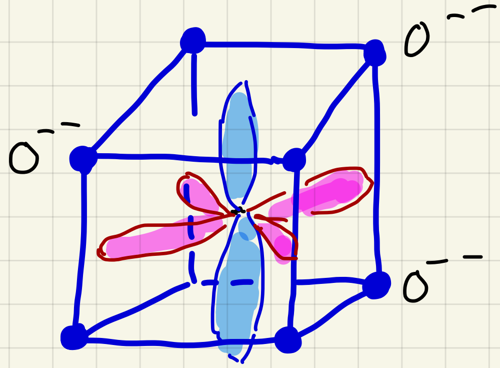
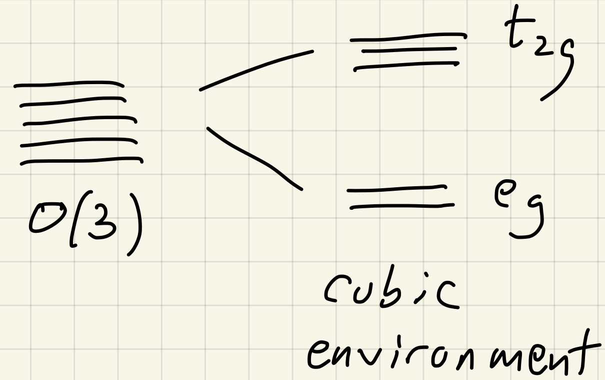



## Lecture 20 (March 9)

### The Stoner model : moment formation in itinerant systems

The noninteracting electron gas (see §5.4) exhibits either paramagnetism ($\chi > 0$) or diamagnetism ($\chi < 0$), but never **ferromagnetism**, in which there is a spontaneous moment formation in the absence of an external field. To account for spontaneous magnetism we must include the effects of interactions, which in our case means the Coulomb interaction. How can a spin-independent Coulomb interaction yield magnetism? Lets consider a specific model,

$$\hat{H} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \left( \overset{e^{iA_{ij}}}{c^\dagger_{i\sigma} c_{j\sigma}} + \overset{e^{-iA_{ij}}}{c^\dagger_{j\sigma} c_{i\sigma}} \right) + U \sum_i \overset{c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} c_{i\uparrow}}{\hat{n}_{i\uparrow} \hat{n}_{i\downarrow}} + \mu_B \vec{H} \cdot \sum_{i,\alpha,\beta} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

known as the **Hubbard model**. Note that the interaction term, written in red, is purely local and does not fall off as $1/|\vec{R}_i - \vec{R}_j|$ as is the case for the actual Coulomb potential. We can wave our hands and appeal to screening, but perhaps it is best not to insist that the Hubbard model is realistic. The interaction term, for fixed total electron number per site $n \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, favors a magnetic moment:

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{1}{4}(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 - \frac{1}{4}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2$$

This is minimized by making $|\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}|$ as large as possible. I.e. $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is minimized by a maximally polarized situation where $\hat{n}_{i\uparrow} = n$ , $\hat{n}_{i\downarrow} = 0$.

**Stoner mean field theory : ferromagnetism**

The idea here is to write $\hat{n}_{i\sigma} = \langle \hat{n}_{i\sigma} \rangle + \delta \hat{n}_{i\sigma}$, where $\langle n_{i\sigma} \rangle$ is the thermodynamic average, which we assume to be site-independent in the case of ferromagnetism. We then have $\delta \hat{n}_{i\sigma} = \hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle$ and

$$\begin{aligned}
\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} &= (\langle \hat{n}_{i\uparrow} \rangle + \delta \hat{n}_{i\uparrow})(\langle \hat{n}_{i\downarrow} \rangle + \delta \hat{n}_{i\downarrow}) \\
&= \langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \delta \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \delta \hat{n}_{i\uparrow} + \overbrace{\delta \hat{n}_{i\uparrow} \delta \hat{n}_{i\downarrow}}^{(\text{flucts})^2} \\
&= -\langle \hat{n}_{i\uparrow} \rangle \langle \hat{n}_{i\downarrow} \rangle + \langle \hat{n}_{i\uparrow} \rangle \hat{n}_{i\downarrow} + \langle \hat{n}_{i\downarrow} \rangle \hat{n}_{i\uparrow} + \mathcal{O}(\delta \hat{n}^2) \\
&= \frac{1}{4}(m^2 - n^2) + \frac{1}{2} n (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + \frac{1}{2} m (\hat{n}_{i\uparrow} - \hat{n}_{i\uparrow}) + \cancel{\mathcal{O}(\delta \hat{n}^2)}
\end{aligned}$$

