TKM2 Übungsblatt 1: Lösungen

April 27, 2012

1 **Fermionic Correlation Functions**
Most of the solutions for this problem follow the exact same route as the problem for bosonic correlation functions, which were presented during last weeks Übung. However, for completeness I shall present the full solutions with the appropriate changes (which turn out to only correspond to differing signs at various places).

a) We may rewrite the expressions $c_{\boldsymbol{k}}\rho = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)}\rho c_{\boldsymbol{k}}$ and $c_{\boldsymbol{k}}^\dagger \rho = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)}\rho c_{\boldsymbol{k}}^\dagger$ in the form

$$e^{\beta(H-\mu N)} c_{\boldsymbol{k}} e^{-\beta(H-\mu N)} = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)} c_{\boldsymbol{k}}, \qquad e^{\beta(H-\mu N)} c_{\boldsymbol{k}}^\dagger e^{-\beta(H-\mu N)} = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)} c_{\boldsymbol{k}}^\dagger \tag{1}$$

Comparing the left-hand side with the left-hand side of the Hadamard Lemma, we can identify $X = \beta(H-\mu N)$ and $Y = c_{\boldsymbol{k}}$ or $Y = c_{\boldsymbol{k}}^\dagger$. Next, we compute the commutators

$$[X,Y] = [\beta(H-\mu N), c_{\boldsymbol{k}}] = \sum_{\boldsymbol{k}'} \beta(\epsilon_{\boldsymbol{k}'}-\mu)\left[c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'}, c_{\boldsymbol{k}}\right] = \sum_{\boldsymbol{k}'} \beta(\epsilon_{\boldsymbol{k}'}-\mu)\left(a_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} c_{\boldsymbol{k}} - c_{\boldsymbol{k}} c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'}\right) \tag{2}$$

and

$$[X,Y] = [\beta(H-\mu N), c_{\boldsymbol{k}}^\dagger] = \sum_{\boldsymbol{k}'} \beta(\epsilon_{\boldsymbol{k}'}-\mu)\left[a_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'}, c_{\boldsymbol{k}}^\dagger\right] = \sum_{\boldsymbol{k}'} \beta(\epsilon_{\boldsymbol{k}'}-\mu)\left(c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} c_{\boldsymbol{k}}^\dagger - c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'}\right) \tag{3}$$

So far everything is exactly the same as for the bosonic case. The only difference comes in the next step (though the result turns out to be the same).

The last term in the brackets of these expressions can be rewritten using the fermionic *anti*-commutation relations

$$c_{\boldsymbol{k}} c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'} c_{\boldsymbol{k}} - c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}} c_{\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'} c_{\boldsymbol{k}} + c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} c_{\boldsymbol{k}} \tag{4}$$

and

$$c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} = -c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}'} = -\delta_{\boldsymbol{k},\boldsymbol{k}'} c_{\boldsymbol{k}}^\dagger + c_{\boldsymbol{k}'}^\dagger c_{\boldsymbol{k}'} c_{\boldsymbol{k}}^\dagger \tag{5}$$

The last terms in these two expressions cancel the first term in the previous expressions so we are left with

$$[H, c_{\boldsymbol{k}}] = -\beta(\epsilon_{\boldsymbol{k}}-\mu)c_{\boldsymbol{k}}, \qquad [H, c_{\boldsymbol{k}}^\dagger] = -(\epsilon_{\boldsymbol{k}}-\mu)c_{\boldsymbol{k}}^\dagger \tag{6}$$

In terms of the superoperator ad_X we can interpret this as $c_{\boldsymbol{k}}$ being an eigenoperator of ad_X with eigenvalue $-\beta(\epsilon_{\boldsymbol{k}}-\mu)$. We thus have for the right-hand side of the Hadamard Lemma

$$e^{\mathrm{ad}_X} c_{\boldsymbol{k}} = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)} c_{\boldsymbol{k}}, \qquad e^{\mathrm{ad}_X} c_{\boldsymbol{k}}^\dagger = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)} c_{\boldsymbol{k}}^\dagger \tag{7}$$

Which thus proves (1).

b) For fermionic operators we have relations similar (upto difference in sign) as with the bosonic operators:

$$\langle c_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} \rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} - \langle c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_1} \rangle \tag{8}$$

(**notice sign difference compared to bosonic case**) and

$$\langle c_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} \rangle = e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)} \langle c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_1} \rangle. \tag{9}$$

The first follows directly from the *anti*-commutation relations $c_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} - c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_1}$, while the second follows from the relation $c^\dagger_{\boldsymbol{k}_2}\rho = e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}\rho c^\dagger_{\boldsymbol{k}_2}$ together with the cyclic property of the trace. By subtracting the left-hand side and the right-hand sides from the two relations we obtain

$$(1 + e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}) \langle c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_1} \rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{10}$$

and thus

$$\langle c^\dagger_{\boldsymbol{k}_2} c_{\boldsymbol{k}_1} \rangle = \frac{1}{1 + e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}} \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{11}$$

It then follows from the second relation that

$$\langle c_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_2} \rangle = \frac{e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}}{1 + e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}} \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{12}$$

Notice that $\langle n_{\boldsymbol{k}} \rangle = \langle c^\dagger_{\boldsymbol{k}} c_{\boldsymbol{k}} \rangle = n_F(\epsilon_{\boldsymbol{k}})$ where $n_F(x)$ is the Fermi-Dirac distribution, and $\langle c_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} \rangle = \langle 1 - n_{\boldsymbol{k}} \rangle = 1 - n_F(\epsilon_{\boldsymbol{k}})$.

