- This is an individual homework. Each submission must have been worked out and written up by the submitting student.
- This homework is an open-book assessment. Students are permitted to use lecture slides, notes, exercises, and any other provided resource materials to solve the problems.
- Some problems may require students to generate plots. For this, students may utilize any offline or online plotting tools of their choice.
- Each homework set contains questions worth a total of 20 points. You may gain extra point(s) by solving the optional questions. But the maximum you can get in one homework is 20.
- A digital copy of the homework solutions, whether handwritten or typed, must be submitted through the Moodle assignment section by Wednesday, December 11th, 2024, at 09:59 PM.
- The homework will be assessed within a reasonable timeframe, and students may discuss their assessments during the exercise sessions.

Coherence length of Cooper pairs

The purpose of this exercise is to determine the coherence length ℓ_c of the Cooper pairs. To this end, we use the expansion of the BCS state into states with a fixed number of particles (see course):

$$|\Phi_{BCS}\rangle = \sum_{N=0,2,4\cdots} |\Phi_N\rangle, \qquad \text{with} \qquad |\Phi_N\rangle = C\left(\sum_{\boldsymbol{k}} g_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\right)^{N/2} |0\rangle \tag{1}$$

where $C = \frac{1}{(N/2)!}\left(\prod_{\boldsymbol{p}} u_{\boldsymbol{p}}\right)$, $g_{\boldsymbol{k}} = \frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}}$, $u^2_{\boldsymbol{k}} = \frac{1}{2}\left(1+\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)$, $v^2_{\boldsymbol{k}} = \frac{1}{2}\left(1-\frac{\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)$, $E_{\boldsymbol{k}} = \sqrt{\xi^2_{\boldsymbol{k}}+\Delta^2}$ and $\xi_{\boldsymbol{k}} = \frac{k^2}{2m} - \epsilon_F$.

(a) Show that Φ_N can be decomposed into a product of two-particle wave functions

$$\langle \boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N|\Phi_N\rangle \sim \mathcal{A}\cdot\Big(\psi(\boldsymbol{r}_1\sigma_1,\boldsymbol{r}_2\sigma_2)\psi(\boldsymbol{r}_3\sigma_3,\boldsymbol{r}_4\sigma_4)\cdots\psi(\boldsymbol{r}_{N-1}\sigma_{N-1},\boldsymbol{r}_N\sigma_N)\Big), \tag{2}$$

where

- $\psi(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')$ is the two-particle wave function given by $\psi(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') = \varphi(\boldsymbol{r}-\boldsymbol{r}')\eta_\uparrow(\sigma)\eta_\downarrow(\sigma')$,
- $\eta_{\sigma'}(\sigma) = \delta_{\sigma,\sigma'}$ is the spin wave function,
- $\varphi(\boldsymbol{r})$ is the spatial wave function defined by

$$\varphi(\boldsymbol{r}) = \frac{1}{\sqrt{\Omega}}\sum_{\boldsymbol{k}} g_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{3}$$

- $\mathcal{A}$ is the antisymmetrisation operator, defined by its action on a function $f(\boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N)$

$$\mathcal{A} \cdot f(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \cdots, \boldsymbol{r}_N\sigma_N) = \frac{1}{N!} \sum_{p \in S_N} s_p f(\boldsymbol{r}_{p(1)}\sigma_{p(1)}, \boldsymbol{r}_{p(2)}\sigma_{p(2)}, \cdots, \boldsymbol{r}_{p(N)}\sigma_{p(N)}), \tag{4}$$

- S_N is the set of permutations with N terms,
- and finally $s_p = (-1)^p = \pm 1$ is the signature of the permutation p.

Remember that

$$\begin{aligned} |\phi_1, \phi_2, \ldots, \phi_N\rangle &\equiv \frac{1}{\sqrt{N!}} \sum_{p \in S_N} \zeta^p |\phi_{p(1)}\rangle \otimes |\phi_{p(2)}\rangle \otimes \ldots \otimes |\phi_{p(n)}\rangle \qquad (5) \\ &= c^\dagger_{\phi_1} c^\dagger_{\phi_2} \ldots c^\dagger_{\phi_N} |0\rangle \end{aligned}$$

where $\zeta = -1$ for fermions and $\zeta = +1$ for bosons. For example, in real-space representation,

$$|\boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N\rangle = \Psi^\dagger(\boldsymbol{r}_1\sigma_1) \cdots \Psi^\dagger(\boldsymbol{r}_N\sigma_N)|0\rangle$$

where Ψ is the field operator

$$\Psi^\dagger(\boldsymbol{r}\sigma) \equiv c^\dagger_{\boldsymbol{r}\sigma} = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} c^\dagger_{\boldsymbol{k}\sigma}$$

such that

$$\langle \boldsymbol{r}\sigma | \boldsymbol{k}\sigma' \rangle = \frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \delta_{\sigma\sigma'} = \frac{1}{\sqrt{\Omega}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \eta_\sigma(\sigma') \tag{6}$$

[3 points]

