Phys 726 – Lecture 7

Degenerate Electron Gas

$$\hat{H} = \sum_{\vec{k},\alpha} \frac{\hbar^2 k^2}{2m} c^\dagger_{\vec{k}\alpha} c_{\vec{k}\alpha} + \frac{e^2}{2V} \sum_{\vec{k}\vec{k}'} \sum_{\substack{\alpha \\ \beta}} \frac{4\pi}{q^2} c^\dagger_{\vec{k}+\vec{q}\alpha} c^\dagger_{\vec{k}'\beta} c_{\vec{k}'+\vec{q},\beta} c_{\vec{k}\alpha}$$

$\vec{q} \neq 0$

charge neutrality
($q=0$ component cancels
the positive background)

* We argued that the kinetic term dominates at high density ($r_s \ll 1$) and the Coulomb term at low density ($r_s \gg 1$)

* At the extremal values, the ground states are the Fermi Sea

$$|F\rangle = \left(\prod_{k<k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} \right) |vac\rangle \quad \text{for } r_s = 0$$

and the Wigner Crystal

$$|W\rangle = \left(\prod_{\vec{R} \in BCC} \hat{\psi}^\dagger(\vec{R}) \right) |vac\rangle \quad \text{for } r_s = \infty$$

* Last class, we treated these as trial wave functions for the ground state at intermediate values of r_s

→ comparison of variational energies

$$E[|F\rangle] = \langle F|\hat{H}|F\rangle = \frac{Ne^2}{2a_0}\left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \cdots\right)$$

$$E[|W\rangle] = \langle W|\hat{H}|W\rangle = \frac{Ne^2}{2a_0}\left(-\frac{1.79}{r_s} + \frac{2.66}{r_s^{3/2}} + \cdots\right)$$

lattice summation of electrostatic repulsion for point charges in the body-centered cubic arrangement

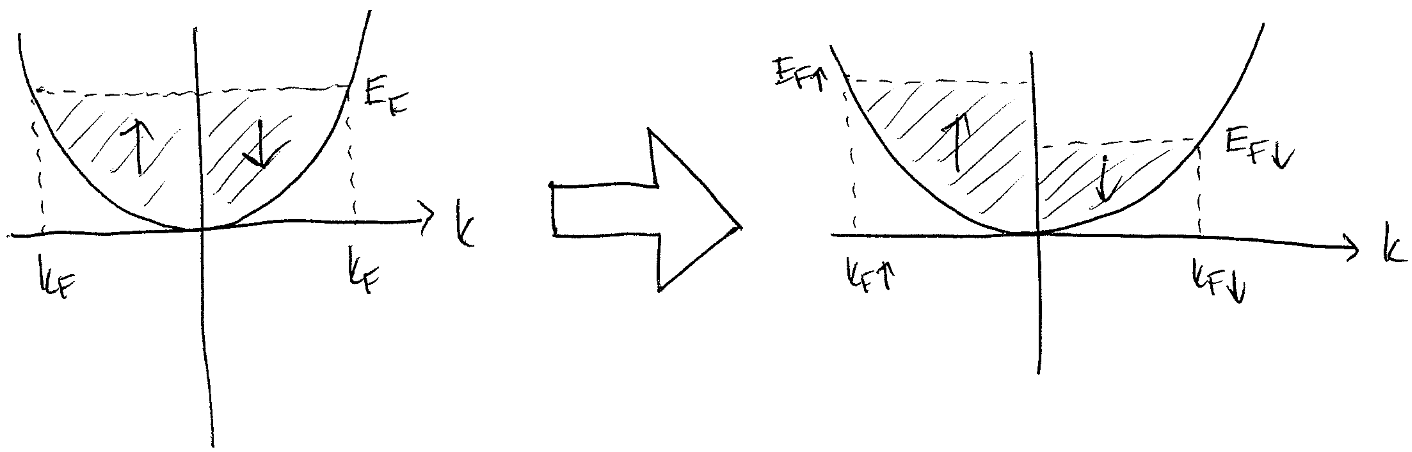
kinetic contribution from quantum zero-point motion