c) To evaluate the correlation function $\langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle$ we shall follow a similar route as in the calculation before. Let us write

$$\begin{aligned}
\langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle &= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle - \langle c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_1} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle \\
&= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle + \langle c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_4} \rangle \\
&= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4} \langle c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} \rangle - \langle c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} c^\dagger_{\boldsymbol{k}_1} \rangle
\end{aligned} \tag{13}$$

(**notice all the sign-differences compared to the bosonic case**). The last term in the right-hand side of the last line is simply a cyclic permutation of the expression on the left-hand side (with an additional minus sign). Using the property $c^\dagger_{\boldsymbol{k}_1}\rho = e^{\beta(\epsilon_{\boldsymbol{k}_1}-\mu)}\rho c^\dagger_{\boldsymbol{k}_1}$ together with the cyclic property of the trace we get

$$(1 + e^{\beta(\epsilon_{\boldsymbol{k}_1}-\mu)}) \langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4} \rangle + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4} \langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} \rangle \tag{14}$$

Recalling the results from the previous problem we can now write this result in a compact form

$$\begin{aligned}
\langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle &= \langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_2} \rangle \langle c^\dagger_{\boldsymbol{k}_3} c_{\boldsymbol{k}_4} \rangle + \langle c^\dagger_{\boldsymbol{k}_1} c_{\boldsymbol{k}_4} \rangle \langle c_{\boldsymbol{k}_2} c^\dagger_{\boldsymbol{k}_3} \rangle \\
&= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \delta_{\boldsymbol{k}_3,\boldsymbol{k}_4} n_F(\epsilon_{\boldsymbol{k}_1}) n_F(\epsilon_{\boldsymbol{k}_3}) + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4} \delta_{\boldsymbol{k}_2,\boldsymbol{k}_3} n_F(\epsilon_{\boldsymbol{k}_1}) \left(1 - n_F(\epsilon_{\boldsymbol{k}_3})\right)
\end{aligned} \tag{15}$$

So in the end, the only sign difference compared to the bosonic case comes from the last term ($1 - n_F$ as opposed to $1 + n_B$).

2 | Density-density correlation function

a) The average of the density operator can be written in the form

$$
\begin{aligned}
\langle n(\boldsymbol{r})\rangle = \langle \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\rangle &= \frac{1}{V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}\langle c^\dagger_{\boldsymbol{k}_1}c_{\boldsymbol{k}_2}\rangle \\
&= \frac{1}{V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}n_F(\epsilon_{\boldsymbol{k}_1}) \\
&= \frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}}) \\
&= \frac{N}{V}
\end{aligned} \tag{16}
$$

b) We have

$$
\begin{aligned}
\langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle &= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\langle c^\dagger_{\boldsymbol{k}_1}c_{\boldsymbol{k}_2}c^\dagger_{\boldsymbol{k}_3}c_{\boldsymbol{k}_4}\rangle \\
&= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\boldsymbol{k}_3,\boldsymbol{k}_4}n_F(\epsilon_{\boldsymbol{k}_1})n_F(\epsilon_{\boldsymbol{k}_3}) \\
&\quad+\frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_3}n_F(\epsilon_{\boldsymbol{k}_1})\left(1-n_F(\epsilon_{\boldsymbol{k}_3})\right) \\
&= \frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_F(\epsilon_{\boldsymbol{k}_1})\sum_{\boldsymbol{k}_3} n_F(\epsilon_{\boldsymbol{k}_3}) \\
&\quad+\frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_F(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sum_{\boldsymbol{k}_3}\left(1-n_F(\epsilon_{\boldsymbol{k}_3})\right)e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')} \\
&= \left(\frac{N}{V}\right)^2 + \frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_F(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sum_{\boldsymbol{k}_3}\left(1-n_F(\epsilon_{\boldsymbol{k}_3})\right)e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')}
\end{aligned} \tag{17}
$$

And thus the density-density correlation function is given by

$$
\begin{aligned}
&\langle \Delta n(\boldsymbol{r})\Delta n(\boldsymbol{r}')\rangle = \langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle - \langle n\rangle^2 \\
&\qquad= \frac{1}{V}\sum_{\boldsymbol{k}_1} n_F(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\left(\frac{1}{V}\sum_{\boldsymbol{k}_3} e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')} - \frac{1}{V}\sum_{\boldsymbol{k}_3} n_F(\epsilon_{\boldsymbol{k}_3})e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right)
\end{aligned} \tag{18}
$$

Using the identity $\frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta(\boldsymbol{r}-\boldsymbol{r}')$ we get

$$
\begin{aligned}
\langle \Delta n(\boldsymbol{r})\Delta n(\boldsymbol{r}')\rangle &= \delta(\boldsymbol{r}-\boldsymbol{r}')\frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}}) - \left|\frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2 \\
&= \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle - \left|\frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2
\end{aligned} \tag{19}
$$

The first term we again recognize as the *auto-correlation* term and the second term is proportional to the **pair-correlation** term for fermions

$$h_F(\boldsymbol{r}-\boldsymbol{r}') = -\frac{1}{\langle n\rangle^2}\left|\frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2 \tag{20}$$

Apart from the different distribution functions in this expression, the fermionic pair-correlation has a **negative sign**, i.e. bosons have positive pair-correlations while fermions have negative pair-correlations. This is a consequence of the **Pauli-Exclusion Principle**.