where

$$n \equiv \langle \hat{n}_{i\uparrow} \rangle + \langle \hat{n}_{i\downarrow} \rangle$$

$$m \equiv \langle \hat{n}_{i\downarrow} \rangle - \langle \hat{n}_{i\uparrow} \rangle$$

We further assume

$$\langle n_{i\sigma} \rangle = \frac{1}{2} n - \frac{1}{2} \sigma m \qquad \text{(independent of } i\text{)}$$

The mean field grand canonical Hamiltonian is then

$$\hat{K}^{MF} = -\frac{1}{2}\sum_{i,j}\sum_{\sigma} t_{ij}\left(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}\right) - \left(\mu - \tfrac{1}{2}Un\right)\sum_{i,\sigma} c^\dagger_{i\sigma}c_{i\sigma}$$

$$+ \left(\mu_B H + \tfrac{1}{2}Um\right)\sum_{i,\sigma}\sigma\, c^\dagger_{i\sigma}c_{i\sigma} + \frac{1}{4}N_s\, U(m^2 - n^2)$$

$\leftarrow$ # of lattice sites

We've taken $\vec{H} = H\hat{z}$, without loss of generality. Note:

- The chemical potential is shifted down to $\bar{\mu} \equiv \mu - \frac{1}{2}Un$.
- The effective magnetic field is $H_{eff} = H + \dfrac{Um}{2\mu_B}$.
  We define $\Delta \equiv \mu_B H_{eff} = \mu_B H + \frac{1}{2}Um$.

The grand potential per lattice site is then

$$\omega = \frac{1}{4}U(m^2-n^2) - \frac{1}{2}k_BT\int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\left\{\ln\left(1+e^{(\bar{\mu}-\varepsilon-\Delta)/k_BT}\right) + \ln\left(1+e^{(\bar{\mu}-\varepsilon+\Delta)/k_BT}\right)\right\}$$

where $g(\varepsilon)$ is the DOS per site for both spin polarizations. Thus $[g(\varepsilon)] = E^{-1}$. We compute the Gibbs free energy density

$$\varphi = \omega + \mu n = \omega + \bar{\mu}n + \frac{1}{2}Un^2$$

and so

$$\varphi = \frac{1}{4}U(n^2+m^2) + \bar{\mu}n - \frac{1}{2}k_BT\int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\left\{\ln\left(1+e^{(\bar{\mu}-\varepsilon-\Delta)/k_BT}\right) + \ln\left(1+e^{(\bar{\mu}-\varepsilon+\Delta)/k_BT}\right)\right\}$$

Note $\varphi = \varphi(n, T, H)$ is not a function of $\mu$ or $m$. Thus we must set

① $\dfrac{\partial \varphi}{\partial \bar{\mu}} = 0 \Rightarrow$

$$n = \frac{1}{2}\int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\left\{ f(\varepsilon-\Delta-\bar{\mu}) + f(\varepsilon+\Delta-\bar{\mu}) \right\}$$

② $\dfrac{\partial \varphi}{\partial m} = 0 \Rightarrow$

$$m = \frac{1}{2}\int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\left\{ f(\varepsilon-\Delta-\bar{\mu}) - f(\varepsilon+\Delta-\bar{\mu}) \right\}$$

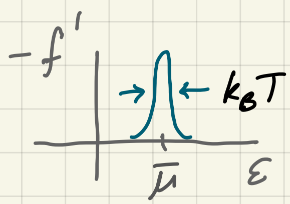
We assume $\Delta = \mu_B H + \frac{1}{2} U m$ is small, and we expand ① in powers of $\Delta$:

$$n = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\left\{ f(\varepsilon-\bar{\mu}) + \frac{1}{2} f''(\varepsilon-\bar{\mu})\,\Delta^2 + \frac{1}{24} f''''(\varepsilon-\bar{\mu})\,\Delta^4 + \ldots \right\}$$

