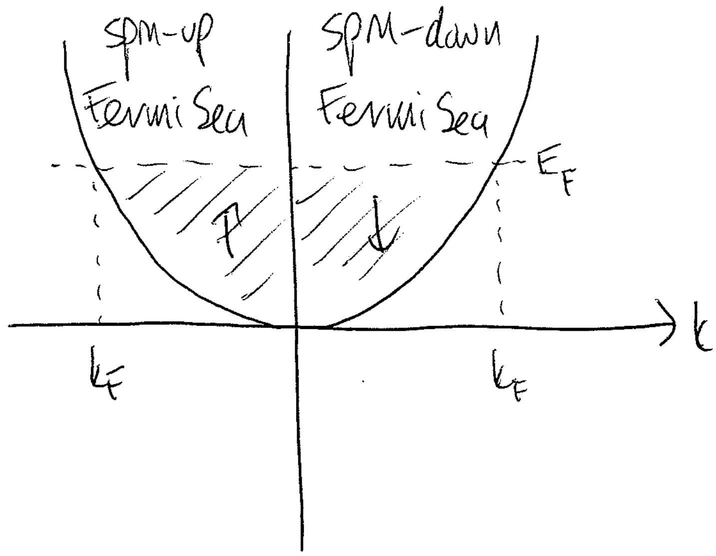
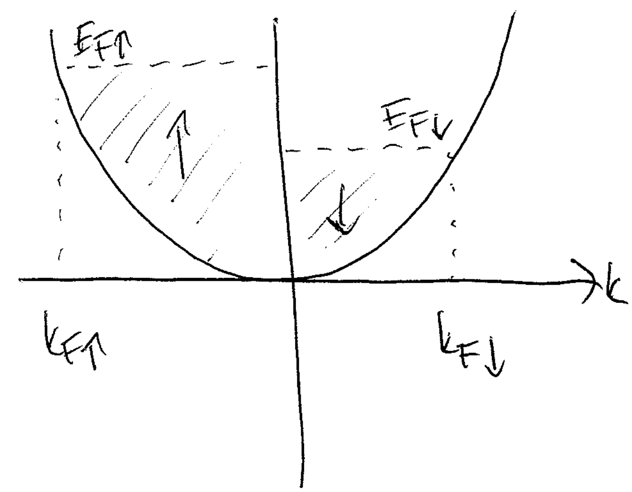
Phys 726 - Lecture 8

Induced polarization and linear response

* We showed that, at the level of a variational calculation, repulsive interactions can cause a Fermionic system to spontaneously polarize





$$\frac{E}{N} = \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}E_F \qquad\qquad \frac{E_\alpha}{N_\alpha} = \frac{3}{5}\frac{\hbar^2 k_{F\alpha}^2}{2m} = \frac{3}{5}E_{F\alpha} \quad \text{for each of } \alpha = \uparrow, \downarrow$$

$$E = \frac{3}{5}E_F \cdot N \qquad\qquad E = \frac{3}{5}\left(E_{F\uparrow}N_\uparrow + E_{F\downarrow}N_\downarrow\right)$$

$$\sim \left(N_\uparrow^{2/3+1} + N_\downarrow^{2/3+1}\right)$$

→ population imbalance $\Delta N = N_\uparrow - N_\downarrow \neq 0$

→ kinetic energy

$$E(\Delta N) \sim (N + \Delta N)^{5/3} + (N + \Delta N)^{5/3}$$

$$= E(0) + (\text{const.} > 0)\cdot(\Delta N)^2$$

is a monotonically increasing function of ΔN

but compensated at large r_s by the exchange contribution of the Coulomb repulsion term

* Polarization can also be induced by application of an external magnetic field

→ $\vec{B}$ couples to all the spins through a term $-\vec{B}\cdot\vec{M}$, where

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

is the total magnetization

→ expand $\hat{\psi}_\alpha = \sum_k \phi_k(\vec{r})\, c_{k\alpha}$ in one-body eigenstates to obtain