→ We expect to find a critical value of r_s above which the Fermi Liquid freezes into the Wigner Crystal

→ accompanied by a symmetry reduction so that only discrete translations and rotations are allowed

Itinerant Ferromagnet

* Another possibility is the spontaneous polarization of spins in the Fermi Liquid



$$|F\rangle = \left(\prod_{k<k_F} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow}\right)|vac\rangle \qquad |F'\rangle = \left(\prod_{k<k_{F\uparrow}} c^\dagger_{k\uparrow}\right)\left(\prod_{k<k_{F\downarrow}} c^\dagger_{k\downarrow}\right)|vac\rangle$$

Constant total density $n = \frac{N}{V} = n_\uparrow + n_\downarrow$ across the two species with population imbalance $\delta n = n_\uparrow - n_\downarrow$

i.e. $\frac{N_\uparrow}{V} = \frac{n+\delta n}{2}$ and $\frac{N_\downarrow}{V} = \frac{n-\delta n}{2}$

Density for spin-α particles

$$n_\alpha = \frac{N_\alpha}{V} = \int \frac{d^3k}{(2\pi)^3} \langle F' | c^\dagger_{k\alpha} c_{k\alpha} | F' \rangle$$

$$= \int_0^{k_{F\alpha}} \frac{4\pi k^2 dk}{8\pi^3} = \frac{1}{2\pi^2} \cdot \frac{1}{3} k_{F\alpha}^3 \Rightarrow \boxed{k_{F\alpha} = (6\pi^2 n_\alpha)^{1/3}}$$

Total kinetic energy

$$E_0 = \frac{V}{8\pi^3} \int_0^{k_{F\uparrow}} 4\pi k^2 dk \, \frac{\hbar^2 k^2}{2m} + \frac{V}{8\pi^3} \int_0^{k_{F\downarrow}} 4\pi k^2 dk \cdot \frac{\hbar^2 k^2}{2m}$$

$$= \frac{V\hbar^2}{20\pi^2 m} \left(k_{F\uparrow}^5 + k_{F\downarrow}^5 \right) = \frac{V\hbar^2 (6\pi^2)^{5/3}}{20\pi^2 m} \left(n_\uparrow^{5/3} + n_\downarrow^{5/3} \right)$$

$$= \frac{V\hbar^2 (6\pi^2)^{5/3}}{20\pi^2 m} \left[\left(\frac{n+\delta n}{2} \right)^{5/3} + \left(\frac{n-\delta n}{2} \right)^{5/3} \right]$$

$$= \frac{V\hbar^2 (3\pi^2)^{5/3}}{20\pi^2 m} n^{5/3} \underbrace{\left[\left(1+\frac{\delta n}{n}\right)^{5/3} + \left(1-\frac{\delta n}{n}\right)^{5/3} \right]}_{2 + \frac{10}{9}\left(\frac{\delta n}{n}\right)^2 + O\left(\frac{\delta n}{n}\right)^4}$$

$$\left(\frac{N}{V}\right)^{5/3} = \frac{N}{V} n^{2/3}$$

$$= N \frac{\hbar^2 (3\pi^2)^{5/3}}{10\pi^2 m} \left(1 + \frac{5}{9} \left(\frac{\delta n}{n} \right)^2 + \cdots \right) \cdot n^{2/3}$$

$$n^{2/3} = \left(\frac{N}{V}\right)^{2/3} = \left(\frac{N}{\frac{4}{3}\pi r_0^3 N}\right)^{2/3} = \left(\frac{3}{4\pi r_0^3}\right)^{2/3}$$

$$= \left(\frac{3}{4\pi}\right)^{2/3} \frac{1}{r_0^2} = \left(\frac{3}{4\pi}\right)^{2/3} \frac{1}{a_0^2 r_s^2}$$

