The Fourier transform of $n(\vec{r})$ is thus

$$\hat{n}(\vec{q}) = \int d^3r \, e^{-i\vec{q}\cdot\vec{r}} \, n(\vec{r}) =$$

$$= \frac{1}{V} \sum_{\vec{k},\vec{k}'} \underbrace{\int d^3\vec{r} \, e^{i\vec{r}\cdot(\vec{k}-\vec{k}'-\vec{q})}}_{= V \delta_{\vec{k}-\vec{k}',\vec{q}}} a^+_{\vec{k}'} a_{\vec{k}}$$

$$= \sum_{\vec{k}} a^+_{\vec{k}-\vec{q}} \, a_{\vec{k}}$$

5° Correlation functions

Correlation functions are the main tools for probing the spatial and temporal structure of many-body states.

a) Single particle correlation function

The single particle correlation function of a state $|\Phi\rangle$ is defined by

$$g^{(1)}(\vec{r}, \vec{r}\,') = \langle \Phi | \psi^+(\vec{r}) \, \psi(\vec{r}) | \Phi \rangle$$

<u>Interpretation:</u> $|g^{(1)}(\vec{r},\vec{r}')|^2$ is the probability that moving a particle from $\vec{r}'$ to $\vec{r}$ will recover the same quantum state

In momentum representation

$$g^{(1)}(\vec{r},\vec{r}') = \frac{1}{V} \sum_{\vec{k},\vec{k}'} e^{-i\vec{k}\cdot\vec{r}+i\vec{k}'\cdot\vec{r}'} \langle \Phi | a^\dagger_{\vec{k}} a_{\vec{k}'} | \Phi \rangle$$

This will be evaluated in the exercises for non-interacting fermions and bosons.

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b) <u>Pair correlation function</u>

The pair correlation function quantifies the probability to observe a particle at $\vec{r}_1$ and another one at $\vec{r}_2$. Assuming translational invariance this depends only on the relative coordinate $\vec{r} = \vec{r}_1 - \vec{r}_2$ and can be written as

$$g^{(2)}(\vec{r}) = \frac{V}{N(N-1)} \left\langle \sum_{\alpha\neq\beta=1}^{N} \delta(\vec{r} - \vec{r}_\alpha + \vec{r}_\beta) \right\rangle$$

Since the number of terms in the sum is $N(N-1) = N^2 - N$, the normalization is such that

$$\frac{1}{V}\int d^3r\, g^{(2)}(\vec{r}) = \frac{1}{N(N-1)} \sum_{\alpha\neq\beta=1}^{N} 1 = 1$$

$g^{(2)}(\vec{r})$ is closely related to the density-density correlation function $C(\vec{r})$ defined by

$$C(\vec{r}) = \langle n(\vec{r})\, n(0)\rangle = \langle n(\vec{r}+\vec{r}\,')\, n(\vec{r}\,')\rangle$$

which is independent of $\vec{r}\,'$ by translational invariance. Recall that

$$n(\vec{r}) = \sum_{\alpha=1}^{N} \delta(\vec{r}-\vec{r}_\alpha)$$

and hence

$$C(\vec{r}) = \langle \sum_{\alpha,\beta=1}^{N} \delta(\vec{r}+\vec{r}\,'-\vec{r}_\alpha)\,\delta(\vec{r}\,'-\vec{r}_\beta)\rangle =$$

$$= \frac{1}{V}\int d^3r'\, \langle \sum_{\alpha,\beta=1}^{N} \underbrace{\delta(\vec{r}+\vec{r}\,'-\vec{r}_\alpha)\,\delta(\vec{r}\,'-\vec{r}_\beta)}\rangle$$

integrate over $\vec{r}\,'$ $\qquad = \delta(\vec{r}+\vec{r}_\beta-\vec{r}_\alpha)\,\delta(\vec{r}\,'-\vec{r}_\beta)$

$$= \frac{1}{V}\langle \sum_{\alpha,\beta=1}^{N} \delta(\vec{r}+\vec{r}_\beta-\vec{r}_\alpha)\rangle =$$

$$= \frac{N(N-1)}{V^2}\, g^{(2)}(\vec{r}) + \frac{N}{V}\,\delta(\vec{r}) \;, \quad \frac{N}{V} = n$$

mean particle density

It follows that

$$C(\vec{r}) = \langle \Phi | \psi^+(\vec{r}) \underbrace{\psi(\vec{r}) \psi^+(0)}_{= \delta(\vec{r}) \mp \psi^+(0)\psi(\vec{r})} \psi(0) | \Phi \rangle$$

$$= \underbrace{\langle \Phi | \psi^+(\vec{r}) \psi(0) | \Phi \rangle}_{= \rho^{(1)}(0) = n} \delta(\vec{r}) \mp$$

$$\mp \langle \Phi | \psi^+(\vec{r}) \psi^+(0) \psi(\vec{r}) \psi(0) | \Phi \rangle =$$

$$= n\,\delta(\vec{r}) + \underbrace{\langle \Phi | \psi^+(\vec{r}) \psi^+(0) \psi(0) \psi(\vec{r}) | \Phi \rangle}_{n^2 \rho^{(2)}(\vec{r}) \qquad (N \gg 1)}$$

$$\Rightarrow \quad \rho^{(2)}(\vec{r}-\vec{r}\,') = \frac{1}{n^2} \langle \Phi | \psi^+(\vec{r}) \psi^+(\vec{r}\,') \psi(\vec{r}\,') \psi(\vec{r}) | \Phi \rangle$$

which is valid for bosons and fermions.

