M1- Sciences de la Matière, A. A. 2022-2023
Superconductivity, superfluidity and magnetism
Tommaso Roscilde, Fabio Mezzacapo, Youssef Trifa

TD7bis: Fermions – coherence properties and pairing

1 Quantum coherence in a fermion gas

We here consider the correlation function of first and second order in a fermion gas.

1.1

Considering an ideal spinless Fermi gas in $d = 3$, we want to calculate the one-body density matrix (or first-order correlation function)

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \langle \hat{\psi}^\dagger(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}') \rangle \quad . \tag{1}$$

Using the momentum representation of the field operators

$$\hat{\psi}(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \hat{c}_{\boldsymbol{k}} \tag{2}$$

and considering that, at $T = 0$, the Fermi gas occupies a Fermi sphere of radius k_F in momentum space, show that $g^{(1)}(\boldsymbol{r}, \boldsymbol{r}')$ reads

$$g^{(1)}(\boldsymbol{r}, \boldsymbol{r}') = \frac{1}{2\pi^2 R^2} \left[\frac{\sin(k_F R)}{R} - k_F \cos(k_F R) \right] \tag{3}$$

where $R = |\boldsymbol{r} - \boldsymbol{r}'|$. Sketch the behavior of $g^{(1)}$ for $R \to \infty$ and comment on the physical meaning of this limit. Taking the opposite limit $g^{(1)}(R \to 0)$ show that $k_F = (6\pi^2 n)^{1/3}$ where $n = N/V$ is the density of the spinless Fermi gas.

1.2

We consider a generic $S = 1/2$ Fermi gas, and we introduce the *pair correlation function*

$$g^{(2)}(\boldsymbol{r}, \boldsymbol{r}') = V \langle \hat{\psi}_\downarrow^\dagger(\boldsymbol{r}) \hat{\psi}_\uparrow^\dagger(\boldsymbol{r}) \hat{\psi}_\uparrow(\boldsymbol{r}') \hat{\psi}_\downarrow(\boldsymbol{r}') \rangle \quad . \tag{4}$$

Using the momentum representation of the field operators, and considering a system in which the momentum is conserved, show that, for $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$

$$g^{(2)}(\boldsymbol{r}, \boldsymbol{r}') \approx \frac{1}{V} \sum_{\boldsymbol{k}} \langle \hat{\mathcal{S}}_{\boldsymbol{k}}^\dagger \hat{\mathcal{S}}_{\boldsymbol{k}} \rangle \; + \; \text{(rapidly oscillating terms)} \tag{5}$$

where we have introduced the operator

$$\hat{\mathcal{S}}_{\boldsymbol{k}}^\dagger = \frac{1}{\sqrt{2}} \left(\hat{c}_{\boldsymbol{k}\uparrow}^\dagger \hat{c}_{-\boldsymbol{k}\downarrow}^\dagger - \hat{c}_{\boldsymbol{k}\downarrow}^\dagger \hat{c}_{-\boldsymbol{k}\uparrow}^\dagger \right) \quad . \tag{6}$$

1.3

Consider the two-particle wavefunction $|\psi\rangle = \hat{\mathcal{S}}^\dagger_{\boldsymbol{k}}|0\rangle$. Remembering that, for fermions

$$\psi(\boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma) = \frac{1}{\sqrt{2}} \left(\langle \boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma'| - \langle \boldsymbol{r}', \sigma'; \boldsymbol{r}, \sigma| \right) |\psi\rangle \tag{7}$$

show that $\psi(\boldsymbol{r}, \sigma; \boldsymbol{r}', \sigma)$ describes two particles with opposite momenta and with spins forming a singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ (Cooper pair). Conclude on the relationship between the pair correlation function and the density of Cooper pairs.

1.4

We return to the ideal Fermi gas, this time with spin. Show that, for this system

$$g^{(2)}(\boldsymbol{r}, \boldsymbol{r}') = V g^{(1)}_{\uparrow}(\boldsymbol{r}, \boldsymbol{r}') g^{(1)}_{\downarrow}(\boldsymbol{r}, \boldsymbol{r}') \quad . \tag{8}$$

How does this function decay for $|\boldsymbol{r} - \boldsymbol{r}'| \to \infty$? Conclude on the density of pairs in the ideal Fermi gas.

2 Quantum-mechanical description of electron-electron interactions mediated by phonons

Consider the electron gas in a metal. A minimal model describing both the (non-interacting) electrons, the phonons of the ion lattice, and their interaction, is the following Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el} + \hat{\mathcal{H}}_{\rm el-ph} \tag{9}$$

where

$$\begin{aligned} \hat{\mathcal{H}}_{\rm ph} &= \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \; \hat{b}^\dagger_{\boldsymbol{q}} \hat{b}_{\boldsymbol{q}} \\ \hat{\mathcal{H}}_{\rm el} &= \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \; \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}_{\boldsymbol{k},\sigma} \\ \hat{\mathcal{H}}_{\rm el-ph} &= \gamma \sum_{\boldsymbol{k},\boldsymbol{q},\sigma} \left(\hat{b}^\dagger_{\boldsymbol{q}} \; \hat{c}^\dagger_{\boldsymbol{k}-\boldsymbol{q},\sigma} \hat{c}_{\boldsymbol{k},\sigma} + \text{h.c.} \right) \end{aligned} \tag{10}$$

The last term describes the elementary quantum mechanical processes of interaction between an electron and the ion lattice: an electron emits or aborbs a phonon from the lattice, thereby losing/gaining a momentum $\hbar\boldsymbol{q}$. A pictorial way to represent this process is the one shown in Fig. 1.