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

Same structure as the one-body kinetic energy (bilinear in $c^\dagger, c$ and diagonal in momentum k)

→ free to choose spin quantization axis so that it aligns with the field: $\vec{B} = B\vec{e}_z$.
Then

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

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

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

* Hamiltonian for free electrons in an applied field (ignoring orbital coupling!) is

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

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

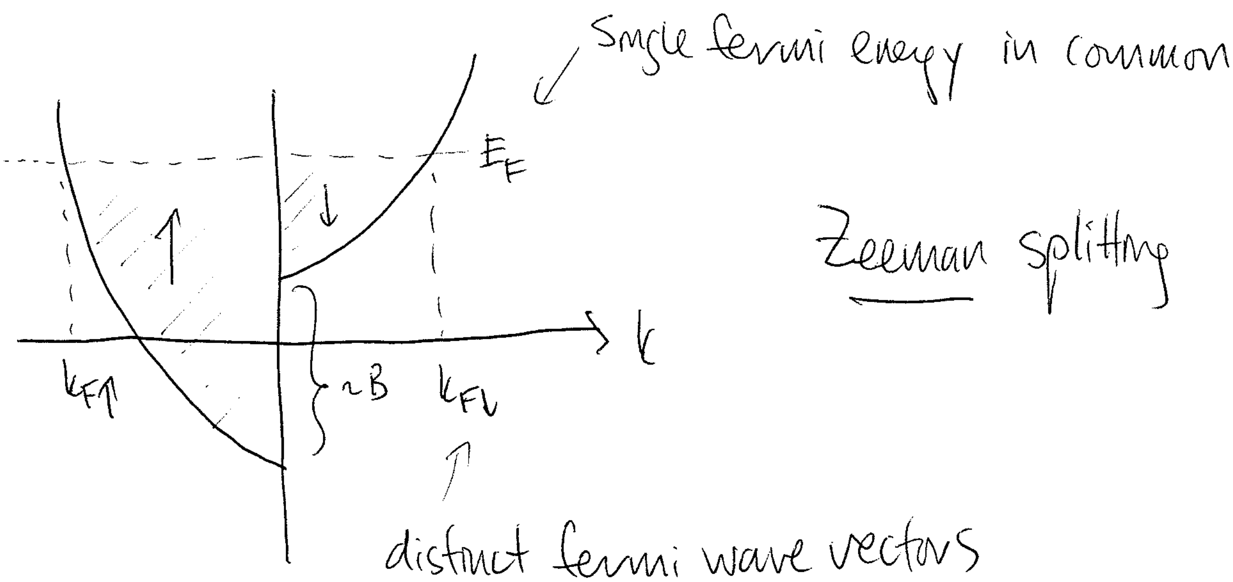
→ symmetry of the model is broken by hand: swapping ↑ and ↓ doesn't leave the system invariant so long as $B \neq 0$

* Rewrite as the sum of an up-spin and down-spin Hamiltonian with shifted dispersion

$$\hat{H} = \sum_{k}\sum_{\alpha} \varepsilon_{k\alpha} \hat{n}_{k\alpha}$$

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

* For $B > 0$



Zeeman splitting

→ ground state

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

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

with energy eigenvalue

$$\hat{H}|F_B\rangle = E_0(B)|F_B\rangle$$

and $E_0(B) = \sum_k \sum_\alpha \varepsilon_{k\alpha}\,\theta(E_F - \varepsilon_{k\alpha})$

$$E_0(B) = \sum_k \sum_{\alpha=\uparrow,\downarrow} \varepsilon_{k\alpha}\, \theta(E_F - \varepsilon_{k\alpha})$$

$$= \sum_k \sum_{n=\pm1} \left(\varepsilon_k - \frac{nB}{2}\right) \theta\left(E_F - \varepsilon_k + \frac{n}{2}B\right)$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