Solution: We have

$$\begin{aligned} |\Phi_N\rangle &= C\Big(\sum_{\boldsymbol{k}} g_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow}\Big)^{N/2} |0\rangle \\ &= C \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_{N/2}} \big(g_{\boldsymbol{k}_1} \ldots g_{\boldsymbol{k}_{N/2}}\big)\, c^\dagger_{\boldsymbol{k}_1\uparrow} c^\dagger_{-\boldsymbol{k}_1\downarrow} \cdots c^\dagger_{\boldsymbol{k}_{N/2}\uparrow} c^\dagger_{-\boldsymbol{k}_{N/2}\downarrow} |0\rangle \\ &= C \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_{N/2}} \big(g_{\boldsymbol{k}_1} \ldots g_{\boldsymbol{k}_{N/2}}\big)\, |\boldsymbol{k}_1 \uparrow, -\boldsymbol{k}_1 \downarrow, \ldots, \boldsymbol{k}_{N/2} \uparrow, -\boldsymbol{k}_{N/2} \downarrow\rangle \end{aligned}$$

and therefore:

$$\begin{aligned} &\langle \boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots \boldsymbol{r}_N\sigma_N | \Phi_N\rangle = C \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_{N/2}} \big(g_{\boldsymbol{k}_1} \ldots g_{\boldsymbol{k}_{N/2}}\big) \sum_p s_p \\ &\times \langle \boldsymbol{r}_{p_1}\sigma_{p_1} | \boldsymbol{k}_1 \uparrow\rangle \, \langle \boldsymbol{r}_{p_2}\sigma_{p_2} | -\boldsymbol{k}_1 \downarrow\rangle \ldots \langle \boldsymbol{r}_{p_{N-1}}\sigma_{p_{N-1}} | \boldsymbol{k}_{N/2} \uparrow\rangle \, \langle \boldsymbol{r}_{p_N}\sigma_{p_N} | -\boldsymbol{k}_{N/2} \downarrow\rangle \end{aligned}$$

where $p_i \equiv p(i)$. Here we used the fact that

$$\begin{aligned} \langle \phi_1, \ldots, \phi_N | \varphi_1, \ldots, \varphi_N\rangle &= \frac{1}{N!} \sum_{p,q \in S_N} \zeta^{p+q} \langle \phi_{p(1)} | \varphi_{q(1)}\rangle \cdot \cdots \cdot \langle \phi_{p(N)} | \varphi_{q(N)}\rangle \\ &= \frac{1}{N!} \sum_{p,q \in S_N} \zeta^{p+q} \langle \phi_{p\cdot q^{-1}(1)} | \varphi_1\rangle \cdot \cdots \cdot \langle \phi_{p\cdot q^{-1}(N)} | \varphi_N\rangle \\ &= \sum_{r \in S_N} \zeta^r \langle \phi_{r(1)} | \varphi_1\rangle \cdot \cdots \cdot \langle \phi_{r(N)} | \varphi_N\rangle. \end{aligned}$$

Using the formula $\langle \boldsymbol{r}\sigma|\boldsymbol{k}\sigma'\rangle = \delta_{\sigma\sigma'}\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}} = \eta_{\sigma'}(\sigma)\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$, we obtain

$$\begin{aligned}\langle \boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots \boldsymbol{r}_N\sigma_N|\Phi_N\rangle &= C\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\ldots,\boldsymbol{k}_{N/2}}\left(g_{\boldsymbol{k}_1}\ldots g_{\boldsymbol{k}_{N/2}}\right)\sum_p s_p\\ &\quad\times\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}_1\cdot\boldsymbol{r}_{p_1}}\eta_\uparrow(\sigma_{p_1})\frac{1}{\sqrt{\Omega}}e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}_{p_2}}\eta_\downarrow(\sigma_{p_2})\\ &\quad\vdots\\ &\quad\times\frac{1}{\sqrt{\Omega}}e^{i\boldsymbol{k}_{N/2}\cdot\boldsymbol{r}_{p_{N-1}}}\eta_\uparrow(\sigma_{p_{N-1}})\frac{1}{\sqrt{\Omega}}e^{-i\boldsymbol{k}_{N/2}\cdot\boldsymbol{r}_{p_{N-1}}}\eta_\downarrow(\sigma_{p_N})\end{aligned}$$

