3.1.6 Application of the Wick theorem: density correlations of free fermions

First, let us illustrate the application of the Wick theorem with calculating the density-density correlation function $\langle n(x)n(y)\rangle$ in a free-fermion gas (without spin). The density operator may be expressed as

$$n(x) = a^+(x)a(x)\,, \tag{3.1.36}$$

which leads to the Wick-theorem result for the correlation function

$$\langle n(x)n(y)\rangle = \langle a^+(x)a(x)a^+(y)a(y)\rangle = \langle a^+(x)a(x)\rangle\langle a^+(y)a(y)\rangle + \langle a^+(x)a(y)\rangle\langle a(x)a^+(y)\rangle$$
$$= G(0)^2 - |G(x-y)|^2 + G(0)\delta(x-y)\,, \tag{3.1.37}$$

where we have defined

$$G(x-y) = \langle a^+(x)a(y)\rangle \tag{3.1.38}$$

(in particular, $G(0) = n$ is the average particle density).

The contractions can be conveniently represented diagrammatically (Fig. 5). [The third delta-term in (3.1.37) is not shown: it corresponds to one particle contributing to both $n(x)$ and $n(y)$].

The "Green function" $G(x)$ has the form shown in Fig. 6. In 3D at zero temperature, it can be calculated exactly:

$$G(R) = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{kR}} n_F(\varepsilon_k) = \frac{1}{2\pi^2 R^3}\left[\sin(k_F R) - (k_F R)\cos(k_F R)\right]\,. \tag{3.1.39}$$

Note that the resulting correlation function $\langle n(x)n(y)\rangle$ (Fig. 6) vanishes at $x \to y$, in agreement with the Pauli principle. It oscillates at the wave vector $2k_F$ (*Friedel oscillations*).

3.1.7 Application of the Wick theorem: perturbative energy of interaction (Hartree–Fock)

Consider now a spinless Fermi gaz with the interaction (3.1.24). Let us calculate the interaction energy in a perturbative way, to the first order in V.

If we write the Hamiltonian as

$$H = H_0 + V\,, \tag{3.1.40}$$

then we can expand all the thermodynamic quantities with respect to V. The (grand-canonical) partition function (with $\beta = 1/T$)

$$Z = \operatorname{tr} e^{-\beta(H_0+V)} = \operatorname{tr} e^{-\beta H_0} - \beta \operatorname{tr} V e^{-\beta H_0} + O(V^2) = Z_0(1 - \beta\langle V\rangle_0 + O(V^2))\,. \tag{3.1.41}$$
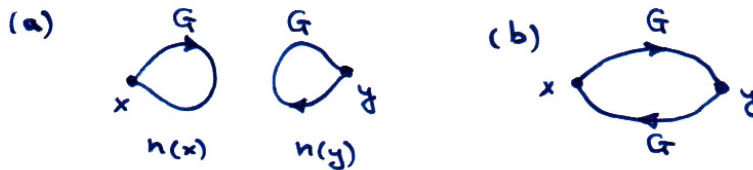

Figure 5: Two diagrams contributing to the correlation function $\langle n(x)n(y)\rangle$.
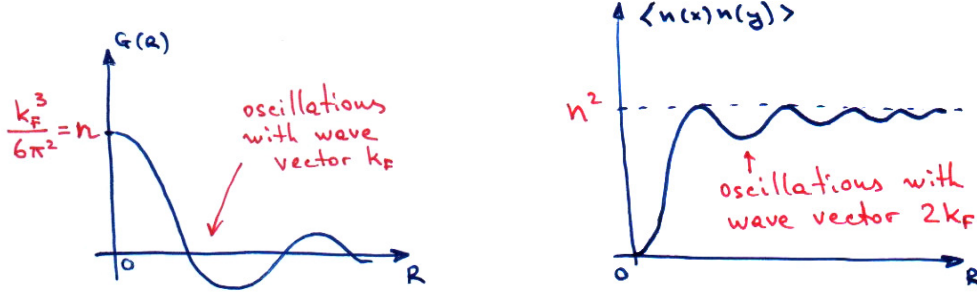
Figure 6: Qualitative sketches of $G(R)$ and $\langle n(x)n(y)\rangle$.