$$= V \int \frac{d^3k}{(2\pi)^3} \sum_{n=\pm1} \Big[\underbrace{\int d\varepsilon\, \delta(\varepsilon - \varepsilon_k)}_{=1} \Big] \left(\varepsilon_k - \frac{nB}{2}\right) \theta\left(E_F - \varepsilon_k + \frac{n}{2}B\right)$$

$$= V \sum_{n=\pm1} \int d\varepsilon \Big[\underbrace{\int \frac{d^3k}{(2\pi)^3} \delta(\varepsilon - \varepsilon_k)}_{\substack{\text{density of states} \\ D(\varepsilon)}} \Big] \left(\varepsilon_k - \frac{n}{2}B\right) \theta\left(E_F - \varepsilon_k + \frac{n}{2}B\right)$$

$$= V \sum_{n=\pm1} \int d\varepsilon\, D(\varepsilon) \left(\varepsilon - \frac{n}{2}B\right) \theta\left(E_F - \varepsilon + \frac{n}{2}B\right)$$

shift variable of integration $\varepsilon \to \varepsilon + \frac{n}{2}B$

$$= V \sum_{n=\pm1} \int d\varepsilon\, D\left(\varepsilon + \frac{n}{2}B\right) \varepsilon\, \theta(E_F - \varepsilon)$$

* Expand in powers of B, making use of the fact that $n = \pm 1$ implies

$$n^{\text{even}} = 1 \quad \text{and} \quad n^{\text{odd}} = n$$

$$D(\varepsilon + \tfrac{n}{2}B) = D(\varepsilon) + \tfrac{n}{2}B\,D'(\varepsilon) + \frac{1}{2}\left(\frac{n}{2}B\right)^2 D''(\varepsilon) + \frac{1}{6}\left(\frac{n}{2}B\right)^3 D'''(\varepsilon) + \cdots$$

$$= D(\varepsilon) + \tfrac{1}{2}nB\,D'(\varepsilon) + \frac{B^2}{8}D''(\varepsilon) + \frac{1}{48}nB^3 D'''(\varepsilon) + \cdots$$

and

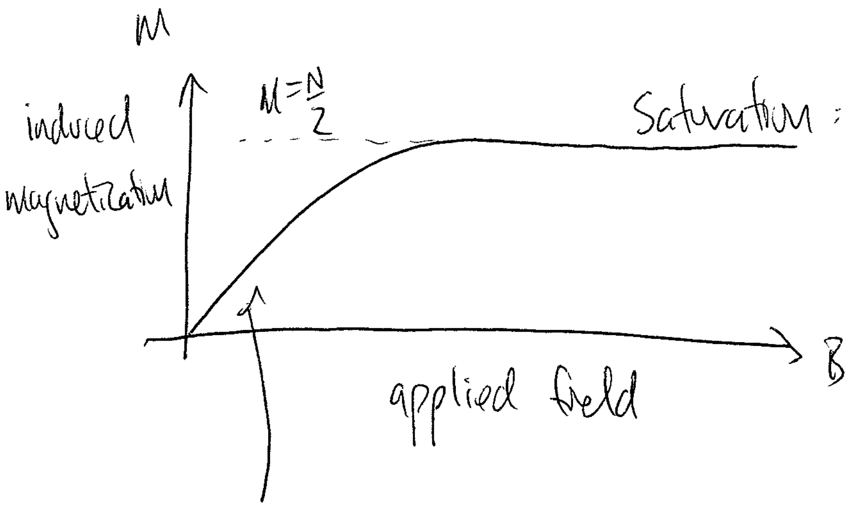
$$\sum_{n=\pm 1} D(\varepsilon + \tfrac{n}{2}B) = 2D(\varepsilon) + \frac{B^2}{4}D''(\varepsilon) + O(B^4)$$

$$\text{So } E_0(B) = V\int d\varepsilon \left[2D(\varepsilon) + \frac{B^2}{4}D''(\varepsilon) + O(B^4)\right]\varepsilon\,\theta(E_F - \varepsilon)$$

$$= \underbrace{2V\int_{-\infty}^{E_F} d\varepsilon\, D(\varepsilon)\varepsilon}_{\text{Zero-field kinetic energy } E_0(0)} + \frac{V}{4}B^2\int_{-\infty}^{E_F} d\varepsilon\, D''(\varepsilon)\varepsilon + O(B^4)$$

