Phys 726 – Lecture 20

Attractive vs. Repulsive interactions

* Coulomb interactions are repulsive
  → on the lattice, we've been modelling the screened Coulomb potential with an onsite energy cost U

i.e. $$\hat{H}_{\text{Coulomb}} \sim \sum_{i<j} \frac{e^{-\lambda r_{ij}}}{r_{ij}} \rightsquigarrow U \sum_i n_{i\uparrow} n_{i\downarrow}$$

→ there are various re-writings of this term, which represent different ordering "channels".

e.g. In the magnetic channel,

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

$$= \hat{n}_\uparrow + \hat{n}_\downarrow - 2\hat{n}_\uparrow \hat{n}_\downarrow$$

Hence

$$U\hat{n}_\uparrow \hat{n}_\downarrow = \frac{U}{2}\hat{n} - \frac{U}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)^2$$

and

$$\hat{H} = \hat{H}_0 + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$$= \hat{H}_0 + \frac{U}{2}\sum_i \left(\hat{n}_i - (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 \right)$$

$$= \hat{H}_0 + \frac{U}{2}\hat{N} - \frac{U}{2}\sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2$$

$U>0$ favours $\langle \hat{n}_{i\uparrow} \rangle \neq \langle \hat{n}_{i\downarrow} \rangle$

this is a constant for fixed particle number; otherwise it can be absorbed into a chemical ~~poten~~ potential

→ consider the mean-field decoupling of this magnetic channel

$$(\hat{n}_\uparrow - \hat{n}_\downarrow)^2 = 4\hat{M}\hat{M}$$

$$\simeq 4\left[\langle \hat{M} \rangle \hat{M} + \hat{M}\langle \hat{M} \rangle - \langle \hat{M} \rangle^2 \right]$$

$$= 8\langle \hat{M} \rangle \hat{M} - 4\langle \hat{M} \rangle^2$$

where $\hat{M} = \frac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow) = \frac{1}{2} c^\dagger \sigma^z c$

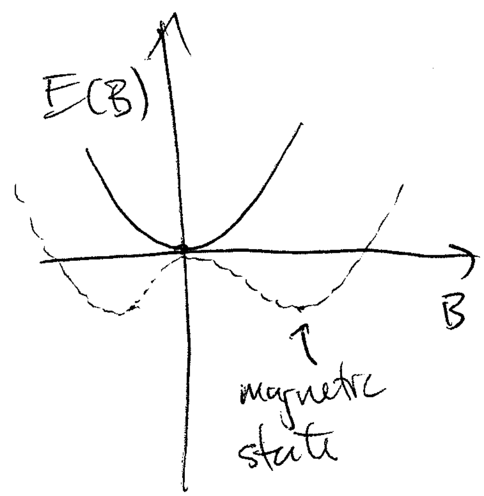
Then

$$-\frac{U}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)^2 \simeq -4U\langle \hat{M} \rangle \hat{M} + 2U \langle \hat{M} \rangle^2$$

$$= -B\hat{M} + \frac{B^2}{8U}$$

where $B = 4U\langle \hat{M} \rangle$ is an effective local field

So $\hat{H}_{MF} = \hat{H}_0 - B\hat{M} + \frac{B^2}{8U}$



and the variation energy

$$E(B) = \langle \psi | \hat{H}_0 - B\hat{M} | \psi \rangle + \frac{B^2}{8U}$$

may have a minimum at $B=0$ or some $B \neq 0$

→ Now consider what we call the "pairing" channel

$$\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$$

swap

$$= - c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\uparrow} c_{i\downarrow}$$

swap

$$= + c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow} c_{i\uparrow} \equiv \hat{A}^{\dagger}_i A_i$$

where $\hat{A}_i = c_{i\downarrow} c_{i\uparrow}$

So

$$U n_{i\uparrow} n_{i\downarrow} = U \hat{A}^{\dagger}_i \hat{A}_i$$

$$\simeq U \langle A_i \rangle^{*} \hat{A}_i + U \hat{A}^{\dagger}_i \langle A_i \rangle - U |\langle \hat{A}_i \rangle|^2$$

$$= \Delta^{*} \hat{A}_i + \Delta \hat{A}^{\dagger}_i - \frac{|\Delta|^2}{U}$$

→ Move the description to k-space

$$\hat{A}_j = c_{j\downarrow} c_{j\uparrow} = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{R}_j} c_{k\downarrow} \cdot \frac{1}{\sqrt{N}} \sum_{k'} e^{i\vec{k}'\cdot\vec{R}_j} c_{k'\uparrow}$$

$$= \frac{1}{N} \sum_{kk'} e^{i(\vec{k}+\vec{k}')\cdot\vec{R}_j} c_{k\downarrow} c_{k'\uparrow}$$

so that $\displaystyle \sum_j \hat{A}_j = \sum_{kk'} \left(\frac{1}{N} \sum_j e^{i(k+k')\cdot R_j} \right) c_{k\downarrow} c_{k'\uparrow} = \sum_k c_{k\downarrow} c_{-k\uparrow}$

and $\displaystyle U \sum_j n_{j\uparrow} n_{j\downarrow} \simeq \Delta^* \sum_k c_{k\downarrow} c_{-k\uparrow} + \Delta \sum_k c^+_{-k\uparrow} c^+_{k\downarrow} - N \frac{|\Delta|^2}{U}$

