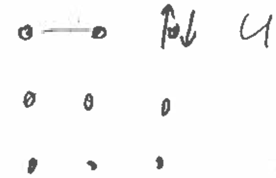
LECTURE 14

The Hubbard model and the magnetic instability of the electron gas.



$$H = \sum_{i,j,\sigma} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} \qquad n_{j\sigma} = c^{\dagger}_{j\sigma} c_{j\sigma}$$

hopping between sites — on-site interaction

- simplest model for interacting electrons on the lattice

Momentum space representation: $H = H_0 + H_1$

$$H_0 = \sum_{p\sigma} \varepsilon_p\, c^{\dagger}_{p\sigma} c_{p\sigma}$$

$$H_1 = \frac{U}{N} \sum_{pp'q} c^{\dagger}_{p+q\uparrow} c_{p\uparrow}\, c^{\dagger}_{p'-q\downarrow} c_{p'\downarrow}$$

- Kubo formula for the magnetic susceptibility tensor

- to investigate magnetic properties couple to external B-field

$$H_{ext} = -\int \vec{B}(\vec{x},t) \cdot \vec{\sigma}(\vec{x})\, d^3x$$

$\vec{\sigma}(\vec{x})$ - electron spin density operator

$$\vec{\sigma}(\vec{x}) = \sum_{x_{el}} \delta(\vec{x} - \vec{x}_{el})\, \vec{\sigma}_{el}$$

$$\left.\begin{array}{l} \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \\ \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{array}\right\} \text{Pauli matrices}$$

- use units such that

$\mu_B = e\hbar/2mc = 1$

- In second quantization we have

$$\vec{\sigma}(\vec{x}) = \sum_j \delta(\vec{x} - \vec{x}_j)\, \psi_j^{+} \vec{\sigma} \psi_j \qquad \psi_j = \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix}$$

$$= \sum_j \delta(\vec{x} - \vec{x}_j)\, c^{\dagger}_{j\alpha} \vec{\sigma}_{\alpha\beta} c_{j\beta}$$

$$= \sum_q e^{i\vec{q}\cdot\vec{x}} \sum_p c^{\dagger}_{p+q\alpha} \vec{\sigma}_{\alpha\beta} c_{p\beta}$$

- Define spin raising & lowering operators:

$$\sigma^{\pm} = \frac{1}{2}(\sigma^x \pm i\sigma^y)$$

$$\left(\begin{array}{l} \sigma^{+}(\vec{x}) = \sum_q e^{i\vec{x}\cdot\vec{q}} \sum_p c^{\dagger}_{p+q\uparrow} c_{p\downarrow} \\ \sigma^{-}(\vec{x}) = \sum_q e^{i\vec{x}\cdot\vec{q}} \sum_p c^{\dagger}_{p+q\downarrow} c_{p\uparrow} \end{array}\right)$$

- We are interested in mag. moment induced by $\vec{B}$.

$$\langle \vec{\sigma}(\vec{x},t)\rangle = \langle \Psi(t)|\,\vec{\sigma}(\vec{x})\,|\Psi(t)\rangle$$

– to leading order in $\vec{B}$ we find (usual steps)

$$\langle \sigma^i(\vec{x},t)\rangle = \langle \sigma^i(\vec{x},t)\rangle_{B=0} +$$
$$+ \sum_j \int dt' \int d^3x' \; \chi^{ij}(\vec{x}-\vec{x}', t-t')\, B^j(\vec{x}',t')$$
$$\chi^{ij}(\vec{x}-\vec{x}', t-t') = i\,\theta(t-t')\langle [\sigma^i(\vec{x},t), \sigma^j(\vec{x}',t')]\rangle$$

Kubo formula for mag. susceptibility

- We'll be interested in

$$\chi^{-+}(\vec{x}-\vec{x}', t-t') = i\theta(t-t')\langle[\sigma^-(\vec{x},t), \sigma^+(\vec{x}',t')]\rangle$$
$$= \sum_{pq} e^{i\vec{q}\cdot\vec{x}}\, \chi^{-+}(\vec{p},\vec{q},t)$$

$$\chi^{-+}(\vec{p},\vec{q},t) = i\theta(t)\langle[c^+_{p+q\downarrow}(t)\, c_{p\uparrow}(t), \sigma^+(0,0)]\rangle$$

- Following standard steps to evaluate χ^{-+} within FD expansion (details in the textbook)

$$\chi^{+-} =$$

"ladder diagram"

We obtain:

$$\chi^{-+}(\vec{p},\vec{q};\omega) = \frac{(f_{p\uparrow} - f_{p+q\downarrow})\left[1 + \frac{U}{N}\chi^{-+}(\vec{q},\omega)\right]}{\omega + \tilde{\varepsilon}_{p+q\uparrow} - \tilde{\varepsilon}_{p\downarrow}} \qquad (*)$$

$$\chi^{-+}(\vec{q},\omega) = \sum_p \chi^{-+}(\vec{p},\vec{q};\omega)$$

$$\tilde{\varepsilon}_{p\sigma} = \varepsilon_p - \frac{U}{N}\sum_{p'} f_{p',\bar{\sigma}} \qquad \bar{\sigma} = -\sigma$$

