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13.1Stoner instability

Consider a 3D Fermi gas with point-like interactions:

$$H = T + V = \sum_{k\sigma} \left(\frac{k^2}{2m_e} - \mu \right) n_{k\sigma} + u \int \psi_{\uparrow}^{\dagger}(x) \psi_{\downarrow}^{\dagger}(x) \psi_{\downarrow}(x) \psi_{\uparrow}(x) d^3x,$$

or, completely in the momentum representation

$$H = \sum_{k\sigma} \left(\frac{k^2}{2m_e} - \mu \right) n_{k\sigma} + \frac{u}{V} \sum_{k_1, k_2, q} c^{\dagger}_{k_1 + q, \uparrow} c^{\dagger}_{k_2 - q, \downarrow} c_{k_2, \downarrow} c_{k_1, \uparrow},$$

after substitution $\psi_{\sigma}(x) = V^{-1/2} \sum_{k} e^{-ikx} c_{k,\sigma}$. The density of states. The density of states at the Fermi Energy for the non-interacting system

$$2\int \frac{d^3k}{(2\pi)^3} = \int d\varepsilon \ D(\varepsilon), \quad \Leftrightarrow \quad D(\varepsilon) = 2\int \frac{d^3k}{(2\pi)^3} \delta(\varepsilon - \varepsilon_k) = \frac{\sqrt{2}}{\pi^2} m_{\rm e}^{3/2} \sqrt{\varepsilon},$$

with $\varepsilon_k = \frac{1}{2m_e}k^2$. Considering that $n = \frac{N}{V} = \frac{2}{6\pi^2}k_F^3$, we have

$$D_{\rm F} \stackrel{\rm def}{=} D(\varepsilon_{\rm F}) = \frac{3^{1/3}}{2\pi^{4/3}} m_{\rm e} \left(\frac{N}{V}\right)^{1/3}.$$

For an interacting gas, as a first approximation, we can simply replace the mass $m \to m_{\text{eff}}$.

The Hartree-Fock approximation. Consider one parameter family of states $|m\rangle$:

$$m = \frac{1}{V} (N_{\uparrow} - N_{\downarrow})$$
$$n = \frac{1}{V} (N_{\uparrow} + N_{\downarrow})$$

which have a fixed magnetisation m and density n, as trial states to find the magnetisation m which minimises the energy $E(m) = \langle m|H|m\rangle$. For kinetic energy term¹

$$\langle m|T|m\rangle = \sum_{k,\sigma}^{k_{\rm F}} \left(\frac{k^2}{2m_{\rm e}} - \mu\right) n_{k\sigma} = \sum_{\sigma} V \int \frac{d^3k}{(2\pi)^3} \left(\frac{k^2}{2m_{\rm e}} - \mu\right) \theta(\varepsilon_{\rm F}(\sigma) - \varepsilon_k) = \frac{1}{m_{\rm e}} \left(\frac{\pi^4}{V^2}\right)^{1/3} \left(N_{\uparrow}^{5/3} + N_{\downarrow}^{5/3}\right) + \frac{1}{2}\mu N,$$

with $N_{\uparrow,\downarrow} = \frac{N}{2} \left(1 \pm \frac{m}{n}\right)$. And, by Wick's theorem, for interaction energy

$$\langle m|V|m\rangle = \frac{u}{V}\sum_{k_1,k_2,q}\langle c^{\dagger}_{k_1+q,\uparrow}c_{k_1,\uparrow}\rangle\langle c^{\dagger}_{k_2-q,\downarrow}c_{k_2,\downarrow}\rangle - \frac{u}{V}\sum_{k_1,k_2,q}\langle c^{\dagger}_{k_1+q,\uparrow}c_{k_2,\downarrow}\rangle\langle c^{\dagger}_{k_2-q,\downarrow}c_{k_1,\uparrow}\rangle = \frac{u}{V}\sum_{k_1,k_2}n_{k_1\uparrow}n_{k_2\downarrow} = \frac{u}{V}N_{\uparrow}N_{\downarrow}.$$

Thus the expression for energy is

$$E(m) = \frac{1}{m_e} \left(\frac{\pi^4}{V^2}\right)^{1/3} \left(\frac{N}{2}\right)^{5/3} \left(\left(1 + \frac{m}{n}\right)^{5/3} + \left(1 - \frac{m}{n}\right)^{5/3}\right) + \frac{uN^2}{4V} \left(1 - \frac{m^2}{n^2}\right)$$

$$D_F E(m)/V = \left(\frac{9}{20} + \frac{1}{4}uD_F\right)n^2 + \left(\frac{1 - uD_F}{4}\right)m^2 + \frac{1}{108}\frac{m^4}{n^2} + o(m^4).$$