so that

$$\begin{aligned}\langle \boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots \boldsymbol{r}_N\sigma_N|\Phi_N\rangle &= C\sum_p s_p\\ &\quad\times\frac{1}{\Omega}\sum_{\boldsymbol{k}_1}g_{\boldsymbol{k}_1}e^{i\boldsymbol{k}_1\cdot(\boldsymbol{r}_{p_1}-\boldsymbol{r}_{p_2})}\eta_\uparrow(\sigma_{p_1})\eta_\downarrow(\sigma_{p_2})\\ &\quad\times\frac{1}{\Omega}\sum_{\boldsymbol{k}_2}g_{\boldsymbol{k}_2}e^{i\boldsymbol{k}_2\cdot(\boldsymbol{r}_{p_3}-\boldsymbol{r}_{p_4})}\eta_\uparrow(\sigma_{p_3})\eta_\downarrow(\sigma_{p_4})\\ &\quad\vdots\\ &\quad\times\frac{1}{\Omega}\sum_{\boldsymbol{k}_{N/2}}g_{\boldsymbol{k}_{N/2}}e^{i\boldsymbol{k}_{N/2}\cdot(\boldsymbol{r}_{p_{N-1}}-\boldsymbol{r}_{p_N})}\eta_\uparrow(\sigma_{p_{N-1}})\eta_\downarrow(\sigma_{p_N})\\ &= \frac{C}{\Omega^{N/4}}\sum_p s_p\psi(\boldsymbol{r}_{p_1}\sigma_{p_1}, \boldsymbol{r}_{p_2}\sigma_{p_2})\psi(\boldsymbol{r}_{p_3}\sigma_{p_3}, \boldsymbol{r}_{p_4}\sigma_{p_4})\ldots\psi(\boldsymbol{r}_{p_{N-1}}\sigma_{p_{N-1}}, \boldsymbol{r}_{p_N}\sigma_{p_N})\\ \Rightarrow \langle \boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2, \ldots \boldsymbol{r}_N\sigma_N|\Phi_N\rangle &\propto \mathcal{A}\cdot\Big(\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)\psi(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\ldots\psi(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N)\Big)\end{aligned}$$

(b) Show that it is possible to express Eq. (2) in terms of antisymmetric wave functions:

$$\langle \boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N|\Phi_N\rangle \sim \mathcal{A}\cdot\Big(\psi_a(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)\psi_a(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\psi_a(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N)\Big)$$

where the antisymmetric two-particle wave function ψ_a is defined by

$$\psi_a(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') = \frac{1}{\sqrt{2}}\Big(\eta_\uparrow(\sigma)\eta_\downarrow(\sigma') - \eta_\downarrow(\sigma)\eta_\uparrow(\sigma')\Big)\ \varphi(\boldsymbol{r}-\boldsymbol{r}')$$

[2 points]

Solution: We can antisymmetrise the two-particle wave function. Indeed, using

$$\mathcal{A}\cdot f(\cdots, \boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j, \cdots) = -\mathcal{A}\cdot f(\cdots, \boldsymbol{r}_j\sigma_j, \boldsymbol{r}_i\sigma_i, \cdots)$$

we have

$$\begin{aligned}\mathcal{A}\cdot f(\cdots, \boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j, \cdots) &= \frac{1}{2}\Big(\mathcal{A}\cdot f(\cdots, \boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j, \cdots) - \mathcal{A}\cdot f(\cdots, \boldsymbol{r}_j\sigma_j, \boldsymbol{r}_i\sigma_i, \cdots)\Big)\\ &= \mathcal{A}\cdot\frac{1}{2}\Big(f(\cdots, \boldsymbol{r}_i\sigma_i, \boldsymbol{r}_j\sigma_j, \cdots) - f(\cdots, \boldsymbol{r}_j\sigma_j, \boldsymbol{r}_i\sigma_i, \cdots)\Big)\end{aligned}$$

Hence, for particles 1 and 2,

$$\begin{aligned}\langle \boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N|\Phi_N\rangle &\propto \mathcal{A}\cdot\Big(\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)\psi(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\Big) \\ &= \frac{1}{2}\mathcal{A}\cdot\Big(\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)\psi(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\psi(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N) \\ &\quad -\psi(\boldsymbol{r}_2\sigma_2, \boldsymbol{r}_1\sigma_1)\psi(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\psi(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N)\Big) \\ &= \frac{1}{\sqrt{2}}\mathcal{A}\cdot\Big(\frac{\psi(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)-\psi(\boldsymbol{r}_2\sigma_2, \boldsymbol{r}_1\sigma_1)}{\sqrt{2}} \\ &\quad \times\psi(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\psi(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N)\Big)\end{aligned}$$

By performing the same operation for the pairs of particles $(3,4),(5,6),\cdots,(N-1,N)$, we obtain

$$\langle \boldsymbol{r}_1\sigma_1, \cdots, \boldsymbol{r}_N\sigma_N|\Phi_N\rangle \propto \mathcal{A}\cdot\Big(\psi_a(\boldsymbol{r}_1\sigma_1, \boldsymbol{r}_2\sigma_2)\psi_a(\boldsymbol{r}_3\sigma_3, \boldsymbol{r}_4\sigma_4)\cdots\psi_a(\boldsymbol{r}_{N-1}\sigma_{N-1}, \boldsymbol{r}_N\sigma_N)\Big)$$

with the antisymmetrised two-particle wave function

$$\begin{aligned}\psi_a(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') &= \frac{\psi(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma')-\psi(\boldsymbol{r}'\sigma', \boldsymbol{r}\sigma)}{\sqrt{2}} \\ &= \frac{1}{\sqrt{2}}\left(\varphi(\boldsymbol{r}-\boldsymbol{r}')\eta_\uparrow(\sigma)\eta_\downarrow(\sigma') - \underbrace{\varphi(\boldsymbol{r}'-\boldsymbol{r})}_{=\varphi(\boldsymbol{r}-\boldsymbol{r}')}\eta_\uparrow(\sigma')\eta_\downarrow(\sigma)\right) \\ &= \frac{1}{\sqrt{2}}\varphi(\boldsymbol{r}-\boldsymbol{r}')\Big(\eta_\uparrow(\sigma)\eta_\downarrow(\sigma') - \eta_\downarrow(\sigma)\eta_\uparrow(\sigma')\Big)\end{aligned}$$