* We've arrived at what's called the Bardeen-Cooper-Schrieffer (BCS) Hamiltonian

$$\hat{H} = \underset{\substack{\uparrow \\ \text{band structure for a} \\ \text{translationally invariant system}}}{\hat{H}_0} + U \sum_j \hat{n}_{j\uparrow} n_{j\downarrow}$$

$$\simeq \sum_k \left\{ \varepsilon_k c^+_{k\uparrow} c_{k\uparrow} + \varepsilon_k c^+_{k\downarrow} c_{k\downarrow} + \Delta^* c_{k\downarrow} c_{-k\uparrow} + \Delta c^+_{-k\uparrow} c^+_{k\downarrow} - \frac{|\Delta|^2}{U} \right\}$$

In the grand canonical ensemble,

$$\hat{H}_{MF} - \mu \hat{N} = \sum_k \Big\{ (\varepsilon_k - \mu) c^{\dagger}_{k\uparrow} c_{k\uparrow} + (\varepsilon_k - \mu) \underbrace{c^{\dagger}_{k\downarrow} c_{k\downarrow}}_{=1 - c_{k\downarrow} c^{\dagger}_{k\downarrow}}$$

$$+ \Delta^{*} c_{k\downarrow} c_{-k\uparrow} + \Delta c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} - \frac{|\Delta|^2}{U} \Big\}$$

$$= \sum_k \Big\{ (\varepsilon_k - \mu) c^{\dagger}_{k\uparrow} c_{k\uparrow} + \Delta c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow}$$

$$+ \Delta^{*} \underbrace{c_{-k\downarrow} c_{k\uparrow}} - (\varepsilon_k - \mu) \underbrace{c_{-k\downarrow} c_{-k\downarrow}} + (\varepsilon_k - \mu) - \frac{|\Delta|^2}{U} \Big\}$$

inversion symmetry
$\varepsilon_{-k} = \varepsilon_k$

$$= \sum_k \begin{pmatrix} c^{\dagger}_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^{*} & \mu - \varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix} + \text{const}$$

we've eliminated the four-fermion terms, but this is not bilinear in the way we know how to solve

* Is there a set of transformed operators $\gamma, \gamma^\dagger$ that will diagonalize the Hamiltonian? (i.e. $\hat{H} - \mu\hat{N} \simeq \sum_{k,n} E_{k,n} \gamma_{kn}^\dagger \gamma_{kn}$)

→ There is, but we have to express γ as a linear combination of c and $c^\dagger$ terms

→ The bare electron is no longer a natural excitation in this model

NB $[\hat{H}_{MF}, \hat{N}] \neq 0$

→ Introduce a unitary transformation

$$\mathcal{U} = \begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix} \qquad \mathcal{U}^{-1} = \begin{pmatrix} u^* & -v \\ v^* & u \end{pmatrix}$$

with $\det(\mathcal{U}) = |u|^2 + |v|^2 = 1$

such that

$$\gamma = \begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix} = \mathcal{U}^{-1} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix}$$

<u>EXERCISE</u>: Show that the $\gamma, \gamma^\dagger$ ops are fermions

$$\{\gamma_n, \gamma_m^\dagger\} = (|u|^2 + |v|^2)\delta_{nm} = \delta_{nm}$$

Then

$$H_{MF} - \mu N = \sum_k \begin{pmatrix} c_{k\uparrow}^\dagger & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^* & \mu - \varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{pmatrix} \cdots$$

$$= \sum_k \begin{pmatrix} \gamma_{k1}^\dagger & \gamma_{k2}^\dagger \end{pmatrix} \underbrace{\begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^* & \mu - \varepsilon_k \end{pmatrix} \begin{pmatrix} u^* & -v \\ v^* & u \end{pmatrix}} \begin{pmatrix} \gamma_{k1} \\ \gamma_{k2} \end{pmatrix} \cdots$$

$$= \left(\begin{array}{c|c} (\varepsilon_k - \mu)(|u|^2 - |v|^2) + 2\,\mathrm{Re}\,\Delta v^* u & -2(\varepsilon_k - \mu) u v - \Delta v^2 + \Delta u^2 \\ \hline -2(\varepsilon_k - \mu) u^* v^* - \Delta v^{*2} + \Delta^* u^{*2} & -(\varepsilon_k - \mu)(|u|^2 - |v|^2) - 2\,\mathrm{Re}\,\Delta u v^* \end{array}\right)$$

$$\equiv \begin{pmatrix} E_{k1} & 0 \\ 0 & E_{k2} \end{pmatrix} \quad \text{diagonalize}$$