It looks like a second-order phase transition in Landau's theory, only with interaction u instead of T – quantum phase transition. Magnetisation

$$m(u) = \pm \sqrt{\frac{27}{2}} \theta(uD_{\rm F} - 1) n \sqrt{uD_{\rm F} - 1}.$$

Stoner criterion. The critical value of the dimensionless interaction strength for the gas developing a spontaneous magnetisation $m \neq 0$ within the HF approximation

$$uD_{\rm F} > 1, \quad \Rightarrow \quad u_{\rm crit} = \frac{1}{D_{\rm F}}.$$

The critical exponent

$$m \sim \theta(u - u_{\text{crit}}) \left(\frac{u - u_{\text{crit}}}{u_{\text{crit}}}\right)^{\beta},$$

corresponds to the $\beta = 1/2$, as in the classical Ising model – second order phase transition.

¹Here I don't write $5^{-1}3^{5/3}2^{-1/3} \approx 0.99 \approx 1$, but take into account in calculations.

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13.2 Bogoliubov rotation and gap equation at zero temperature

Let us consider the BCS Hamiltonian

$$H = \sum_{k\sigma} \xi_k c_{k\sigma}^{\dagger} c_{k\sigma} + \frac{1}{\Omega} \sum_{kk'} V_{kk'} c_{k'\uparrow}^{\dagger} c_{-k'\downarrow}^{\dagger} c_{-k\downarrow} c_{k\uparrow},$$

where $\xi_k = \varepsilon_k - \mu$ is the single particle energy with respect to the chemical potential μ . We introduce the creation operators for Bogoliubov quasiparticles, denoted $\gamma_{k\sigma}^{\dagger}$, via the Bogoliubov rotation

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} \sin\theta_k & -\cos\theta_k \\ \cos\theta_k & \sin\theta_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix}, \qquad \tan\theta_k = \frac{\Delta_k}{E_k - \xi_k},$$

where $\Delta_k = -\frac{1}{\Omega} \sum_k V_{kk'} \langle c_{-k\downarrow} c_{k'\uparrow} \rangle$ is the gap function and $E_k = \sqrt{\Delta_k^2 + \xi_k^2}$. It's usefull to have

$$\begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \sin\theta_k & \cos\theta_k \\ -\cos\theta_k & \sin\theta_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} u_p & v_p \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^{\dagger} \end{pmatrix}$$

The Bogoliubov quasiparticles satisfy the usual fermionic anti-commutation relations (1):

$$\begin{split} &\{\gamma_{k\uparrow},\gamma_{k'\downarrow}\} = \sin\theta_k\cos\theta_{-k'}\delta_{k,-k'} - \cos\theta_k\sin\theta_{-k'}\delta_{k,-k'} = 0, \\ &\{\gamma_{k\sigma},\gamma_{k'\sigma'}\} = \left\{\sin\theta_kc_{k\uparrow} - \cos\theta_kc_{-k\downarrow}^{\dagger}, \ \sin\theta_{k'}c_{k'\uparrow} - \cos\theta_{k'}c_{-k'\downarrow}^{\dagger}\right\} = 0, \\ &\{\gamma_{k\uparrow}, \ \gamma_{k'\uparrow}^{\dagger}\right\} = \sin\theta_k\sin\theta_{k'}\delta_{kk'} + \cos\theta_k\cos\theta_{k'}\delta_{kk'} = \delta_{kk'}. \end{split}$$

Hamiltonian. In the mean-field approximation, the BCS Hamiltonian takes the form

$$H \approx \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma} - \sum_k \left(\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \bar{\Delta}_k c_{-k\downarrow} c_{k\uparrow} + \mathrm{const} \right),$$

introducing operators of the form

$$A_k \stackrel{\text{def}}{=} c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger}, \qquad B_k \stackrel{\text{def}}{=} c_{-k\downarrow} c_{k\uparrow},$$

the mean-field approximation amounts to approximating

$$(A_{k'} - \langle A_{k'} \rangle) (B_k - \langle B_k \rangle) \approx 0.$$

i.e. neglecting fluctuations around the expectation values in quadratic order. The interaction (2)

$$\begin{split} V &= \frac{1}{\Omega} \sum_{kk'} V_{kk'} A_{k'} B_k = \frac{1}{\Omega} \sum_{kk'} A_{k'} \langle B_k \rangle + \frac{1}{\Omega} \sum_{kk'} V_{kk'} \langle A_k' \rangle B_k - \frac{1}{\Omega} \sum_{kk'} \langle A_{k'} \rangle \langle B_k \rangle \\ &= - \sum_{k'} \Delta_{k'} A_{k'} - \sum_{k} \bar{\Delta}_k B_k + \text{const.} \end{split}$$