$$E_0 = N \frac{\hbar^2}{m a_0^2} \frac{(3\pi^2)^{5/3}}{10\pi^2} \cdot \left(\frac{3}{4\pi}\right)^{2/3} \frac{1}{r_s^2} \left(1 + \frac{5}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots\right)$$

$$= N \frac{\hbar^2}{m a_0^2} \frac{3}{10} \left(\frac{9\pi}{4}\right)^{2/3} \cdot \frac{1}{r_s^2} \left(1 + \frac{5}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots\right)$$

$$= N \frac{e^2}{2a_0} \frac{3}{5} \left(\frac{9\pi}{4}\right)^{2/3} \frac{1}{r_s^2} \left(1 + \frac{5}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots\right)$$

Average Coulomb energy

$$\Delta E = \frac{e^2}{2V} \sum_{\substack{kk' \\ q\neq 0}} \sum_{\alpha\beta} \frac{4\pi}{q^2} \langle F' | \overbrace{c^\dagger_{k+q\,\alpha}\, c^\dagger_{k'\beta}\, c_{k'+q\,\beta}\, c_{k\alpha}}^{\sim \delta_{q,0}} | F' \rangle$$

$$= \frac{e^2}{2V} \sum_{\substack{kk' \\ q\neq 0}} \sum_{\alpha\beta} \frac{4\pi}{q^2} \left(- \delta_{kk'} \delta_{\alpha\beta}\, \theta(k_{F\alpha} - k)\, \theta(k_{F\alpha} - |k+q|) \right)$$

$$= -\frac{2\pi e^2}{V} \sum_{k,q\neq 0} \sum_\alpha \frac{1}{q^2}\theta(k_{F\alpha}-k)\,\theta(k_{F\alpha}-|k+q|)$$

$$= -2\pi e^2 V \sum_\alpha \int \frac{d^3k}{(2\pi)^3}\int \frac{d^3q}{(2\pi)^3}\frac{1}{q^2}\,\theta(k_{F\alpha}-k)\,\theta(k_{F\alpha}-|k+q|)$$

$$= -\frac{2\pi e^2}{(2\pi)^6} V \sum_\alpha \int 4\pi q^2 dq \cdot \frac{1}{q}\underbrace{\int d^3k\,\theta(k_{F\alpha}-k)\,\theta(k_{F\alpha}-|k+q|)}_{\frac{4}{3}\pi k_{F\alpha}^3\left(1-\frac{3}{2}x+\frac{1}{2}x^3\right)\theta(1-x)}$$

where $x = \dfrac{q}{2k_{F\alpha}}$

$$= -\frac{2\pi e^2}{(2\pi)^6} V \sum_\alpha \int \underbrace{4\pi dq}_{=8\pi k_{F\alpha} dx} \cdot \frac{4}{3}\pi k_{F\alpha}^3\left(1-\frac{3}{2}x+\frac{1}{2}x^3\right)\theta(1-x)$$

$$= -\frac{e^2}{(2\pi)^5} V \sum_\alpha 8\pi k_{F\alpha}\cdot\frac{4}{3}\pi k_{F\alpha}^3 \underbrace{\int_0^1\left(1-\frac{3}{2}x+\frac{1}{2}x^3\right)dx}$$

$$= \left[x - \frac{3}{4}x^2 + \frac{1}{8}x^3\right]_0^1$$

$$= 1 - \frac{3}{4} + \frac{1}{8}$$

$$= \frac{8}{8} - \frac{6}{8} + \frac{1}{8} = \frac{3}{8}$$

$$= -\frac{e^2}{(2\pi)^5} V \frac{8}{3} (2\pi)^2 \sum_\alpha k_{F\alpha}^4 \cdot \frac{3}{8} = -\frac{e^2}{(2\pi)^3} V \sum_\alpha (6\pi^2 n_\alpha)^{4/3}$$

$$= -\frac{e^2}{(2\pi)^3} V (6\pi^2)^{4/3} \left[n_\uparrow^{4/3} + n_\downarrow^{4/3} \right]$$