(c) The coherence length ℓ_c of the pair is then calculated from the average radius ρ of the wave function ψ

$$\ell_c^2 \simeq \rho^2 = \frac{\langle\psi|\hat{R}^2|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int \varphi^*(\boldsymbol{R})R^2\varphi(\boldsymbol{R})d^3R}{\int \varphi^*(\boldsymbol{R})\varphi(\boldsymbol{R})d^3R} \tag{7}$$

1. Show that ρ^2 can be written as:

$$\rho^2 = \frac{\int d^3k(\boldsymbol{\nabla}_k g_{\boldsymbol{k}})^2}{\int d^3k g_{\boldsymbol{k}}^2} \tag{8}$$

[3 points]

Hint: when you integrate over a sphere of radius $|\mathbf{k}| \to \infty$, you may need to approximate $E_k \approx \xi_k\left(1+\frac{\Delta^2}{2\xi_k^2}\right)$.

Solution: Switching to the continuous limit for $\boldsymbol{k}$:

$$\begin{aligned}\int \varphi^*(\boldsymbol{R})R^2\varphi(\boldsymbol{R})d^3R &= \frac{\Omega}{(2\pi)^6}\int d^3R\int d^3k g_{\boldsymbol{k}}\boldsymbol{R}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\cdot\int d^3p g_{\boldsymbol{p}}\boldsymbol{R}e^{-i\boldsymbol{p}\cdot\boldsymbol{R}} \\ &= \frac{\Omega}{(2\pi)^6}\int d^3R\int d^3k g_{\boldsymbol{k}}\boldsymbol{\nabla}_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\cdot\int d^3p g_{\boldsymbol{p}}\boldsymbol{\nabla}_{\boldsymbol{p}}e^{-i\boldsymbol{p}\cdot\boldsymbol{R}}\end{aligned}$$

However, $\nabla_{\boldsymbol{k}}(f(\boldsymbol{k})g(\boldsymbol{k})) = f(\boldsymbol{k})\nabla_{\boldsymbol{k}}g(\boldsymbol{k}) + g(\boldsymbol{k})\nabla_{\boldsymbol{k}}f(\boldsymbol{k})$. Therefore we have:

$$\int d^3k g_{\boldsymbol{k}}\boldsymbol{\nabla}_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}} = \int d^3k\boldsymbol{\nabla}_{\boldsymbol{k}}\left(g_{\boldsymbol{k}}e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\right) - \int d^3k(\boldsymbol{\nabla}_{\boldsymbol{k}}g_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$$

We then use Gauss's theorem (the divergence theorem) on the first term

$$\int d^3k \boldsymbol{\nabla}_{\boldsymbol{k}} \left(g_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\right) = \int dS g_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \boldsymbol{e_r}$$

We need to integrate over a sphere of radius $|\boldsymbol{k}| \to \infty$. Yet, $g_{\boldsymbol{k}} \to 0$ when $\xi_k > \xi_{k_F} + \omega_D$. More precisely, recall the expression of g_k, u_k and v_k (recall that $\xi_k = \frac{k^2}{2m} - \epsilon_F$). You see that for very large k, $E_k \simeq \xi_k + \frac{1}{2}\frac{\Delta^2}{\xi_k}$. By expanding, one gets that

$$g_{\boldsymbol{k}} = \frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} \simeq \frac{m\Delta}{\boldsymbol{k}^2} \tag{9}$$

Since the surface $dS \simeq 4\pi k^2$, we are essentially integrating $e^{i\boldsymbol{k}\cdot\boldsymbol{R}}$ on the sphere, which gives zero.
We thus have

$$\int d^3k \boldsymbol{\nabla}_{\boldsymbol{k}} \left(g_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{R}}\right) = 0$$