We define $\bar{\mu} = \bar{\mu}_0 + \delta\bar{\mu}$ and expand further in $\delta\bar{\mu}$, with

$$n = \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon) f(\varepsilon-\bar{\mu}_0)$$

which implicitly yields $\bar{\mu}_0(n,T)$. Defining




$$D(\bar{\mu}) \equiv -\int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon) f'(\varepsilon-\bar{\mu}) \Rightarrow D^{(k)}(\bar{\mu}) = -\int_{-\infty}^{\infty} d\varepsilon\, g^{(k)}(\varepsilon) f'(\varepsilon-\bar{\mu})$$

we obtain, from ①,

$$0 = D(\bar{\mu}_0)\,\delta\bar{\mu} + \frac{1}{2}\left(\Delta^2 + (\delta\bar{\mu})^2\right) D'(\bar{\mu}_0) + \frac{1}{2} D''(\bar{\mu}_0)\,\Delta^2\,\delta\bar{\mu} + \frac{1}{24} D'''(\bar{\mu}_0)\,\Delta^4 + \mathcal{O}(\Delta^6)$$

$$\Rightarrow \delta\bar{\mu} + \frac{1}{2} a_1 (\delta\bar{\mu})^2 + \frac{1}{2} a_1 \Delta^2 + \frac{1}{2} a_2 \Delta^2 \delta\bar{\mu} + \frac{1}{24} a_3 \Delta^4 = 0$$

where $a_k \equiv D^{(k)}(\bar{\mu}_0)/D(\bar{\mu}_0)$ has dimensions $E^{-k}$. Sol$^{\underline{n}}$:

$$\delta\bar{\mu} = -\tfrac{1}{2}a_1\Delta^2 - \tfrac{1}{24}\left(3a_1^2 - 6a_1a_2 + a_3\right)\Delta^4 + \mathcal{O}(\Delta^6)$$

Inserting this into our expression for $\varphi$, we obtain

$$\varphi(n,T,H) = \varphi_0(n,T) + \tfrac{1}{4}Um^2 - \tfrac{1}{2}D(\bar{\mu}_0)\Delta^2 + \frac{1}{24}\left(\frac{3[D'(\bar{\mu}_0)]^2}{D(\bar{\mu}_0)} - D''(\bar{\mu}_0)\right)\Delta^4 + \ldots$$

where

$$\varphi_0(n,T) = \tfrac{1}{4}Un^2 + n\bar{\mu}_0 - \int_{-\infty}^{\infty}\! d\varepsilon\, N(\varepsilon)\, f(\varepsilon - \bar{\mu}_0)$$

and $g(\varepsilon) = N'(\varepsilon)$. Assuming $H$ and $m$ are both small,

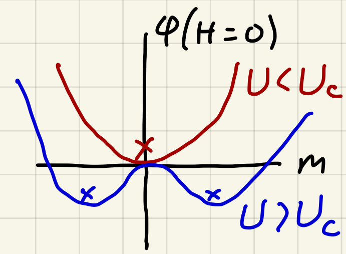
$$\varphi = \varphi_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 - \frac{U\chi_0}{2\mu_B}Hm - \tfrac{1}{2}\chi_0 H^2 + \ldots$$

with $\chi_0 = \mu_B^2 D(\bar{\mu}_0)$ and

$$a = \tfrac{1}{2}U\left(1 - \tfrac{1}{2}UD(\bar{\mu}_0)\right) \quad , \quad b = \frac{1}{96}\left(\frac{3[D'(\bar{\mu}_0)]^2}{D(\bar{\mu}_0)} - D''(\bar{\mu}_0)\right)$$