$$= -\frac{e^2}{(2\pi)^3} V (6\pi^2)^{4/3} \left[\left(\frac{n+\delta n}{2}\right)^{4/3} + \left(\frac{n-\delta n}{2}\right)^{4/3} \right]$$

$$= -\frac{e^2}{(2\pi)^3} V (3\pi^2)^{4/3} \left[(n+\delta n)^{4/3} + (n-\delta n)^{4/3} \right]$$

$$= -\frac{e^2}{(2\pi)^3} V (3\pi^2)^{4/3} n^{4/3} \left[\left(1+\frac{\delta n}{n}\right)^{4/3} + \left(1-\frac{\delta n}{n}\right)^{4/3} \right]$$

$$= -\frac{e^2}{(2\pi)^3} (3\pi^2)^{4/3} V \cdot \left(\frac{N}{V}\right)^{4/3} \left[2 + \frac{4}{9}\left(\frac{\delta n}{n}\right)^2 + O\left(\frac{\delta n}{n}\right)^4 \right]$$

$$= -N \cdot \frac{e^2}{(2\pi)^3} (3\pi^2)^{4/3} \left(\frac{N}{V}\right)^{1/3} \left[2 + \frac{4}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots \right]$$

$$= -N \cdot \frac{e^2}{(2\pi)^3} (3\pi^2)^{4/3} \left(\frac{1}{\frac{4}{3}\pi r_0^3}\right)^{1/3} 2 \left(1 + \frac{2}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots \right)$$

$$= -N \cdot \frac{e^2}{(2\pi)^3} (3\pi^2)(3\pi^2)^{1/3} \left(\frac{3}{4\pi}\right)^{1/3} \frac{1}{a_0 r_s} 2 \left(1 + \frac{2}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots \right)$$

$$= -N \cdot \frac{e^2}{2a_0} \frac{3}{2\pi} \left(\frac{9\pi}{4}\right)^{1/3} \left(1 + \frac{2}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots \right)$$

Sum of all energy contributions

$$\frac{E}{N} = \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2}\left(1+\frac{5}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots\right)\right.$$

$$\left. - \frac{0.916}{r_s}\left(1+\frac{2}{9}\left(\frac{\delta n}{n}\right)^2 + \cdots\right)\right]$$

$$= \frac{e^2}{2a_0}\left\{ \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right] + \left[\frac{1.23}{r_s^2} - \frac{0.204}{r_s}\right]\left(\frac{\delta n}{n}\right)^2 \right\}$$

changes sign when

$$r_s = \frac{1.23}{0.204} = 6.03$$

cf. equilibrium density

$r_s = 4.83$

* Actually two distinct thresholds

→ Variational energy $E[|F'\rangle] < E[|F\rangle]$
for $r_s \geq 5.45$

→ Instability $\frac{\partial^2 E(\delta n)}{\partial(\delta n)^2} < 0$ for $r_s \geq 6.03$

Polarization by external field

* Of course, we can always induce a polarization by applying an external magnetic field

→ spins couple to the field via a term

$$-\vec{B}\cdot\hat{\vec{S}} = -\vec{B}\cdot\frac{1}{2}\sum_{\alpha\beta}\hat{\psi}^\dagger_\alpha(\vec{r})\,\vec{\sigma}_{\alpha\beta}\,\hat{\psi}_\beta(\vec{r})$$

spin of an electron at position $\vec{r}$

$\vec{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ vector of Pauli matrices

→ this is the Zeeman effect

→ here, we'll treat the spin as unitless and measure $\vec{B}$ in units of energy (absorbing $\hbar$, the Bohr magneton, and Landé g-factor)