Let us consider the zero temperature limit when all states with energies below the Fermi-energy (note that $\epsilon_F = \mu(T=0)$) are occupied, i.e.

$$n_F(\epsilon_{\boldsymbol{k}_F}) = \Theta(\epsilon_F - \epsilon_{\boldsymbol{k}}) \tag{21}$$

(Note that we have neglected spin here, if we include spin there would be an additional factor due to degeneracy).

Turning the sum into an integral over spherical coordinates and we have after performing the integration over the angle-variables

$$\frac{1}{V}\sum_{\boldsymbol{k}} n_F(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \frac{1}{(2\pi)^2}\int_0^\infty dk\frac{k\sin(k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|}\Theta(\epsilon_F-\epsilon_k) \tag{22}$$

The step-function cuts the integral at a point k_F: $\epsilon_{k_F} = \epsilon_F$, i.e. the Fermi wavevector. We are then left with performing the integral

$$\int_0^{k_F} dk\frac{k\sin(k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|} = \frac{\sin(k_F|\boldsymbol{r}-\boldsymbol{r}'|) - k_F|\boldsymbol{r}-\boldsymbol{r}'|\cos(k_F|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|^3} \tag{23}$$

Plugging this into the pair-correlation function we have

$$h_F(r) = -\frac{1}{(2\pi)^4}\left|\frac{\sin(k_F r) - k_F r\cos(k_F r)}{r^3}\right|^2 \tag{24}$$

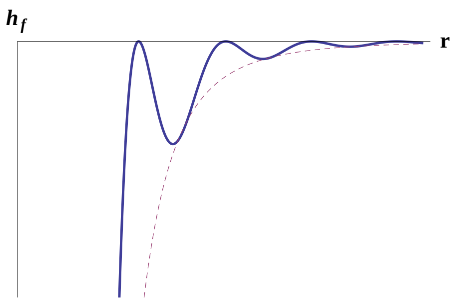

Figure 1: The fermionic pair correlation function at zero temperature. It diverges for small r due to Pauli-Principle then oscillates on the length scale $1/k_F$ but eventually decays as $\sim k_F^2/r^4$(see dashed line).

Additional Notes

For completeness I also provide the calculations for the bosonic case.

1 | Bosonic Correlation Functions

a) We may rewrite the expressions $a_{\boldsymbol{k}}\rho = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)}\rho a_{\boldsymbol{k}}$ and $a^\dagger_{\boldsymbol{k}}\rho = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)}\rho a^\dagger_{\boldsymbol{k}}$ in the form

$$e^{\beta(H-\mu N)}a_{\boldsymbol{k}}e^{-\beta(H-\mu N)} = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)}a_{\boldsymbol{k}}, \qquad e^{\beta(H-\mu N)}a^\dagger_{\boldsymbol{k}}e^{-\beta(H-\mu N)} = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)}a^\dagger_{\boldsymbol{k}} \tag{25}$$

Comparing the left-hand side with the left-hand side of the Hadamard Lemma, we can identify $X = \beta(H-\mu N)$ and $Y = a_{\boldsymbol{k}}$ or $Y = a^\dagger_{\boldsymbol{k}}$. Next, we compute the commutators

$$[X,Y] = [\beta(H-\mu N), a_{\boldsymbol{k}}] = \sum_{\boldsymbol{k}'}\beta(\epsilon_{\boldsymbol{k}'}-\mu)\left[a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}, a_{\boldsymbol{k}}\right] = \sum_{\boldsymbol{k}'}\beta(\epsilon_{\boldsymbol{k}'}-\mu)\left(a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}a_{\boldsymbol{k}} - a_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}\right) \tag{26}$$

and

$$[X,Y] = [\beta(H-\mu N), a^\dagger_{\boldsymbol{k}}] = \sum_{\boldsymbol{k}'}\beta(\epsilon_{\boldsymbol{k}'}-\mu)\left[a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}, a^\dagger_{\boldsymbol{k}}\right] = \sum_{\boldsymbol{k}'}\beta(\epsilon_{\boldsymbol{k}'}-\mu)\left(a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}a^\dagger_{\boldsymbol{k}} - a^\dagger_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}\right) \tag{27}$$

The last term in the brackets of these expressions can be rewritten using the commutation relations

$$a_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'}a_{\boldsymbol{k}} + a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}}a_{\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'}a_{\boldsymbol{k}} + a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}a_{\boldsymbol{k}} \tag{28}$$

and

$$a^\dagger_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'} = a^\dagger_{\boldsymbol{k}'}a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'} = -\delta_{\boldsymbol{k},\boldsymbol{k}'}a^\dagger_{\boldsymbol{k}} + a^\dagger_{\boldsymbol{k}'}a_{\boldsymbol{k}'}a^\dagger_{\boldsymbol{k}} \tag{29}$$

The last terms in these two expressions cancel the first term in the previous expressions so we are left with

$$[\beta(H-\mu N), a_{\boldsymbol{k}}] = -\beta(\epsilon_{\boldsymbol{k}}-\mu)a_{\boldsymbol{k}}, \qquad [\beta(H-\mu N), a^\dagger_{\boldsymbol{k}}] = \beta(\epsilon_{\boldsymbol{k}}-\mu)a^\dagger_{\boldsymbol{k}} \tag{30}$$

For higher order commutators we have e.g.