and

$$\begin{aligned}
\int \varphi^*(\boldsymbol{R}) R^2 \varphi(\boldsymbol{R}) d^3R &= \frac{\Omega}{(2\pi)^6} \int d^3R \int d^3k g_{\boldsymbol{k}} \boldsymbol{R} e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \cdot \int d^3p g_{\boldsymbol{p}} \boldsymbol{R} e^{-i\boldsymbol{p}\cdot\boldsymbol{R}} \\
&= \frac{\Omega}{(2\pi)^6} \int d^3R \int d^3k (\boldsymbol{\nabla}_{\boldsymbol{k}} g_{\boldsymbol{k}}) e^{i\boldsymbol{k}\cdot\boldsymbol{R}} \cdot \int d^3p (\boldsymbol{\nabla}_{\boldsymbol{p}} g_{\boldsymbol{p}}) e^{-i\boldsymbol{p}\cdot\boldsymbol{R}} \\
&= \frac{\Omega}{(2\pi)^6} \int d^3k \int d^3p (\boldsymbol{\nabla}_{\boldsymbol{k}} g_{\boldsymbol{k}}) \cdot (\boldsymbol{\nabla}_{\boldsymbol{p}} g_{\boldsymbol{p}}) \underbrace{\int e^{i(\boldsymbol{k}-\boldsymbol{p})\cdot\boldsymbol{R}} d^3R}_{=(2\pi)^3 \delta_{\boldsymbol{k},\boldsymbol{p}}} \\
&= \frac{\Omega}{(2\pi)^3} \int d^3k (\boldsymbol{\nabla}_{\boldsymbol{k}} g_{\boldsymbol{k}})^2
\end{aligned}$$

For the denominator,

$$\begin{aligned}
\int \varphi^*(\boldsymbol{R}) \varphi(\boldsymbol{R}) d^3R &\simeq \frac{\Omega}{(2\pi)^6} \int d^3k \int d^3p g_k g_p \int d^3R e^{i(\boldsymbol{k}-\boldsymbol{p})\cdot\boldsymbol{R}} \\
&= \frac{\Omega}{(2\pi)^3} \int d^3k \int d^3p g_{\boldsymbol{k}} g_{\boldsymbol{p}} \delta(\boldsymbol{k}-\boldsymbol{p}) \\
&= \frac{\Omega}{(2\pi)^3} \int d^3k g_{\boldsymbol{k}}^2
\end{aligned}$$

Therefore, finally we got the required expression.

2. Then write it as

$$\rho^2 = \frac{\left(\frac{d\xi_k}{dk}\right)^2_{\xi_k=0} \int_0^{\omega_D} d\xi_k \left(\frac{dg_k}{d\xi_k}\right)^2}{\int_0^{\omega_D} g_k^2 d\xi_k}. \tag{10}$$

[3 points]

Hint: For Cooper pairs in the presence of a a Fermi sea, when $\epsilon_k < \epsilon_F$, g_k can be seen as constant and its gradient is zero.

Solution: Again, let's start from the numerator, and use the fact that g_k behaves as

- We consider a set of Cooper pairs in the presence of a a Fermi sea. Therefore, for $\epsilon_{\boldsymbol{k}} < \epsilon_F$, $g_{\boldsymbol{k}}$ is constant and its gradient it zero.
- $\boldsymbol{\nabla}_{\boldsymbol{k}} g_{\boldsymbol{k}}$ only depends on $|\boldsymbol{k}|$, so that we can switch to spherical coordinates and integrate over the angular variables.

Then we have

$$\begin{aligned}
\int \varphi^*(\boldsymbol{R})R^2\varphi(\boldsymbol{R})d^3R &= \frac{\Omega}{2\pi^2}\int_{k_F}^{k_0} dk k^2\left(\frac{dg_k}{dk}\right)^2 \\
&\simeq \frac{\Omega}{2\pi^2}k_F^2\int_{k_F}^{k_0} dk\left(\frac{dg_k}{dk}\right)^2 \\
&= \frac{\Omega}{2\pi^2}k_F^2\int_0^{\omega_D} d\xi_k\left(\frac{dk}{d\xi_k}\right)\left(\frac{d\xi_k}{dk}\frac{dg_k}{d\xi_k}\right)^2 \\
&\simeq \frac{\Omega}{2\pi^2}k_F^2\left(\frac{d\xi_k}{dk}\right)_{\xi_k=0}\int_0^{\omega_D} d\xi_k\left(\frac{dg_k}{d\xi_k}\right)^2
\end{aligned}$$

For the denominator,

$$\begin{aligned}
\int \varphi^*(\boldsymbol{R})\varphi(\boldsymbol{R})d^3R &\simeq \frac{\Omega}{2\pi^2}k_F^2\int_{k_F}^{k_0} dk g_k^2 \\
&\simeq \frac{\Omega}{2\pi^2}k_F^2\left(\frac{dk}{d\xi_k}\right)_{\xi_k=0}\int_0^{\omega_D} g_k^2 d\xi_k
\end{aligned}$$

3. Calculate the integral, then using the weak-coupling approximation ($\Delta \ll \omega_D$) as well as

$$\left(\frac{d\xi_k}{dk}\right)_{\xi_k=0} = \hbar v_F \tag{11}$$

infer that

$$\ell_c \sim \frac{\hbar v_F}{\Delta}. \tag{12}$$

[3 points]