Since $\varphi$ is not a function of $m$, we must have

$$0 = \frac{\partial\varphi}{\partial m} = am + bm^3 - \frac{U\chi_0}{2\mu_B}H$$




For small $m, H$ we find

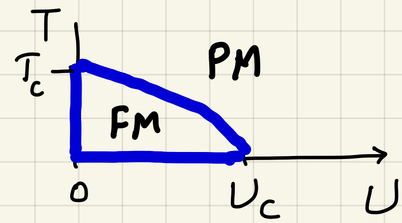
$$m = \frac{U\chi_0}{2\mu_B a}H = \frac{\chi_0}{\mu_B}\cdot\frac{H}{1 - U/U_c}$$

with $U_c = 2/D(\bar{\mu}_0)$. Note $a = \tfrac{1}{2}U\left(1 - \frac{U}{U_c}\right)$ so $a(U<U_c)>0$ while $a(U>U_c)<0$. The magnetization density is $M = \mu_B m$

and thus

$$\chi = \frac{M}{H}\bigg|_{H\to 0} = \frac{\chi_0}{1-U/U_c} \leftarrow \text{"Stoner enhancement"}$$

When $H=0$ we may still get $m\neq 0$ provided $U>U_c$, in which case $a<0$. We find then




$$m(U) = \pm\left(\frac{U}{2bU_c}\right)^{1/2}\sqrt{U-U_c}$$

This exhibits the usual $\beta = 1/2$ mean field order parameter exponent. For $U>U_c$, the eqn for $T_c$ is: $D(\bar{\mu}_0, T_c) = \frac{2}{U}$.

**Stoner antiferromagnetism:**

It's easy to see that near half filling $(n=1)$, on a bipartite lattice, the ground state should be antiferromagnetic. This follows from second order perturbation theory in the hopping matrix element $t$ (setting $\vec{H}=0$):

$$E_0(t) = E_0(t=0) + \langle G|\hat{T}|G\rangle + \sum_n{}' \frac{|\langle n|\hat{T}|G\rangle|^2}{E_0-E_n} + \cdots$$

Here $|G\rangle$ is the $t=0$ ground state, which at $n=1$ is massively degenerate. Any state $|G\rangle$ with $\hat{n}_i|G\rangle = |G\rangle$, i.e. one electron per site, is a ground state, with $E_0=0$. Excited states contain some sites with $n_i=0$ or $n_i=2$, such that $\langle \hat{n}_i\rangle = 1$ on average.

Consider the ferromagnetic state $|F\rangle = |\uparrow\uparrow\uparrow\cdots\uparrow\rangle$

for which $\hat{n}_{i\sigma}|F\rangle = \delta_{\sigma,+}|F\rangle$. Note $S_{tot} = \frac{1}{2}N_s$ for this state, and it is a "highest weight" state with $S^z_{tot} = +S_{tot}$. We can obtain the full set of $2S_{tot}+1 = N_s+1$ ferromagnetic states by successively applying $\hat{S}^-_{tot} = \sum_{j=1}^{N} \hat{S}^-_j$ to $|F\rangle$. Now the kinetic energy operator is

$$\hat{T} = -\sum_{\langle ij\rangle}\sum_{\sigma}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right)$$

which preserves spin polarization in the hopping process. Thus, $\hat{T}|F\rangle = 0$ since Pauli blocking prevents any two $\uparrow$ spins from sharing any given site. Thus, $E_0 = 0$ **to all orders in perturbation theory in $t$**. In other words, $\hat{H}|F\rangle = 0$ and $|F\rangle$ is an eigenstate of the Hubbard Hamiltonian $\hat{H}$ (again, set $\vec{H}=0$).

Next, consider the model on a bipartite lattice. In this case we can form the two sublattice antiferromagnetic state $|AF\rangle = |\uparrow\downarrow\uparrow\downarrow\cdots\rangle$ where

$$\hat{n}_{i\sigma}|AF\rangle = \left(\delta_{i,A}\delta_{\sigma,+} + \delta_{i,B}\delta_{\sigma,-}\right)|AF\rangle$$