* The Hamiltonian will be augmented by a term that couples $\vec{B}$ to all the spins

$$-\vec{B}\cdot\int d^3r\ \frac{1}{2}\sum_{\alpha\beta}\hat{\psi}^\dagger_\alpha(\vec{r})\,\vec{\sigma}_{\alpha\beta}\,\hat{\psi}_\beta(\vec{r})$$

$$= -\vec{B}\cdot \int d^3r\ \frac{1}{2}\sum_{\alpha\beta}\left(\sum_k \phi_k(\vec{r})^* c_{k\alpha}^\dagger\right)\sigma_{\alpha\beta}\left(\sum_{k'}\phi_{k'}(\vec{r})c_{k'\beta}\right)$$

$$= -\vec{B}\cdot \frac{1}{2}\sum_{\alpha\beta}\sum_{kk'}\underbrace{\left(\int d^3r\ \phi_k(\vec{r})^*\phi_{k'}(\vec{r})\right)}_{\substack{\delta_{kk'} \\ \text{by completeness}}} c_{k\alpha}^\dagger\vec{\sigma}_{\alpha\beta}c_{k'\beta}$$

$$= -\vec{B}\cdot\frac{1}{2}\sum_{\alpha\beta}\sum_k c_{k\alpha}^\dagger\vec{\sigma}_{\alpha\beta}c_{k\beta}$$

* If we choose $\vec{B} = B\vec{e}_z$, then

$$-\frac{B}{2}\sum_{\alpha\beta}\sum_k c_{k\alpha}^\dagger\sigma^z_{\alpha\beta}c_{k\beta}$$

$$= -\frac{B}{2}\sum_{\alpha\beta}\sum_k c_{k\alpha}^\dagger\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_{\alpha\beta}c_{k\beta}$$

$$= -\frac{B}{2}\sum_k\left(c_{k\uparrow}^\dagger c_{k\uparrow} - c_{k\downarrow}^\dagger c_{k\downarrow}\right)$$

$$= -\frac{B}{2}\left(\hat{N}_\uparrow - \hat{N}_\downarrow\right)$$

magnetization ~ spin-up, spin-down population imbalance

* Consider the Hamiltonian of free electrons in this applied field

$$\hat{H} = \sum_k \sum_\alpha \frac{\hbar^2 k^2}{2m} c_{k\alpha}^\dagger c_{k\alpha} - \frac{B}{2} \sum_k \sum_{\alpha\beta} c_{k\alpha}^\dagger \sigma_{\alpha\beta}^z c_{k\beta}$$

$$= \sum_k \frac{\hbar^2 k^2}{2m} (\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow}) - \frac{B}{2} \sum_k (\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow})$$

→ what happens under the transformation $\uparrow \leftrightarrow \downarrow$?

$$\hat{H} \rightarrow \sum_k \frac{\hbar^2 k^2}{2m} (\hat{n}_{k\downarrow} + \hat{n}_{k\uparrow}) - \frac{B}{2} \sum_k (\hat{n}_{k\downarrow} - \hat{n}_{k\uparrow})$$

$$= \sum_k \frac{\hbar^2 k^2}{2m} (\hat{n}_{k\uparrow} + \hat{n}_{k\downarrow}) + \frac{B}{2} \sum_k (\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow})$$

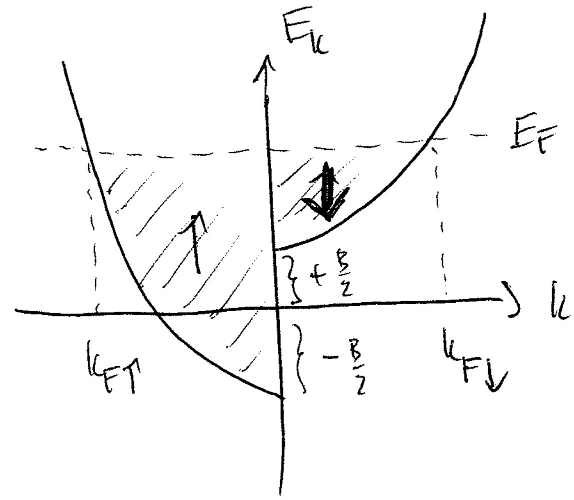
* When $B \neq 0$, exchanging up and down spins is no longer a symmetry of the model.