Solution: Remember that

$$g_{\boldsymbol{k}} = \sqrt{\frac{E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}+\xi_{\boldsymbol{k}}}} = \sqrt{\frac{E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}+\xi_{\boldsymbol{k}}}}\sqrt{\frac{E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}}} = \frac{E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}}{\sqrt{E_{\boldsymbol{k}}^2-\xi_{\boldsymbol{k}}^2}} = \frac{1}{\Delta}\left(E_{\boldsymbol{k}}-\xi_{\boldsymbol{k}}\right)$$

so we have

$$\begin{aligned}
\left(\frac{dg_k}{d\xi_k}\right)^2 &= \frac{1}{\Delta^2}\left(\frac{d}{d\xi_k}\left(E-\xi_k\right)\right)^2 \\
&= \frac{1}{\Delta^2}\left(\frac{d}{d\xi_k}\left(\sqrt{\xi_k^2+\Delta^2}-\xi_k\right)\right)^2 \\
&= \frac{1}{\Delta^2}\left(1+\frac{\xi_k^2}{\xi_k^2+\Delta^2}-2\frac{\xi_k}{\sqrt{\xi_k^2+\Delta^2}}\right)
\end{aligned}$$

and

$$\begin{aligned}
\int_0^{\omega_D} d\xi_k\left(\frac{dg_k}{d\xi_k}\right)^2 &= \frac{1}{\Delta^2}\left[\xi_k+(\xi_k-\Delta\arctan\frac{\xi_k}{\Delta})-2\sqrt{\xi_k^2+\Delta^2}\right]_0^{\omega_D} \\
&= \frac{1}{\Delta^2}\left(2\omega_D-\Delta\arctan\frac{\omega_D}{\Delta}+2\sqrt{\omega_D^2+\Delta^2}+2\Delta\right).
\end{aligned}$$

But $\Delta = 2\omega_D e^{\frac{-1}{Vg_F}}$ (see course), so that in the weak coupling limit $\Delta \ll \omega_D \Rightarrow \sqrt{\omega_D^2 + \Delta^2} \simeq \omega_D$ and

$$\int_0^{\omega_D} d\xi_k \left(\frac{dg_k}{d\xi_k}\right)^2 \simeq \frac{2-\frac{\pi}{2}}{\Delta}$$

Thus we have, with $\left(\frac{d\xi_k}{dk}\right)_{\xi_k=0} = \hbar v_F$, and

$$\int \varphi^*(\boldsymbol{R}) R^2 \varphi(\boldsymbol{R}) d^3R = \frac{\Omega k_F^2 \hbar v_F}{\pi^2 \Delta}\left(1 - \frac{\pi}{4}\right).$$

Similarly, we have

$$\begin{aligned}
\int \varphi^*(\boldsymbol{R})\varphi(\boldsymbol{R}) d^3R &\simeq \frac{\Omega}{2\pi^2} k_F^2 \int_{k_F}^{k_0} dk g_k^2 \\
&\simeq \frac{\Omega}{2\pi^2} k_F^2 \left(\frac{dk}{d\xi_k}\right)_{\xi_k=0} \int_0^{\omega_D} g_k^2 d\xi_k \\
&= \frac{\Omega}{2\pi^2} \frac{k_F^2}{\hbar v_F} \int_0^{\omega_D} \left(\frac{\sqrt{\Delta^2+\xi_k^2} - \xi_k}{\Delta}\right)^2 d\xi_k \\
&= \frac{\Omega}{2\pi^2} \frac{k_F^2}{\hbar v_F \Delta^2} \int_0^{\omega_D} \left(\Delta^2 + 2\xi_k^2 - 2\xi_k\sqrt{\Delta^2+\xi_k^2}\right) d\xi_k \\
&= \frac{\Omega}{2\pi^2} \frac{k_F^2}{\hbar v_F \Delta^2} \left[\xi_k \Delta^2 + \frac{2}{3}\xi_k^3 - \frac{2}{3}(\Delta^2+\xi_k^2)\sqrt{\Delta^2+\xi_k^2}\right]_0^{\omega_D} \\
&= \frac{\Omega}{2\pi^2} \frac{k_F^2}{\hbar v_F \Delta^2} \left(\omega_D \Delta^2 + \frac{2}{3}\omega_D^3 - \frac{2}{3}(\Delta^2+\omega_D^2)\sqrt{\Delta^2+\omega_D^2} + \frac{2}{3}\Delta^3\right)
\end{aligned}$$

But $\Delta \ll \omega_D \Rightarrow \sqrt{1+\left(\frac{\Delta}{\omega_D}\right)^2} \simeq 1 + \Delta^2/(2\omega_D^2)$, and we get

$$\int \varphi^*(\boldsymbol{R})\varphi(\boldsymbol{R}) d^3R \simeq \frac{\Omega k_F^2 \Delta}{3\pi^2 \hbar v_F}.$$

Finally,

$$\ell_c^2 \simeq \frac{\int \varphi^*(\boldsymbol{R}) R^2 \varphi(\boldsymbol{R}) d^3R}{\int \varphi^*(\boldsymbol{R})\varphi(\boldsymbol{R}) d^3R} \sim \frac{\hbar^2 v_F^2}{\Delta^2}$$

Usually, $\ell_c \sim 10^3$ Å, which should be compared with the lattice constant $\sim$1Å ($\sim$ distance between the centers of mass of the pairs). Thereby, the spatial extent of the Cooper pairs is considerably larger than the distance between their centers of mass, and we cannot assume that they are independent.