$$[\beta(H-\mu N), [\beta(H-\mu N), a_{\boldsymbol{k}}]] = -\beta(\epsilon_{\boldsymbol{k}}-\mu)[\beta(H-\mu N), a_{\boldsymbol{k}}] = (-\beta(\epsilon_{\boldsymbol{k}}-\mu))^2 a_{\boldsymbol{k}} \tag{31}$$

and so on. In terms of the superoperator ad_X we can interpret this as $a_{\boldsymbol{k}}$ being an eigen-operator of ad_X with eigenvalue $-\beta(\epsilon_{\boldsymbol{k}}-\mu)$:

$$\mathrm{ad}_X a_{\boldsymbol{k}} = -\beta(\epsilon_{\boldsymbol{k}}-\mu)a_{\boldsymbol{k}}, \qquad \mathrm{ad}^n_X a_{\boldsymbol{k}} = (-\beta(\epsilon_{\boldsymbol{k}}-\mu))^n a_{\boldsymbol{k}} \tag{32}$$

and similarly for $a^\dagger_{\boldsymbol{k}}$. We thus have for the right-hand side of the Hadamard Lemma

$$e^{\mathrm{ad}_X}a_{\boldsymbol{k}} = e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)}a_{\boldsymbol{k}}, \qquad e^{\mathrm{ad}_X}a^\dagger_{\boldsymbol{k}} = e^{\beta(\epsilon_{\boldsymbol{k}}-\mu)}a^\dagger_{\boldsymbol{k}} \tag{33}$$

Which thus proves (25).

b) Let us first note two relationships

$$\langle a_{\boldsymbol{k}_1}a^\dagger_{\boldsymbol{k}_2}\rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} + \langle a^\dagger_{\boldsymbol{k}_2}a_{\boldsymbol{k}_1}\rangle \tag{34}$$

and

$$\langle a_{\boldsymbol{k}_1}a^\dagger_{\boldsymbol{k}_2}\rangle = e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}\langle a^\dagger_{\boldsymbol{k}_2}a_{\boldsymbol{k}_1}\rangle. \tag{35}$$

The first follows directly from the commutation relations $a_{\boldsymbol{k}_1} a^\dagger_{\boldsymbol{k}_2} = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} + a^\dagger_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}$, while the second follows from the relation $a^\dagger_{\boldsymbol{k}_2}\rho = e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}\rho a^\dagger_{\boldsymbol{k}_2}$ together with the cyclic property of the trace. By subtracting the left-hand side and the right-hand sides from the two relations we obtain

$$(1 - e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)})\langle a^\dagger_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}\rangle = -\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{36}$$

and thus

$$\langle a^\dagger_{\boldsymbol{k}_2} a_{\boldsymbol{k}_1}\rangle = \frac{-1}{1 - e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{37}$$

It then follows from the second relation that

$$\langle a_{\boldsymbol{k}_1} a^\dagger_{\boldsymbol{k}_2}\rangle = \frac{-e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}}{1 - e^{\beta(\epsilon_{\boldsymbol{k}_2}-\mu)}}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} \tag{38}$$

Notice that $\langle n_{\boldsymbol{k}}\rangle = \langle a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}\rangle = n_B(\epsilon_{\boldsymbol{k}})$ where $n_B(x)$ is the Bose-Einstein distribution, and $\langle a_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}}\rangle = \langle 1 + n_{\boldsymbol{k}}\rangle = 1 + n_B(\epsilon_{\boldsymbol{k}})$.

c) To evaluate the correlation function $\langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle$ we shall follow a similar route as in the calculation before. Let us write

$$\begin{aligned}\langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle &= -\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle + \langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_1} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle \\ &= -\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle + \langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_4}\rangle \\ &= -\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle - \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3}\rangle + \langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4} a^\dagger_{\boldsymbol{k}_1}\rangle\end{aligned} \tag{39}$$

The last term in the right-hand side of the last line is simply a cyclic permutation of the expression on the left-hand side. Using the property $a^\dagger_{\boldsymbol{k}_1}\rho = e^{\beta(\epsilon_{\boldsymbol{k}_1}-\mu)}\rho a^\dagger_{\boldsymbol{k}_1}$ together with the cyclic property of the trace we get

$$(1 - e^{\beta(\epsilon_{\boldsymbol{k}_1}-\mu)})\langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle = -\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle - \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3}\rangle \tag{40}$$

Recalling the results from the previous problem we can now write this result in a compact form

$$\begin{aligned}\langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle &= \langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2}\rangle\langle a^\dagger_{\boldsymbol{k}_3} a_{\boldsymbol{k}_4}\rangle + \langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_4}\rangle\langle a_{\boldsymbol{k}_2} a^\dagger_{\boldsymbol{k}_3}\rangle \\ &= \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\boldsymbol{k}_3,\boldsymbol{k}_4} n_B(\epsilon_{\boldsymbol{k}_1}) n_B(\epsilon_{\boldsymbol{k}_3}) + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_3} n_B(\epsilon_{\boldsymbol{k}_1})\left(1 + n_B(\epsilon_{\boldsymbol{k}_3})\right)\end{aligned} \tag{41}$$