Moving on to quasiparticles, we find (3)

$$H = \sum_{k} \begin{pmatrix} c_{k\uparrow}^{\dagger} & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \xi_{k} & -\Delta_{k} \\ -\Delta_{k} & \xi_{k} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^{\dagger} \end{pmatrix} + \text{const}$$

$$= \sum_{k} \begin{pmatrix} \gamma_{k\uparrow}^{\dagger} & \gamma_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \sin\theta_{k} & \cos\theta_{k} \\ -\cos\theta_{k} & \sin\theta_{k} \end{pmatrix} \begin{pmatrix} \xi_{k} & -\Delta_{k} \\ -\Delta_{k} & \xi_{k} \end{pmatrix} \begin{pmatrix} \sin\theta_{k} & -\cos\theta_{k} \\ \cos\theta_{k} & \sin\theta_{k} \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^{\dagger} \end{pmatrix} + \text{const}$$

$$\stackrel{?}{=} \sum_{k} \begin{pmatrix} \gamma_{k\uparrow}^{\dagger} & \gamma_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \tilde{E}_{k} & 0 \\ 0 & -\tilde{E}_{k} \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma_{-k\downarrow}^{\dagger} \end{pmatrix},$$

with

$$\tilde{E}_k = \xi_k - 2\xi_k \cos(\theta_k)^2 + 2\Delta_k \sin\theta_k \cos\theta_k = \frac{\xi_k^2 + \Delta_k^2}{E_k} = E_k.$$

With $\Delta_k = \Delta$ we could plot the dispersion relation (fig. 1).

Ground state. The BCS state

$$|gs\rangle = \prod_{k} \left(\sin \theta_k + \cos \theta_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} \right) |0\rangle,$$

has zero Bogoliubov quasiparticles (4):

$$\begin{split} \gamma_{k\uparrow} \left| \mathrm{gs} \right\rangle &= \left(\sin \theta_k c_{k\uparrow} - \cos \theta_k c_{-k\downarrow}^{\dagger} \right) \prod_k \left(\sin \theta_k + \cos \theta_k c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} \right) \left| 0 \right\rangle \\ &= \sin \theta_k c_{k\uparrow} c_{k\uparrow}^{\dagger} c_{-k\downarrow}^{\dagger} \left| 0 \right\rangle - \cos \theta_k \sin \theta_k c_{-k\downarrow}^{\dagger} \left| 0 \right\rangle = 0, \end{split}$$

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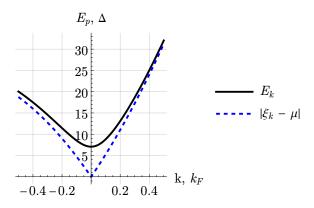


Figure 1: The dispersion relation

so $|gs\rangle$ is ground state of the mean field approximation of H. Actually the $|gs\rangle$ could be observed by

$$|gs\rangle \stackrel{\text{n}}{=} \prod_{k} \gamma_{-k\downarrow} \gamma_{k\downarrow} |0\rangle.$$

In this state

$$E(\theta_k) = \langle gs|H|gs \rangle = \sum_k 2\xi_k \cos^2 \theta_k + \frac{1}{4\Omega} \sum_{kk'} V_{kk'} \sin(2\theta_k) \sin(2\theta_{k'}),$$

and we could find θ_k just by minimizing the energy

$$\frac{\partial}{\partial \theta_q} E(\theta_k) = \frac{1}{\Omega} \cos(2\theta_q) \sum_k V_{qk} \sin(2\theta_k) - 2\xi_q \sin(2\theta_q) = 0.$$

Using this relation we could simplify expression (5)

$$\Delta_k = -\frac{1}{\Omega} \sum_{k'} V_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle_{\mathrm{gs}} = -\frac{1}{2\Omega} \sum_{k'} V_{kk'} \sin(2\theta_{k'}) = -\frac{1}{\Omega} \sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2E_{k'}},$$

the zero temperature gap equation.