Instead $(\vec{B}, \uparrow, \downarrow) \rightarrow (-\vec{B}, \downarrow, \uparrow)$ is a symmetry

* Collect the common one-body terms

$$\hat{H} = \sum_k \left\{ \left(\frac{\hbar^2 k^2}{2m} - \frac{B}{2} \right) \hat{n}_{k\uparrow} + \left(\frac{\hbar^2 k^2}{2m} + \frac{B}{2} \right) \hat{n}_{k\downarrow} \right\}$$

$B > 0$



Ground state

$$|F_B\rangle = \left(\prod_{k<k_{F\uparrow}} c^\dagger_{k\uparrow} \right) \left(\prod_{k<k_{F\downarrow}} c^\dagger_{k\downarrow} \right) |vac\rangle$$

$$= \left(\prod_{\frac{\hbar^2 k^2}{2m} - \frac{B}{2} < E_F} c^\dagger_{k\uparrow} \right) \left(\prod_{\frac{\hbar^2 k^2}{2m} + \frac{B}{2} < E_F} c^\dagger_{k\downarrow} \right) |vac\rangle$$

with energy

$$\langle F_B | \hat{H} | F_B \rangle = \sum_k \left\{ \left(\frac{\hbar^2 k^2}{2m} - \frac{B}{2} \right) \theta\left(E_F - \frac{\hbar^2 k^2}{2m} + \frac{B}{2} \right) + \left(\frac{\hbar^2 k^2}{2m} + \frac{B}{2} \right) \theta\left(E_F - \frac{\hbar^2 k^2}{2m} - \frac{B}{2} \right) \right\}$$

$$= V \int \frac{d^3k}{(2\pi)^3} \left\{ \left(\frac{\hbar^2 k^2}{2m} - \frac{B}{2} \right) \theta\left(E_F - \frac{\hbar^2 k^2}{2m} + \frac{B}{2} \right) \right.$$

$$\left. + \left(\frac{\hbar^2 k^2}{2m} + \frac{B}{2} \right) \theta\left(E_F - \frac{\hbar^2 k^2}{2m} - \frac{B}{2} \right) \right\}$$

$$= V \int \frac{d^3k}{(2\pi)^3} \left[\int d\varepsilon \, \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m} \right) \right] \{ \cdots \}$$

$$= V \int d\varepsilon \underbrace{\int \frac{d^3k}{(2\pi)^3} \delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m} \right)}_{\substack{\text{density of states} \\ D(\varepsilon)}} \left\{ \left(\varepsilon - \frac{B}{2} \right) \theta\left(E_F - \varepsilon + \frac{B}{2} \right) + \left(\varepsilon + \frac{B}{2} \right) \theta\left(E_F - \varepsilon - \frac{B}{2} \right) \right\}$$

$$= V \int d\varepsilon \, D(\varepsilon) \left\{ \left(\varepsilon - \frac{B}{2} \right) \theta\left(E_F - \varepsilon + \frac{B}{2} \right) \right.$$

$$\left. + \left(\varepsilon + \frac{B}{2} \right) \theta\left(E_F - \varepsilon - \frac{B}{2} \right) \right\}$$

$$= V \int_{-\infty}^{\varepsilon_F + B/2} d\varepsilon \, D(\varepsilon) \left(\varepsilon - \frac{B}{2} \right) + V \int_{-\infty}^{\varepsilon_F - B/2} d\varepsilon \, D(\varepsilon) \left(\varepsilon + \frac{B}{2} \right)$$

$$= V \int^{\varepsilon_F} d\varepsilon \left(D\left(\varepsilon + \frac{B}{2}\right) + D\left(\varepsilon - \frac{B}{2}\right) \right) \varepsilon = 2V \int^{\varepsilon_F} d\varepsilon \, D(\varepsilon) \varepsilon + V \int^{\varepsilon_F} d\varepsilon \, D''(\varepsilon) \varepsilon \frac{B^2}{4} + \cdots$$