The first order contribution $\langle AF|\hat{T}|AF\rangle = 0$ still vanishes, but the second order contribution is found to be

$$\Delta E_0^{(2)} = -\frac{2t^2}{U} \times N_{links}$$

where $N_{links} = \frac{1}{2} z N_{sites}$, with $z$ the lattice coordination number (i.e. # of nearest neighbors). The calculation is easy. Focus on a given neighboring pair of sites $|\uparrow\downarrow\rangle$ with wolog we take $n_{i\sigma} = \delta_{\sigma,+}$ and $n_{j\sigma} = \delta_{\sigma,-}$. The KE operator $\hat{T}$ can hop the $\uparrow$ spin from $i$ to $j$ or the $\downarrow$ spin from $j$ to $i$, creating an intermediate state $|n\rangle = |\uparrow \downarrow \uparrow \downarrow \cdots \uparrow \downarrow\!\uparrow 0 \downarrow \uparrow \cdots\rangle$, whose potential energy is $U$. Thus, $\Delta E^{(2)}(t) = -2t^2/U$ per link. In fact, the effective AF Hamiltonian in the $n_i = 1$ sector is then

$$\hat{H}_{eff} = J \sum_{\langle ij \rangle} \left( \vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j \right)$$

where $J = 4t^2/U$ is the **superexchange constant.**

**Mean field theory of antiferromagnetism :**

The MF Ansatz is again $\hat{n}_{i\sigma} = \langle \hat{n}_{i\sigma} \rangle + \delta\hat{n}_{i\sigma}$ with

$$\langle \hat{n}_{i\sigma} \rangle = \frac{1}{2} n + \frac{1}{2} \sigma m \, e^{i\vec{Q}\cdot\vec{R}_i}$$

where $\vec{Q}$ is the AF ordering vector. On a hypercubic lattice,

$$\vec{Q} = \left( \frac{\pi}{a}, \frac{\pi}{a}, \ldots, \frac{\pi}{a} \right) \quad \Longrightarrow \quad e^{i\vec{Q}\cdot\vec{R}_i} \equiv \eta_i = \begin{cases} +1 & \text{if } i \in A \\ -1 & \text{if } i \in B \end{cases}$$

Thus, $\langle \hat{n}_{A\uparrow} \rangle = \frac{1}{2}(n+m)$, $\langle \hat{n}_{A\downarrow} \rangle = \frac{1}{2}(n-m)$, $\langle \hat{n}_{B\uparrow} \rangle = \frac{1}{2}(n-m)$, and $\langle \hat{n}_{B\downarrow} \rangle = \frac{1}{2}(n+m)$.

The grand canonical Hamiltonian is

$$\hat{K}^{MF} = -t \sum_{\langle ij \rangle} \sum_{\sigma} \left( c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) - \left( \mu - \tfrac{1}{2} U n \right) \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}$$

$$+ \tfrac{1}{2} U m \sum_{i,\sigma} e^{i \vec{Q} \cdot \vec{R}_{i}} \sigma \, c^\dagger_{i\sigma} c_{i\sigma} + \tfrac{1}{4} N_s U (m^2 - n^2)$$

$$= \frac{1}{2} \sum_{k,\sigma} \begin{pmatrix} c^\dagger_{k\sigma} & c^\dagger_{k+\vec{Q}\sigma} \end{pmatrix} \begin{pmatrix} \varepsilon(k) - \bar{\mu} & \frac{1}{2} \sigma U m \\ \frac{1}{2} \sigma U m & \varepsilon(k+\vec{Q}) - \bar{\mu} \end{pmatrix} \begin{pmatrix} c_{k\sigma} \\ c_{k+\vec{Q}\sigma} \end{pmatrix}$$

$$+ \tfrac{1}{2} N_S U (m^2 - n^2)$$

where $\varepsilon(k) = -t(k) = -2t \sum_{\alpha=1}^{d} \cos(k_\alpha a)$ (d-dim$^l$ cubic).
Thus $\varepsilon(k + \vec{Q}) = -\varepsilon(k)$ and the eigenvalues are

$$\lambda_\pm(k) = \pm \sqrt{\varepsilon^2(k) + \Delta^2} - \bar{\mu}$$

with $\Delta = \frac{1}{2} U m$ and $\bar{\mu} = \mu - \frac{1}{2} U n$ as before. The Gibbs free energy per site is then

$$\varphi = \tfrac{1}{4} U (n^2 + m^2) + \bar{\mu} n + \tfrac{1}{2} k_B T \int_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) \left\{ \ln\left(1 + e^{(\bar{\mu} - \sqrt{\varepsilon^2 + \Delta^2})/k_B T}\right) + \ln\left(1 + e^{(\bar{\mu} + \sqrt{\varepsilon^2 + \Delta^2})/k_B T}\right) \right\}$$

