Lesson 6 - Quantum Many-Body Systems
Unit 6.2 Uniform Fermi gas of non-interacting electrons

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Uniform Fermi gas (I)

The non-interacting uniform Fermi gas is obtained setting to zero the confining potential, i.e.

$$U(\mathbf{r}) = 0 \; , \tag{1}$$

and imposing periodicity conditions on the single-particle wavefunctions, which are plane waves with a spinor

$$\phi(x) = \frac{1}{\sqrt{V}} \; e^{i\mathbf{k}\cdot\mathbf{r}} \; \chi_\sigma \; , \tag{2}$$

where χ_σ is the spinor for spin-up and spin-down along a chosen z asis:

$$\chi_\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \; , \qquad \chi_\downarrow = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \; . \tag{3}$$

At the boundaries of a cube having volume V and side L one has

$$e^{ik_x(x+L)} = e^{ik_x x} \; , \quad e^{ik_y(y+L)} = e^{ik_y y} \; , \quad e^{ik_z(z+L)} = e^{ik_z z} \; . \tag{4}$$

Uniform Fermi gas (II)

It follows that the linear momentum $\mathbf{k}$ can only take on the values

$$k_x = \frac{2\pi}{L} n_x \ , \quad k_y = \frac{2\pi}{L} n_y \ , \quad k_z = \frac{2\pi}{L} n_z \ , \tag{5}$$

where n_x, n_y, n_z are integer quantum numbers. The single-particle energies are given by

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \frac{4\pi^2}{L^2} (n_x^2 + n_y^2 + n_z^2) \ . \tag{6}$$

In the thermodynamic limit $L \to \infty$, the allowed values are closely spaced and one can use the continuum approximation

$$\sum_{n_x, n_y, n_z} \to \int dn_x \ dn_y \ dn_z \ , \tag{7}$$

which implies

$$\sum_{\mathbf{k}} \to \frac{L^3}{(2\pi)^3} \int d^3\mathbf{k} = V \int \frac{d^3\mathbf{k}}{(2\pi)^3} \ . \tag{8}$$

The total number N of fermionic particles is given by

$$N = \sum_{\sigma} \sum_{\mathbf{k}} \Theta \left(\epsilon_F - \epsilon_{\mathbf{k}} \right) \ , \tag{9}$$

Fermi energy of non-interacting electrons (I)

In the continuum limit and choosing spin 1/2 fermions one finds

$$N = \sum_{\sigma=\uparrow,\downarrow} V \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \Theta\left(\epsilon_F - \frac{\hbar^2 k^2}{2m}\right) , \tag{10}$$

from which one gets (the sum of spins gives simply a factor 2) the uniform density

$$\rho = \frac{N}{V} = \frac{1}{3\pi^2} \left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2} . \tag{11}$$

The formula can be inverted giving the Fermi energy ϵ_F as a function of the density ρ, namely

$$\epsilon_F = \frac{\hbar^2}{2m} \left(3\pi^2 \rho\right)^{2/3} . \tag{12}$$

In many applications the Fermi energy ϵ_F is written as

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} , \tag{13}$$

where k_F is the so-called Fermi wave-number, given by

$$k_F = \left(3\pi^2 \rho\right)^{1/3} . \tag{14}$$

Total energy of non-interacting electrons (I)

The total energy E of the uniform and non-interacting Fermi system is given by

$$E = \sum_{\sigma} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \, \Theta \left(\epsilon_F - \epsilon_{\mathbf{k}} \right) \; , \tag{15}$$

and using again the continuum limit with spin 1/2 fermions it becomes

$$E = \sum_{\sigma=\uparrow,\downarrow} V \int \frac{d^3\mathbf{k}}{(2\pi)^3} \, \frac{\hbar^2 k^2}{2m} \, \Theta \left(\epsilon_F - \frac{\hbar^2 k^2}{2m} \right) \; , \tag{16}$$

from which one gets the energy density

$$\mathcal{E} = \frac{E}{V} = \frac{3}{5} \rho \, \epsilon_F = \frac{3}{5} \frac{\hbar^2}{2m} \left(3\pi^2 \right)^{2/3} \rho^{5/3} \tag{17}$$

in terms of the Fermi energy ϵ_F and the uniform density ρ.