Solve for

$$2(\varepsilon_k - \mu) u v = \Delta u^2 - \Delta^* v^2$$

Define $u = e^{i\alpha} \cos\chi$ $\quad \left(|u|^2 + |v|^2 = 1 \right)$

$v = e^{i\beta} \sin\chi$

$\Delta = |\Delta| e^{i\delta}$

$$2(\varepsilon_k-\mu)e^{i(\alpha+\beta)} - |\Delta|\cos^2\chi\, e^{i(\delta+2\alpha)}$$
$$-|\Delta|\sin^2\chi\, e^{i(-\delta+2\beta)}$$

Need $\alpha+\beta = \delta+2\alpha = -\delta+2\beta$

i.e. $\delta = \beta-\alpha$

and $\alpha+\beta$ is unrestricted

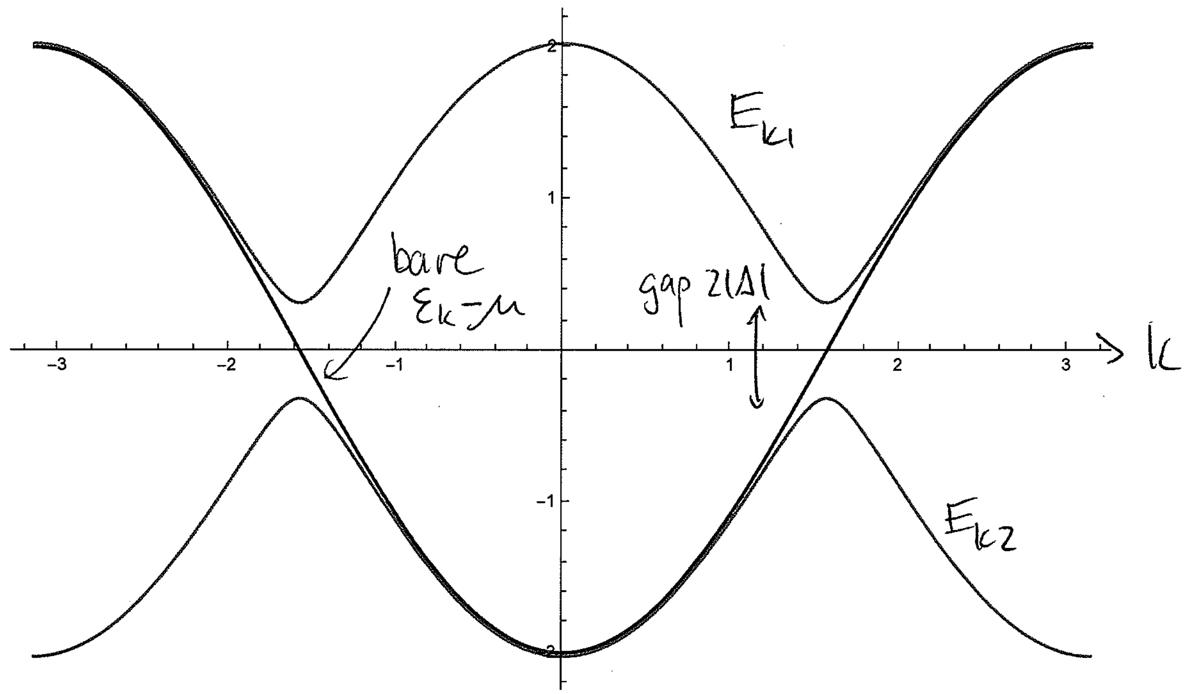
We choose $\alpha = -\beta = -\phi/2$. For χ, we set

$$(\varepsilon_k-\mu)\sin 2\chi = |\Delta|\cos 2\chi$$

or $$\tan 2\chi = \frac{|\Delta|}{\varepsilon_k-\mu}$$

$$\Rightarrow \begin{pmatrix} E_{k1} & 0 \\ 0 & E_{k2} \end{pmatrix} = \begin{pmatrix} \sqrt{(\varepsilon_k-\mu)^2+|\Delta|^2} & 0 \\ 0 & -\sqrt{(\varepsilon_k-\mu)^2+|\Delta|^2} \end{pmatrix}$$

$$E_{k2} = -E_{k1}$$



→ the resulting state is an insulator of Bogoliubov quasiparticles

→ 2Δ is the energy gap associated with breaking a Cooper pair