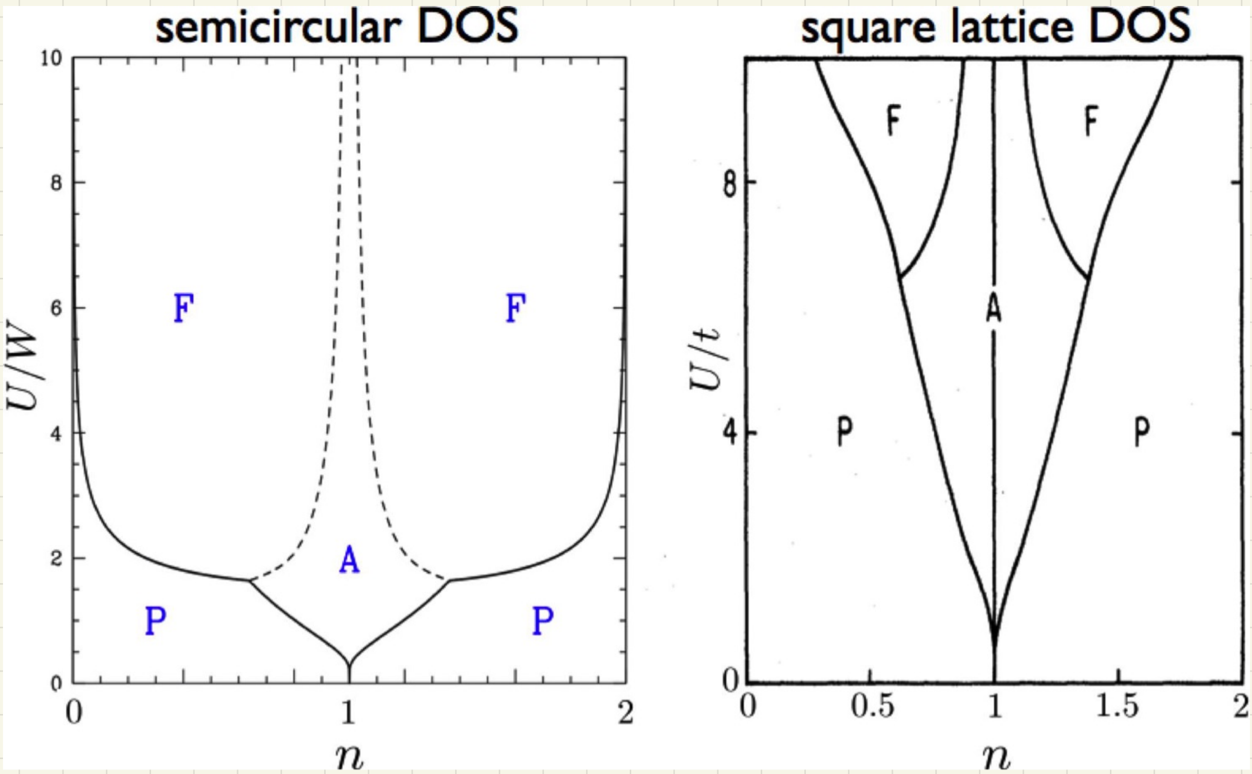
The MF eqns are then

① $$n = \frac{1}{2} \int_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) \left\{ f\left(-\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}\right) + f\left(+\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}\right) \right\}$$

② $$1 = \frac{U}{2} \int_{-\infty}^{\infty} d\varepsilon \, \frac{g(\varepsilon)}{\sqrt{\varepsilon^2 + \Delta^2}} \left\{ f\left(-\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}\right) - f\left(\sqrt{\varepsilon^2 + \Delta^2} - \bar{\mu}\right) \right\}$$

A paramagnetic sol$^{\underline{n}}$ with $m=0$ always exists, in which case ② no longer applies.

**Mean field phase diagrams at $T=0$:**




In fact, FM is quite difficult to obtain in reality and seems to require $U/t \gtrsim 100$ on the square lattice.