Here are some useful integrals:

$$\int \frac{1}{x^2+a^2} dx = \frac{1}{a}\arctan\frac{x}{a} \qquad \text{et} \qquad \int \frac{x^2}{x^2+a^2} dx = x - a\arctan\frac{x}{a}$$

$$\int \frac{x}{\sqrt{x^2+a^2}} dx = \sqrt{x^2+a^2} \qquad \text{et} \qquad \int x\sqrt{x^2+a^2} dx = \frac{1}{3}(x^2+a^2)\sqrt{x^2+a^2}$$

Properties of Hubbard Hamiltonian

Consider the one-dimensional Hubbard model, whose Hamiltonian is given by:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the creation and annihilation operators for an electron at site i with spin σ, $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the number operator for electrons at site i with spin σ, t is the hopping parameter, U is the on-site interaction energy, and $\langle i,j \rangle$ denotes nearest-neighbor sites.

(a) Prove that the total number operator

$$\hat{N} = \sum_i n_i, \quad \text{where } n_i = n_{i\uparrow} + n_{i\downarrow},$$

commutes with the Hamiltonian, i.e., show that:

$$[\hat{N}, H] = 0.$$

[2 points]

Solution: To show that $[\hat{N}, H] = 0$, we compute the commutator explicitly. The total particle number operator is given by:

$$\hat{N} = \sum_j n_j = \sum_j \left(c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow} \right),$$

and the Hamiltonian H has two terms: the hopping term and the interaction term:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

The hopping term is:

$$H_{\text{hop}} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma} \right).$$

The commutator of $\hat{N}$ with H_{hop} is:

$$[\hat{N}, H_{\text{hop}}] = -t \sum_{\langle i,j \rangle, \sigma} \left([\hat{N}, c_{i\sigma}^\dagger c_{j\sigma}] + [\hat{N}, c_{j\sigma}^\dagger c_{i\sigma}] \right).$$

Using the commutator relations:

$$[\hat{N}, c_{i\sigma}] = -c_{i\sigma}, \quad [\hat{N}, c_{i\sigma}^\dagger] = c_{i\sigma}^\dagger,$$

we find:

$$[\hat{N}, c_{i\sigma}^\dagger c_{j\sigma}] = c_{i\sigma}^\dagger c_{j\sigma} - c_{i\sigma}^\dagger c_{j\sigma} = 0,$$

and similarly:

$$[\hat{N}, c_{j\sigma}^\dagger c_{i\sigma}] = 0.$$

Thus:

$$[\hat{N}, H_{\text{hop}}] = 0.$$

The interaction term is:

$$H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

The commutator of $\hat{N}$ with H_{int} is:

$$[\hat{N}, H_{\text{int}}] = U \sum_i [\hat{N}, n_{i\uparrow} n_{i\downarrow}].$$

Since $\hat{N}$ commutes with $n_{i\uparrow}$ and $n_{i\downarrow}$, we have:

$$[\hat{N}, n_{i\uparrow} n_{i\downarrow}] = 0.$$

Thus:

$$[\hat{N}, H_{\text{int}}] = 0.$$

Since $[\hat{N}, H_{\text{hop}}] = 0$ and $[\hat{N}, H_{\text{int}}] = 0$, we conclude:

$$[\hat{N}, H] = 0.$$

This shows that the total particle number $\hat{N}$ is conserved under the Hamiltonian H.

(b) $\hat{N}$ is a conserved quantity. Write the local conservation equation for particle number. Using the Heisenberg equation of motion, find the expression for the corresponding current? **[1 point]**

Solution:

The local conservation equation for particle number is:

$$\frac{dn_i}{dt} + \sum_j J_{ij} = 0,$$

where J_{ij} is the current from site j to site i.

Using the Heisenberg equation of motion:

$$\frac{dn_i}{dt} = \frac{i}{\hbar}[H, n_i],$$

we compute the commutator $[H, n_i]$ with the Hamiltonian:

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

The commutator $[H, n_i]$ receives contributions only from the hopping term:

$$H_{\text{hop}} = -t \sum_{\langle i,j \rangle, \sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right).$$

Expand the commutator:

$$[H_{\text{hop}}, n_i] = -t \sum_{\langle i,j \rangle, \sigma} \left([c^\dagger_{i\sigma} c_{j\sigma}, n_i] + [c^\dagger_{j\sigma} c_{i\sigma}, n_i] \right).$$

For $n_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$, the commutator with the hopping terms evaluates to:

$$[c^\dagger_{i\sigma} c_{j\sigma}, n_i] = -c^\dagger_{i\sigma} c_{j\sigma}, \quad [c^\dagger_{j\sigma} c_{i\sigma}, n_i] = c^\dagger_{j\sigma} c_{i\sigma}.$$

Thus:

$$[H_{\text{hop}}, n_i] = it \sum_{\langle i,j \rangle, \sigma} \left(c^\dagger_{j\sigma} c_{i\sigma} - c^\dagger_{i\sigma} c_{j\sigma} \right).$$