2 | Density-density correlation functions

a) The average of the density operator can be written in the form

$$\begin{aligned}\langle n(\boldsymbol{r})\rangle = \langle \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\rangle &= \frac{1}{V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}\langle a^\dagger_{\boldsymbol{k}_1} a_{\boldsymbol{k}_2}\rangle \\ &= \frac{1}{V}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2} n_B(\epsilon_{\boldsymbol{k}_1}) \\ &= \frac{1}{V}\sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}}) \\ &= \frac{N}{V}\end{aligned} \tag{42}$$

b) We have

$$
\begin{aligned}
\langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle &= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\langle a^\dagger_{\boldsymbol{k}_1}a_{\boldsymbol{k}_2}a^\dagger_{\boldsymbol{k}_3}a_{\boldsymbol{k}_4}\rangle \\
&= \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\boldsymbol{k}_3,\boldsymbol{k}_4}n_B(\epsilon_{\boldsymbol{k}_1})n_B(\epsilon_{\boldsymbol{k}_3}) \\
&+ \frac{1}{V^2}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3,\boldsymbol{k}_4} e^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}}e^{-i(\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}'}\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_3}n_B(\epsilon_{\boldsymbol{k}_1})\left(1+n_B(\epsilon_{\boldsymbol{k}_3})\right) \\
&= \frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_B(\epsilon_{\boldsymbol{k}_1})\sum_{\boldsymbol{k}_3} n_B(\epsilon_{\boldsymbol{k}_3}) \\
&+ \frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_B(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sum_{\boldsymbol{k}_3}\left(1+n_B(\epsilon_{\boldsymbol{k}_3})\right)e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')} \\
&= \left(\frac{N}{V}\right)^2 + \frac{1}{V^2}\sum_{\boldsymbol{k}_1} n_B(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sum_{\boldsymbol{k}_3}\left(1+n_B(\epsilon_{\boldsymbol{k}_3})\right)e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')}
\end{aligned}
\tag{43}
$$

And thus the density-density correlation function is given by

$$
\begin{aligned}
\langle \Delta n(\boldsymbol{r})\Delta n(\boldsymbol{r}')\rangle &= \langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle - \langle n\rangle^2 \\
&= \frac{1}{V}\sum_{\boldsymbol{k}_1} n_B(\epsilon_{\boldsymbol{k}_1})e^{-i\boldsymbol{k}_1\cdot(\boldsymbol{r}-\boldsymbol{r}')}\left(\frac{1}{V}\sum_{\boldsymbol{k}_3} e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')} + \frac{1}{V}\sum_{\boldsymbol{k}_3} n_B(\epsilon_{\boldsymbol{k}_3})e^{i\boldsymbol{k}_3\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right)
\end{aligned}
\tag{44}
$$

Using the identity $\frac{1}{V}\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} = \delta(\boldsymbol{r}-\boldsymbol{r}')$ we get

$$
\begin{aligned}
\langle \Delta n(\boldsymbol{r})\Delta n(\boldsymbol{r}')\rangle &= \delta(\boldsymbol{r}-\boldsymbol{r}')\frac{1}{V}\sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}}) + \left|\frac{1}{V}\sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2 \\
&= \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle + \left|\frac{1}{V}\sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2
\end{aligned}
\tag{45}
$$

The first term is called the *auto-correlation function* and the second part is proportional to the so called **pair-correlation function** for bosons:

$$
h_B(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{\langle n\rangle^2}\left|\frac{1}{V}\sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}})e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2 \tag{46}
$$

Let us consider first the zero temperature limit where the all the N particles are located in the lowest energy state $\boldsymbol{k}=0$:

$$
n_B(\epsilon_{\boldsymbol{k}}) = N\delta_{\boldsymbol{k},0} \tag{47}
$$

In this limit we have the pair-correlation function

$$
h_B(\boldsymbol{r}-\boldsymbol{r}') = \frac{1}{\langle n\rangle^2}\frac{N^2}{V^2} = 1 \tag{48}
$$

This result reflects the long-range order present in the **condensate state** we are considering where all particles are in the same single particle quantum state.

Unified Description - Wicks Theorem

Bosons and Fermions may be treated on the same footing by introducing the parameter $\zeta = \pm 1$, where $\zeta = +$ corresponds to Bosons and $\zeta = -1$ corresponds to Fermions. The (anti-)commutation relations can then be written in the unified form

$$[a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}]_\zeta = \delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{49}$$

where a and $a^\dagger$ now refer to either bosons or fermions and

$$[A, B]_\zeta = AB - \zeta BA \tag{50}$$

denotes the commutator for $\zeta = +1$ and anti-commutator for $\zeta = -1$. Consequently, we have for any operators A and B whose (anti-)commutator is a scalar (this is the case for any combination of choices for A,B between $a_{\boldsymbol{k}}$ and $a^\dagger_{\boldsymbol{k}'}$) we can write

$$\langle AB \rangle = [A, B]_\zeta + \zeta \langle BA \rangle \tag{51}$$

The last term is just a cyclic permutation (upto factor ζ) of the term on the left hand side. For any system at equilibrium with a Hamiltonian quadratic in creation and annihilation operators (here A and B) we have $A\rho = e^{\eta_A(\beta - \epsilon_A)}\rho A$ where $\eta_A = +1$ if A is a creation operator and $\eta_A = -1$ if A is an annihilation operator. Thus we have

$$\langle BA \rangle = e^{\eta_A \beta(\epsilon_A - \mu)} \langle AB \rangle \tag{52}$$

Inserting this into the upper relation one we get

$$\langle AB \rangle = \frac{[A, B]_\zeta}{1 - \zeta e^{\eta_A \beta(\epsilon_A - \mu)}} \tag{53}$$

It is instructive to check this result by entering $A = a^\dagger_{\boldsymbol{k}_1}$ and $B = a_{\boldsymbol{k}_2}$ or the other way around for both fermions and bosons ($\zeta = \pm 1$) and see that it leads to the same result as before. Also note that if A and B are both creation- or annihlation operators, the fact that they (anti-)commute means that this average is zero!