We imagine that the initial configuration of the system consists of two electrons in the anti-symmetrized state $|\psi(0)\rangle = |\boldsymbol{k}, \sigma; \boldsymbol{k}', \sigma'\rangle = \hat{c}^\dagger_{\boldsymbol{k},\sigma} \hat{c}^\dagger_{\boldsymbol{k}',\sigma'} |0\rangle$, moving in the vacuum of phonons. This state is clearly an eigenstate of $\hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el}$. Treating $\hat{\mathcal{H}}_{\rm el-ph}$ as a perturbation, it introduces a finite matrix element between the initial state and a state $|\psi(\boldsymbol{q})\rangle = |\boldsymbol{k} - \boldsymbol{q}, \sigma; \boldsymbol{k}' + \boldsymbol{q}, \sigma'\rangle$. Within second-order perturbation theory, this matrix element reads

$$\langle \psi(\boldsymbol{q}) | \hat{\mathcal{H}} | \psi(0) \rangle \approx \frac{1}{2} \sum_n \left(\frac{1}{E_0 - E_n} + \frac{1}{E_{\boldsymbol{q}} - E_n} \right) \langle \psi(\boldsymbol{q}) | \hat{\mathcal{H}}_{\rm el-ph} | \psi_n \rangle \langle \psi_n | \hat{\mathcal{H}}_{\rm el-ph} | \psi(0) \rangle \tag{11}$$

where $|\psi_n\rangle$ are intermediate eigenstates of $\hat{\mathcal{H}}_{\rm ph} + \hat{\mathcal{H}}_{\rm el}$ different from (and non-degenerate with) $|\psi(\boldsymbol{q})\rangle$ and $|\psi(0)\rangle$. Moreover $E_0 = \epsilon_{\boldsymbol{k}} + \epsilon_{\boldsymbol{k}'}$ and $E_{\boldsymbol{q}} = \epsilon_{\boldsymbol{k}-\boldsymbol{q}} + \epsilon_{\boldsymbol{k}'+\boldsymbol{q}}$.

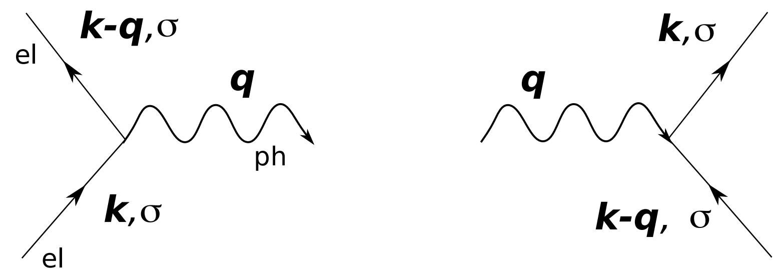

Figure 1: Emission (left) and absorption (right) of a phonon by an electron interacting with the ion lattice.

2.1

Identify the intermediate states $|\psi_n\rangle$ leading to non vanishing contributions in the sum of Eq. (11) , and calculate them. Show that

$$\langle\psi(\boldsymbol{q})|\hat{\mathcal{H}}_{\text{el}-\text{ph}}|\psi(0)\rangle = -\gamma^2 \left[\frac{\hbar\omega_{\boldsymbol{q}}}{(\hbar\omega_{\boldsymbol{q}})^2 - (\epsilon_{\boldsymbol{k}-\boldsymbol{q}} - \epsilon_{\boldsymbol{k}})^2} + \frac{\hbar\omega_{\boldsymbol{q}}}{(\hbar\omega_{\boldsymbol{q}})^2 - (\epsilon_{\boldsymbol{k}'+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}'})^2}\right] \tag{12}$$

Can you relate this matrix element to the process of exchange of (virtual) phonons between the electrons? Why are these phonons *virtual* and not real?

2.2

Write the reduced 2×2 Hamiltonian on the Hilbert space spanned by $|\psi(\boldsymbol{q})\rangle$ and $|\psi(0)\rangle$ (namely the matrix $\langle\psi|\mathcal{H}|\psi'\rangle$ where $|\psi\rangle, |\psi'\rangle = |\psi(\boldsymbol{q})\rangle, |\psi(0)\rangle$). Discuss why the maximum "mixing" between these two states is achieved when $\boldsymbol{q} = 2\boldsymbol{k}$ and $\boldsymbol{k}' = -\boldsymbol{k}$. Show that in this case the matrix element, Eq. (11), takes a negative value $-\Gamma$, with $\Gamma > 0$ to be determined.

2.3

Diagonalising the reduced Hamiltonian described above, show that the minimum energy state in this subspace is

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left(\hat{c}^\dagger_{\boldsymbol{k},\sigma}\hat{c}^\dagger_{-\boldsymbol{k},\sigma'} - \hat{c}^\dagger_{\boldsymbol{k},\sigma'}\hat{c}^\dagger_{-\boldsymbol{k},\sigma}\right)|0\rangle \tag{13}$$

having energy $2\epsilon_{\boldsymbol{k}} - \Gamma$. For what values of σ and σ' is this state non-zero? Comparing with the result of Exercise 1.3, what can you conclude on the nature of the $|\psi_0\rangle$ state? In conclusion, what is the effect of the exchange of phonons between two electrons? Based on the results of Exercise 1.2, how do you expect it to affect the long-distance behavior of the pair correlation function $g^{(2)}$?