* Compute based on the work done in magnetizing the sample

$$E_0(B) = E_0(0) - \int dB \cdot M$$



Saturation: $N_\uparrow = N$, $N_\downarrow = 0$, $M = \frac{1}{2}(N_\uparrow - N_\downarrow) = \frac{N}{2}$

linear regime with slope χ

→ Magnetic susceptibility is defined by

$$\chi = \frac{\partial M}{\partial B} = \chi^{(0)} + \chi^{(1)} B + \chi^{(2)} B^2 + \dots$$

but in the linear regime we often write (somewhat casually)

$$\chi = \chi^{(0)} = \frac{\partial M}{\partial B} = \frac{M}{B}$$

→ so we can identify

$$E_0(B) = E_0(0) - \frac{1}{2} \chi B^2$$

and hence

$$\chi = -\frac{V}{2}\int_{-\infty}^{E_F} D''(\varepsilon)\,d\varepsilon \cdot \varepsilon = +\frac{V}{2}\int_{-\infty}^{E_F} D'(\varepsilon)\,d\varepsilon = \frac{V}{2}D(E_F)$$

* cf. Magnetization as population imbalance

$$\frac{1}{2}(N_\uparrow - N_\downarrow) = \frac{1}{2}\sum_n n V \int \frac{d^3k}{(2\pi)^3}\,\theta\left(E_F - \varepsilon_k + \frac{n}{2}B\right)$$

$$= \frac{1}{2}V \sum_n n \int d\varepsilon\, D(\varepsilon)\,\theta\left(E_F - \varepsilon + \frac{n}{2}B\right)$$

$$= \frac{1}{2}V \sum_n n \int d\varepsilon\, D(\varepsilon)\left[\theta(E_F - \varepsilon) + \frac{n}{2}B\,\delta(E_F - \varepsilon)\right]$$

$$= \frac{1}{2}V \sum_n \int d\varepsilon\, D(\varepsilon)\left[n\,\theta(E_F - \varepsilon) + \frac{n^2}{2}B\,\delta(E_F - \varepsilon)\right]$$

$$\sum_{n=\pm 1} n = 0 \qquad\qquad \sum_{n=\pm 1} n^2 = 2$$

$$= \frac{1}{2}VBD(E_F) \equiv \chi B$$

$\Rightarrow$ Susceptibility $\chi = \frac{1}{2}VD(E_F)$

* Magnetization as population imbalance

$$\frac{1}{2}(N_\uparrow - N_\downarrow) = \frac{1}{2}\sum_n n V \int \frac{d^3k}{(2\pi)^3}\,\theta\left(E_F - \varepsilon_k + \frac{n}{2}B\right)$$

$$= \frac{1}{2} V \sum_n n \int d\varepsilon\, D(\varepsilon)\,\theta\left(E_F - \varepsilon + \frac{n}{2}B\right)$$

$$= \frac{1}{2} V \sum_n n \int d\varepsilon\, D(\varepsilon)\left(\theta(E_F - \varepsilon) + \frac{n}{2}B\,\delta(E_F - \varepsilon)\right)$$

$$= \frac{1}{2} V \sum_n \int d\varepsilon\, D(\varepsilon)\left(\cancelto{0}{n\theta(E_F - \varepsilon)} + \frac{n^2}{2}B\,\delta(E_F - \varepsilon)\right)$$

$$= \frac{1}{2} V B D(E_F) \equiv \chi B$$

$\Rightarrow$ Susceptibility $\chi = \frac{1}{2} V D(E_F)$