If we take higher order correlation functions

$$\begin{aligned} \langle ABCD \rangle &= [A, B]_\zeta \langle CD \rangle + \zeta \langle BACD \rangle \\ &= [A, B]_\zeta \langle CD \rangle + \zeta [A, C] \langle BD \rangle + \zeta^2 \langle BCAD \rangle \\ &= [A, B]_\zeta \langle CD \rangle + \zeta [A, C] \langle BD \rangle + \zeta^2 [A, D] \langle BC \rangle + \zeta^3 \langle BCDA \rangle \end{aligned} \tag{54}$$

where the last term is again a cyclic permutation of the left hand side (upto factor $\zeta^3 = \zeta$). We then have

$$\langle BCDA \rangle = e^{\eta_A \beta(\epsilon_A - \mu)} \langle ABCD \rangle \tag{55}$$

and we get

$$\langle ABCD \rangle = \langle AB \rangle \langle CD \rangle + \zeta \langle AC \rangle \langle BD \rangle + \langle AD \rangle \langle BC \rangle \tag{56}$$

Here I used relation (53) and the fact that any even power of ζ is unity. Again one should check to replace A, B, C and D by the operators form the previous exercises to see that it leads to the same result.

This method can be extended to correlation functions of any order and always reduces to sums of products of two-operator correlation functions. This result, and the combinatorics of how the two-operator correlation-functions appear is commonly referred to as **Wicks Theorem**. This theorem is an indispensable tool when working with high-order correlation functions and it is usually applied in a graphical way that I will briefly describe below.

Let us define a **contraction**

$$\contraction{}{A}{}{B}AB = \langle AB \rangle = \frac{[A,B]_\zeta}{1-\zeta e^{\eta_A \beta(\epsilon_A - \mu)}} \tag{57}$$

Contractions that are entangled, or not "ordered", can be disentangled by interchanging the order of the operators at the cost of potential signs:

$$\contraction{}{A}{B}{C}\contraction[2ex]{A}{B}{C}{D}ABCD = \zeta \contraction{}{A}{}{C}\contraction{AC}{B}{}{D}ACBD \tag{58}$$

For every (nearest neighbour) permutation you must make in order to get the contractions disentangled (or ordered) you put another power of ζ. Wicks theorem then states that any correlation function can be expressed as the sum of all the different full contractions/pairings that can be made, for example for our previous problem of the four-operator correlation function there are three ways to make such contractions

$$\begin{aligned}
\langle ABCD \rangle &= \contraction{}{A}{}{B}\contraction{AB}{C}{}{D}ABCD + \contraction{}{A}{B}{C}\contraction[2ex]{A}{B}{C}{D}ABCD + \contraction[2ex]{}{A}{BC}{D}\contraction{A}{B}{}{C}ABCD \\
&= \contraction{}{A}{}{B}\contraction{AB}{C}{}{D}ABCD + \zeta \contraction{}{A}{}{C}\contraction{AC}{B}{}{D}ACBD + \zeta^2 \contraction{}{A}{}{D}\contraction{AD}{B}{}{C}ADBC \\
&= \langle AB \rangle \langle CD \rangle + \zeta \langle AC \rangle \langle BD \rangle + \zeta^2 \langle AD \rangle \langle BC \rangle
\end{aligned} \tag{59}$$

Pair-correlations

In this section I would like to shed some light on the concept of the pair-correlation function. Let us start by noting that the density-density correlation function can be rewritten in terms of the pair-correlation function in the following way

$$\langle \Delta n(\boldsymbol{r}) \Delta n(\boldsymbol{r}') \rangle = \langle n(\boldsymbol{r}) n(\boldsymbol{r}') \rangle - \langle n \rangle^2 = \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n \rangle + \langle n \rangle^2 h(\boldsymbol{r},\boldsymbol{r}') \tag{60}$$

To understand why we call $h(\boldsymbol{r},\boldsymbol{r}')$ a pair-correlation function let us consider the case of two-particles. The wave-function of the system is given by $\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)$ with the normalization

$$1 = \int d^3 r_1 \int d^3 r_2 |\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|^2 \tag{61}$$

The density operator is given by[1]

$$\hat{n}(\boldsymbol{r}) = \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_1) + \delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_2) \tag{62}$$

where $\hat{\boldsymbol{r}}_i$ is the position operator of particle $i = 1, 2$. The average density is then given by

$$\langle \hat{n}(\boldsymbol{r}) \rangle = \int d^3 r_1 \int d^3 r_2 \Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2) \hat{n}(\boldsymbol{r}) \Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) \tag{63}$$

using $\delta(\boldsymbol{r} - \hat{\boldsymbol{r}}_i)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2) = \delta(\boldsymbol{r} - \boldsymbol{r}_i)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)$ for $i = 1, 2$ we get

$$\langle \hat{n}(\boldsymbol{r}) \rangle = \int d^3 r_2 |\Psi(\boldsymbol{r},\boldsymbol{r}_2)|^2 + \int d^3 r_1 |\Psi(\boldsymbol{r}_1,\boldsymbol{r})|^2 \tag{64}$$

[1] Formally this is an operator valued distribution

If the particles are indistinguishable we have $|\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)|^2 = |\Psi(\boldsymbol{r}_2,\boldsymbol{r}_1)|^2$ and thus

$$\langle\hat{n}(\boldsymbol{r})\rangle = 2\int d^3r' |\Psi(\boldsymbol{r},\boldsymbol{r}')|^2 \tag{65}$$

From the normalization of Ψ we see that $N = \int d^3r\langle\hat{n}(\boldsymbol{r})\rangle = 2$, as it should.

