}$

Although the mean field theory provides a good qualitative understanding of the nature of the transition, the Stoner criterion itself is unreliable. In the lattice system, the density of states is typically set by the bandwidth, i.e. $\nu \sim 1/t$. Therefore, at the Stoner transition where $U/t \sim 1$, the system enters the strongly correlated phase where the interaction can not be considered as a small perturbation. In this regime, the electrons experience an effective interaction renormalised by the screening effect of the charge redistribution. An estimate for the effective interaction $U_{\text{eff}} \sim U/(1+U/t)$ shows that, in the relevant regime, the Stoner criterion becomes replaced by

$$\nu t \geq 1.$$

Typically, for a smoothly varying density of states, $\nu \sim 1/t$ and the inequality is difficult to satisfy. In practice, the Stoner transition to ferromagnetism tends to appear in materials where there is significant enhancement of the density of states near the Fermi energy.

▷ Fluctuations?

Mean-field theory perturbed by both classical and quantum dynamical fluctuations
subject of Hertz-Millis theory (beyond scope of lectures)

Effects depend on proximity to critical region

`phase diagram`