(note that, to the first order, the noncommutativity of H_0 and V does not matter).

For the free energy (the "grand potential"), we thus find

$$\Phi = -T\ln Z = \Phi_0 + \langle V\rangle_0 + O(V^2)\,. \tag{3.1.42}$$

In other words, to the first order, the correction to the free energy equals the average interaction energy calculated in the unperturbed system. Using the Wick theorem, we can express $\langle V\rangle_0$ as the sum of two diagrams (the same as in the previous example), see Fig. 7.

The first diagram gives the classical contribution to the interaction energy:

$$\delta\Phi_1 = \frac{1}{2}\iint dx\,dy\,\langle n(x)\rangle V(x-y)\langle n(y)\rangle = \mathcal{V}\frac{n^2}{2}\int dx\,V(x) = \mathcal{V}\frac{n^2}{2}V_{k=0}\,, \tag{3.1.43}$$

where $\mathcal{V}$ is the total volume of the system.

The second diagram is of the exchange type:

$$\delta\Phi_2 = -\frac{1}{2}\iint dx\,dy\,G(x-y)V(x-y)G(y-x) = -\frac{\mathcal{V}}{2}\iint \frac{d^3k}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}n_k n_{k'}V_{k-k'}\,. \tag{3.1.44}$$

The correction (3.1.44) may be interpreted as a renormalization of energy of each particle by interaction. The correction to the energy of a particle at the momentum k is then

$$\delta\varepsilon_k = -\int \frac{d^3k'}{(2\pi)^3}n_{k'}V_{k-k'}\,. \tag{3.1.45}$$

As we will see later, this correction to the energy corresponds to the Hartree–Fock approximation.

Figure 7: Two diagrams contributing to the perturbative interaction energy: (a) Hartree contribution; (b) exchange contribution.

Problem Set 5

Problem 5.1

(a) In the subsection 3.1.7, we neglected the spin of the electrons. How would the results change, if we include spin?

(b) Consider the model of free electrons with Coulomb interaction. Assume the free-paricle kinetic energy $\varepsilon_k = \hbar^2 k^2/(2m)$ and calculate, at zero temperature, the average interaction energy per particle, using the perturbative expression (3.1.44). Do not forget about spin! Express your result as

$$\delta E = \varepsilon_F \, f \left(\frac{r_s}{a_0} \right),$$

where ε_F is the Fermi energy and r_s/a_0 is the dimensionless parameter introduced in Secion 1.1.5:

$$r_s = \left(\frac{3}{4\pi n} \right)^{1/3}, \qquad a_0 = \frac{\hbar^2}{me^2} = 0.529\text{Å}$$

(a typical distance between electrons in the units of the Bohr radius). Find the function f. If you encounter difficulties in computing integrals, you may either compute them numerically (using your favorite software) or leave them uncomputed as unknown *numerical* coefficients.

Note that we only consider the correction (3.1.44), but not (3.1.43), since the latter is exactly canceled by the background positive charge of the ions.

(c) From the result of part (b), show the stability of a metal: minimize the total energy per electron

$$E_{\text{tot}} = E_{\text{kin}} + \delta E$$

as a function of r_s. The average kinetic energy per particle E_{kin} is proportional to ε_F. Remember that ε_F itself depends on r_s:

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \left(\frac{9\pi}{4} \right)^{2/3} \left(\frac{a_0}{r_s} \right)^2 \text{Ry}, \qquad \text{Ry} = \frac{\hbar^2}{2ma_0^2} \approx 13.6 \, \text{eV}$$

If you have calculated the numerical coefficient in part (b), use it to find the optimal value of r_s. Compare it to the actual values of r_s in alkali metals (Li, Na, K: they are the closest to the free-fermion model).

(d)[*] In the model of free electrons with Coulomb interaction [the same as in parts (b) and (c)], calculate the correction to the energy of a particle at a wave vector k close to the Fermi surface, as given by Eq. (3.1.45). You should find a logarithmic divergence of the Fermi velocity. Show that this divergence comes from the long-range part of the Coulomb potential (since our calculation does not include screening).