The density-density correlation function is given by

$$\begin{aligned}\langle\hat{n}(\boldsymbol{r})\hat{n}(\boldsymbol{r}')\rangle = &\int d^3r_1\int d^3r_2\Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\delta(\boldsymbol{r}-\boldsymbol{r}_1)\delta(\boldsymbol{r}'-\boldsymbol{r}_1)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\\ &+\int d^3r_1\int d^3r_2\Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\delta(\boldsymbol{r}-\boldsymbol{r}_1)\delta(\boldsymbol{r}'-\boldsymbol{r}_2)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\\ &+\int d^3r_1\int d^3r_2\Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\delta(\boldsymbol{r}-\boldsymbol{r}_2)\delta(\boldsymbol{r}'-\boldsymbol{r}_1)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\\ &+\int d^3r_1\int d^3r_2\Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2)\delta(\boldsymbol{r}-\boldsymbol{r}_2)\delta(\boldsymbol{r}'-\boldsymbol{r}_2)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2)\end{aligned} \tag{66}$$

The terms with the same arguments in both delta-functions measure the density of "the same particle" and these terms combine to a term $\delta(\boldsymbol{r}-\boldsymbol{r}')2\int d^3r''|\Psi(\boldsymbol{r},\boldsymbol{r}'')|^2 = \delta(\boldsymbol{r}-\boldsymbol{r})\langle n\rangle$, while the other terms with mixed arguments in the delta functions combine to a term $2|\Psi(\boldsymbol{r},\boldsymbol{r}')$, and thus we have

$$\langle\Delta n(\boldsymbol{r})\Delta n(\boldsymbol{r}')\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle + 2|\Psi(\boldsymbol{r},\boldsymbol{r}')|^2 - \langle n\rangle^2 \tag{67}$$

and the pair-correlation function is given by

$$h(\boldsymbol{r},\boldsymbol{r}') = \frac{\left(2|\Psi(\boldsymbol{r},\boldsymbol{r}')|^2 - \langle n\rangle^2\right)}{\langle n\rangle^2} \tag{68}$$

Since $|\Psi(\boldsymbol{r},\boldsymbol{r}')|^2$ is the probability of finding the particles at $\boldsymbol{r}$ and $\boldsymbol{r}'$ respectively, the term $2|\Psi(\boldsymbol{r},\boldsymbol{r}')|^2$ represents the density of pairs at $\boldsymbol{r}$ and $\boldsymbol{r}'$, which explains why $h(\boldsymbol{r},\boldsymbol{r}')$ is called the pair-correlation function.

Alternatively:
We note that we may rewrite the expression

$$\begin{aligned}\langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle &= \langle\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\rangle\\ &= \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle + \zeta\langle\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})\psi(\boldsymbol{r}')\rangle\\ &= \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle + \langle\psi^\dagger(\boldsymbol{r}')\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\psi(\boldsymbol{r}')\rangle.\end{aligned} \tag{69}$$

If we define the two-particle operators

$$\Phi(\boldsymbol{r},\boldsymbol{r}') = \psi(\boldsymbol{r})\psi(\boldsymbol{r}'), \qquad \Phi^\dagger(\boldsymbol{r},\boldsymbol{r}') = \psi^\dagger(\boldsymbol{r}')\psi^\dagger(\boldsymbol{r}) \tag{70}$$

which can be thought of as creating/annihilating a pair of particles, we can write

$$\langle n(\boldsymbol{r})n(\boldsymbol{r}')\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\langle n\rangle + \langle\Phi^\dagger(\boldsymbol{r},\boldsymbol{r}')\Phi(\boldsymbol{r},\boldsymbol{r}')\rangle \tag{71}$$

The pair-correlation function $h(\boldsymbol{r},\boldsymbol{r}')$ defined in Eq. (60) is then given by

$$h(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\langle n\rangle^2}\Big(\langle\Phi^\dagger(\boldsymbol{r},\boldsymbol{r}')\Phi(\boldsymbol{r},\boldsymbol{r}')\rangle - \langle n\rangle^2\Big) \tag{72}$$

Zero Temperature Limit of Bose-Einstein Distribution Function

The Bose-Einstein distribution function is given by

$$n_B(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} - 1} \tag{73}$$

We notice that for $\epsilon < \mu$ the quantity $e^{\beta(\epsilon-\mu)} < 1$ and so $n_B(\epsilon < \mu) < 0$ which is clearly unphysical. If the minimum of the single particle energies is $\epsilon = \epsilon_0$ we conclude that for bosons we must have $\epsilon_0 \geq \mu$. Usually the lowest energy is by convention taken to be $\epsilon_0 = 0$ and the chemical potential must thus be negative.