Get $\chi^{+}(\vec{q},\omega)$ from by summing both sides over $\vec{p}$:

$$\chi^{-+}(\vec{q},\omega) = \frac{\Gamma^{-+}(\vec{q},\omega)}{1 - U\Gamma^{-+}(\vec{q},\omega)} \qquad (**)$$

$$\Gamma^{-+}(\vec{q},\omega) = \frac{1}{N}\sum_p \frac{f_{p\uparrow} - f_{p+q\downarrow}}{\omega - (\tilde{\varepsilon}_{p\downarrow} - \vec{\varepsilon}_{p+q\uparrow}) + i\varepsilon}$$

- <u>The magnetic instability criterion</u>

- For weak interaction U we expect paramagnetic state with $f_{p\uparrow} = f_{p\downarrow} = f_p$, $\tilde{\varepsilon}_{p\uparrow} = \tilde{\varepsilon}_{p\downarrow} = \varepsilon_p$ and denominator in $(**)$ is <u>nonsingular</u> at $\omega = 0$. (Singularities at $\omega \neq 0$ correspond to collective excitations of the system)
- Vanishing denominator for $\omega = 0$ signals mag. istability

$$\boxed{U\Gamma(\vec{q},0) = 1}$$

where $\Gamma(\vec{q},0) = \frac{1}{N}\sum_p \frac{f_p - f_{p+q}}{\varepsilon_{p+q} - \varepsilon_p}$

(I) <u>Ferromagnetic instability</u> $(\vec{q} \to 0)$ – uniform magnetization

Expand $f_{p+q} \simeq f_p + \vec{q}\cdot\frac{\partial \varepsilon_p}{\partial \vec{p}}\frac{\partial f_p}{\partial \varepsilon_p}$

$\varepsilon_{p+q} \simeq \varepsilon_p + \vec{q}\cdot\frac{\partial \varepsilon_p}{\partial \vec{p}}$

$$\lim_{q\to 0}\Gamma(\vec{q},0) = \frac{1}{N}\sum_p\left(-\frac{\partial f_p}{\partial \varepsilon_p}\right) \xrightarrow{T=0} \underbrace{\frac{1}{N}\sum_p \delta(\varepsilon_p - \varepsilon_F)}_{\mathcal{N}(\varepsilon_F)}$$

DOS at the Fermi energy

$$\boxed{U\,\mathcal{N}(\varepsilon_F) = 1}$$

"Stoner criterion" for ferromag. instability

In 3D $\mathcal{N}(\varepsilon) \sim \sqrt{\varepsilon}$ so for large-enough density and strong enough interaction we expect metals to become ferromagnets.

(II) <u>Antiferromagnetic instability</u>

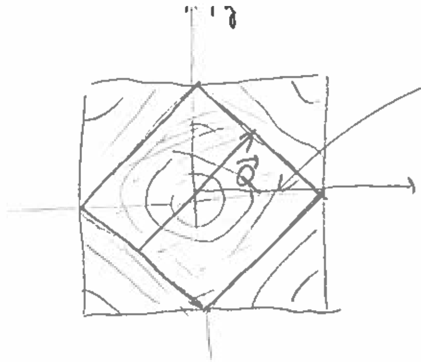
– denominator is zero for $\vec{q} = \vec{Q} \neq 0$.

Consider as an example square lattice in 2D with a nearest neighbor hopping t: $\varepsilon_p = -2t(\cos p_x + \cos p_y)$

For $\vec{Q} = 2\pi\left(\frac{1}{2}, \frac{1}{2}\right)$ "nesting vector"

it holds

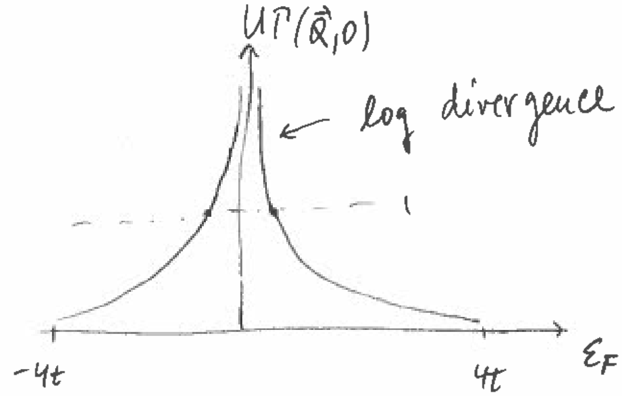
$$\varepsilon_{\vec{p}+\vec{Q}} = -\varepsilon_{\vec{p}}$$



$$\Gamma(\vec{Q},0) = \frac{1}{N}\sum_p \frac{f_p - f_{p+Q}}{\varepsilon_{p+Q} - \varepsilon_p} = \frac{1}{N}\sum_p \frac{f_p - (1-f_p)}{-2\varepsilon_p}$$

$$= -\int_{-4t}^{\varepsilon_F} \frac{N(\varepsilon)}{2\varepsilon}\, d\varepsilon + \int_{-\varepsilon_F}^{4t} \frac{N(\varepsilon)}{2\varepsilon}\, d\varepsilon$$

$$= -\int_{-4t}^{\varepsilon_F} \frac{N(\varepsilon)}{\varepsilon}\, d\varepsilon$$



Conclusion: At $\vec{Q} = (\pi,\pi)$ and close to half-filling the system undergoes an AF instability.

Metal becomes an insulating antiferromagnet.

$f(-\varepsilon) = 1 - f(\varepsilon)$