Substitute this result into the Heisenberg equation of motion:

$$\frac{dn_i}{dt} = t \sum_{\langle i,j \rangle, \sigma} \left(c_{j\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{j\sigma} \right).$$

The current J_{ij} is then:

$$J_{ij} = it \sum_{\sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} - c_{j\sigma}^\dagger c_{i\sigma} \right).$$

(c) It is easy to see that the Hamiltonian is invariant under the transformations:

$$c_{j\sigma} \to e^{-i\theta} c_{j\sigma}, \quad c_{j\sigma}^\dagger \to e^{i\theta} c_{j\sigma}^\dagger.$$

Such a symmetry is called a **global $U(1)$ symmetry**. Given the unitary operator:

$$U = e^{i\theta \hat{N}},$$

compute the transformed operators

$$U c_{j\sigma} U^\dagger \quad \text{and} \quad U c_{j\sigma}^\dagger U^\dagger,$$

and show that they turn out to be $e^{-i\theta} c_{j\sigma}$ and $e^{i\theta} c_{j\sigma}^\dagger$, respectively. **[3 points]**
Hint: You may use the Baker–Campbell–Hausdorff formula.
Solution:
Using the Baker-Campbell-Hausdorff formula:

$$U c_{j\sigma} U^\dagger = e^{i\theta \hat{N}} c_{j\sigma} e^{-i\theta \hat{N}},$$

we expand the transformation as:

$$U c_{j\sigma} U^\dagger = c_{j\sigma} + i\theta [\hat{N}, c_{j\sigma}] + \frac{(i\theta)^2}{2!} [\hat{N}, [\hat{N}, c_{j\sigma}]] + \cdots.$$

From the commutator relations, we know:

$$[\hat{N}, c_{j\sigma}] = -c_{j\sigma}.$$

Substituting this into the expansion:

$$[\hat{N}, [\hat{N}, c_{j\sigma}]] = [\hat{N}, -c_{j\sigma}] = -[\hat{N}, c_{j\sigma}] = c_{j\sigma}.$$

The pattern alternates as:

$$[\hat{N}, [\hat{N}, [\hat{N}, c_{j\sigma}]]] = -c_{j\sigma}, \quad \text{and so on.}$$

Thus, the series sums to:

$$U c_{j\sigma} U^\dagger = c_{j\sigma} \left(1 - i\theta + \frac{(-i\theta)^2}{2!} - \frac{(-i\theta)^3}{3!} + \cdots \right).$$

The expression in parentheses is the Taylor expansion of $e^{-i\theta}$. Therefore:

$$U c_{j\sigma} U^\dagger = e^{-i\theta} c_{j\sigma}.$$

Similarly, for $c^\dagger_{j\sigma}$, we compute:

$$Uc^\dagger_{j\sigma}U^\dagger = e^{i\theta\hat{N}}c^\dagger_{j\sigma}e^{-i\theta\hat{N}},$$

and expand:

$$Uc^\dagger_{j\sigma}U^\dagger = c^\dagger_{j\sigma} + i\theta[\hat{N}, c^\dagger_{j\sigma}] + \frac{(i\theta)^2}{2!}[\hat{N}, [\hat{N}, c^\dagger_{j\sigma}]] + \cdots .$$

Using the commutator:

$$[\hat{N}, c^\dagger_{j\sigma}] = c^\dagger_{j\sigma},$$

the series sums to:

$$Uc^\dagger_{j\sigma}U^\dagger = c^\dagger_{j\sigma}\left(1 + i\theta + \frac{(i\theta)^2}{2!} + \frac{(i\theta)^3}{3!} + \cdots\right).$$

The expression in parentheses is the Taylor expansion of $e^{i\theta}$. Therefore:

$$Uc^\dagger_{j\sigma}U^\dagger = e^{i\theta}c^\dagger_{j\sigma}.$$

(d) **(Optional)** We have shown in the lecture that the effective Hamiltonian for the Hubbard model at half-filling can be written as

$$-\frac{t^2}{U}\sum_{i(j),\sigma'\sigma''} c^\dagger_{i\sigma'}c_{j,\sigma'}n_{j,\sigma}n_{j,-\sigma}c^\dagger_{j,\sigma''}c_{i,\sigma''}.$$

(See Mila's lecture notes, Section 2.3).

In the lecture, we performed explicit calculations for the case

$$\sigma' = \sigma'' = \sigma.$$

Consider the other three cases, i.e.

$$\sigma' = \sigma'' = -\sigma,$$

$$\sigma'' = -\sigma' = \sigma$$

and

$$\sigma'' = -\sigma' = -\sigma,$$

and simplify the effective Hamiltonian (show detailed calculations). **[3 points]**

Solution:

The solution is straightforward once you have determined that

$$c_{j,\sigma}n_{j,\sigma}c^\dagger_{j,\sigma} = (1 - n_{j,\sigma}),$$

$$n_{j,\sigma} + n_{j,-\sigma} = 1$$

and

$$c_{j,\sigma}n_{j,\sigma} = c_{j,\sigma}.$$