In the limit $T \to 0$ or $\beta \to \infty$ we have then two possibilities

$$\lim_{\beta\to\infty} n_B(\epsilon) = \begin{cases} \lim_{\beta\to\infty} e^{-\beta(\epsilon-\mu)} = 0, & (\epsilon-\mu) > 0 \\ \infty, & (\epsilon-\mu) = 0 \end{cases} \tag{74}$$

Thus for $\epsilon > \mu$ the state is not occupied in the zero temperature limit. What about the state with minimal energy $\epsilon_0 = 0$? For a non-zero negative chemical potential this state is not occupied since we have $\epsilon_0 - \mu = -\mu > 0$. On the other hand for $\mu = 0$ we have an infinite occupation which also requires an infinite number of particles. The (average) number of particles N can be held finite if we let $\mu \to 0$ simultaneously as we let $\beta \to \infty$ in such a way that $\beta\mu$ remains finite. In this limit we have for the Bose-Einstein distribution

$$\lim_{\beta\to\infty,\mu\to 0} n_B(\epsilon) = \frac{\delta_{\epsilon,0}}{e^{-\beta\mu} - 1} = \delta_{\epsilon,0} n_B(0) \tag{75}$$

Since $N = \sum_{\boldsymbol{k}} n_B(\epsilon_{\boldsymbol{k}})$ we thus have $n_B(\epsilon_{\boldsymbol{k}=0}) = N$ and[2]

$$n_B(\epsilon_{\boldsymbol{k}}) = N\delta_{\boldsymbol{k},0} \tag{76}$$

Interestingly, a more careful analysis shows that the chemical potential as a function of temperature goes to zero already at a critical temperature $T_c \neq 0$, this signals the phase transition into the **Bose-Einstein Condensate** state where a macroscopically large number of particles occupy the lowest energy state.

High Temperature Limit - Thermal deBroglie Wavelength

If we take the limit $e^{\beta\mu} \ll 1$ then we have for the Fermi/Bose distribution function

$$\frac{1}{e^{\beta(\epsilon-\mu)} \pm 1} = \frac{e^{\beta\mu}}{e^{\beta\epsilon} \pm e^{\beta\mu}} \approx \frac{e^{\beta\mu}}{e^{\beta\epsilon}} = e^{-\beta(\epsilon-\mu)} = n_M(\epsilon) \tag{77}$$

i.e. the Maxwell-Boltzmann distribution.

Then we have $n_{B/F}(\epsilon_{\boldsymbol{k}}) \approx e^{-\beta(\epsilon_{\boldsymbol{k}}-\mu)}$. We then have

$$h_{B/F}(\boldsymbol{r}-\boldsymbol{r}') \approx \pm h_M(\boldsymbol{r}-\boldsymbol{r}') = \pm\frac{e^{2\beta\mu}}{\langle n\rangle^2}\left|\frac{1}{V}\sum_{\boldsymbol{k}} e^{-\beta\epsilon_{\boldsymbol{k}}} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\right|^2 \tag{78}$$

[2] The value of $\beta\mu$ can be evaluated from $n_B(0) = N$ and yields $\beta\mu = -(\ln(N+1) - \ln(N))$.

In the thermodynamic limit we can replace the sum by an integral

$$\frac{1}{V}\sum_{\boldsymbol{k}} = \frac{1}{(2\pi)^3}\int d^3k = \frac{1}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} k^2 dk \tag{79}$$

This gives us

$$h_M(\boldsymbol{r}-\boldsymbol{r}') = \frac{e^{2\beta\mu}}{\langle n\rangle^2}\left|\frac{1}{(2\pi)^2}\int_{-1}^{1} d(\cos\theta)\int_0^{\infty} dk\ k^2 e^{-\beta\epsilon_{\boldsymbol{k}}} e^{i\cos\theta k|\boldsymbol{r}-\boldsymbol{r}'|}\right|^2 \tag{80}$$

Using the integral $\int_{-1}^{1} dx e^{iax} = \int_{-1}^{1} dx \cos(ax) = [\sin(ax)/ax]_{-1}^{1} = 2\sin(a)/a$ we get

$$h_M(\boldsymbol{r}-\boldsymbol{r}') = \frac{e^{2\beta\mu}}{\langle n\rangle^2}\left|\frac{1}{2\pi^2}\int_0^{\infty} dk \frac{k\sin(k|\boldsymbol{r}-\boldsymbol{r}'|)}{|\boldsymbol{r}-\boldsymbol{r}'|} e^{-\beta\epsilon_{\boldsymbol{k}}}\right|^2 \tag{81}$$

For a quadratic dispersion $\epsilon_{\boldsymbol{k}} = \hbar^2k^2/2m$ we can evaluate this expression exactly: Switch integration variables to $x = \lambda k$ with $\lambda = \sqrt{\beta\hbar^2/2m}$ to get an integral of the type $\int_0^{\infty} dx x\sin(bx)e^{-x^2} = \frac{\sqrt{\pi}}{4}be^{-b^2/4}$. The final result is then

$$h_M(\boldsymbol{r}-\boldsymbol{r}') = \frac{e^{2\beta\mu}}{\langle n\rangle^2}\left|\frac{\sqrt{\pi}}{2\pi^2(2\lambda)^2}e^{-\frac{|\boldsymbol{r}-\boldsymbol{r}'|^2}{(2\lambda)^2}}\right|^2 = \frac{e^{2\beta\mu}}{4\pi^3}\frac{1}{(2\lambda)^4}e^{-\frac{|\boldsymbol{r}-\boldsymbol{r}'|^4}{(2\lambda)^4}} \tag{82}$$

The important thing to notice here is that the correlations decay on a length-scale known as the **thermal de Broglie wavelength**

$$\lambda \sim \lambda_T = \frac{\hbar}{\sqrt{2\pi m k_B T}} \tag{83}$$