III. Bosonic systems

1° Free bosons

Consider non-interacting bosons with spin 0. Then the particles are fully characterized by their momenta and the general N-particle state is of the form

$$\left.\begin{array}{l} |\Phi\rangle = |n_{\vec{k}_1}, n_{\vec{k}_2}, \ldots\rangle \;, \quad \sum_{\vec{k}} n_{\vec{k}} = N \\ n_{\vec{k}} : \text{number of particles with momentum } \hbar\vec{k} \end{array}\right\}$$

- Density:

$$\langle \Phi | n(\vec{r}) | \Phi \rangle = \langle \Phi | \psi^\dagger(\vec{r}) \psi(\vec{r}) | \Phi \rangle =$$

$$= \frac{1}{V} \sum_{\vec{k},\vec{k}'} e^{-i\vec{r}\cdot(\vec{k}-\vec{k}')} \underbrace{\langle \Phi | a^\dagger_{\vec{k}} a_{\vec{k}'} | \Phi \rangle}_{= n_{\vec{k}} \delta_{\vec{k}'\vec{k}}} =$$

$$= \frac{1}{V} \sum_{\vec{k}} n_{\vec{k}} = \frac{N}{V} = n \quad \text{spatially uniform}$$

- Pair correlation function:

$$n^2 g^{(2)}(\vec{r}-\vec{r}') = \langle \Phi | \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}') \psi(\vec{r}') \psi(\vec{r}) | \Phi \rangle =$$

$$= \frac{1}{V^2} \sum_{\substack{\vec{k},\vec{q},\\ \vec{k}',\vec{q}'}} e^{-i(\vec{k}\cdot\vec{r} + \vec{q}\cdot\vec{r}' - \vec{k}'\cdot\vec{r} - \vec{q}'\cdot\vec{r}')} \langle \Phi | a^\dagger_{\vec{k}} a^\dagger_{\vec{q}} a_{\vec{q}'} a_{\vec{k}'} | \Phi \rangle$$

Nonzero contributions:

$$\left.\begin{array}{lll} \text{(i)} & \vec{k}' = \vec{k},\ \vec{q}' = \vec{q} & \text{no exchange} \\ \text{(ii)} & \vec{q}' = \vec{k},\ \vec{k}' = \vec{q} & \text{exchange} \end{array}\right\}$$

Moreover the cases $\vec{k} \neq \vec{q}$ and $\vec{k} = \vec{q}$ have to be distinguished. This yields

$$\langle \Phi | a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{q}'} a_{\vec{k}'} | \Phi \rangle = (1 - \delta_{\vec{k}\vec{q}}) \Big[\delta_{\vec{k}\vec{k}'} \delta_{\vec{q}\vec{q}'} \times$$

$$\times \langle \Phi | a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{q}} a_{\vec{k}} | \Phi \rangle + \delta_{\vec{k}\vec{q}'} \delta_{\vec{k}'\vec{q}} \langle \Phi | a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{k}} a_{\vec{q}} | \Phi \rangle \Big]$$

$$+ \delta_{\vec{k}\vec{q}} \delta_{\vec{k}\vec{k}'} \delta_{\vec{q}\vec{q}'} \langle \Phi | a^+_{\vec{k}} a^+_{\vec{k}} a_{\vec{k}} a_{\vec{k}} | \Phi \rangle$$

For $\vec{q} \neq \vec{k}$ we can commute:

$$a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{q}} a_{\vec{k}} = a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{k}} a_{\vec{q}} = a^+_{\vec{k}} a_{\vec{k}} a^+_{\vec{q}} a_{\vec{q}} = N_{\vec{k}} N_{\vec{q}}$$

whereas for $\vec{q} = \vec{k}$

$$a^+_{\vec{k}} \underbrace{a^+_{\vec{k}} a_{\vec{k}}}_{} a_{\vec{k}} = N^2_{\vec{k}} - N_{\vec{k}}$$

$$= a_{\vec{k}} a^+_{\vec{k}} - 1\!\!1$$

$$\Rightarrow \langle \Phi | a^+_{\vec{k}} a^+_{\vec{q}} a_{\vec{q}'} a_{\vec{k}'} | \Phi \rangle = (1 - \delta_{\vec{k}\vec{q}}) \Big[\delta_{\vec{k}\vec{k}'} \delta_{\vec{q}\vec{q}'} +$$

$$+ \delta_{\vec{k}\vec{q}'} \delta_{\vec{k}'\vec{q}} \Big] n_{\vec{k}} n_{\vec{q}} + \delta_{\vec{k}\vec{q}} \delta_{\vec{k}\vec{k}'} \delta_{\vec{q}\vec{q}'} (n^2_{\vec{k}} - n_{\vec{k}})$$

$$\Rightarrow n^2 g^{(2)}(\vec{r} - \vec{r}') = \frac{1}{V^2} \Big\{ \sum_{\substack{\vec{k},\vec{q} \\ \vec{k} \neq \vec{q}}} \Big(1 + \underset{\substack{\uparrow \\ \text{exchange}}}{e^{-i(\vec{k}-\vec{q})\cdot(\vec{r}-\vec{r}')}} \Big) n_{\vec{k}} n_{\vec{q}}$$

$$+ \sum_{\vec{k}} n_{\vec{k}} \underset{\substack{\uparrow \\ \text{multiple occupancy}}}{(n_{\vec{k}} - 1)} \Big\} = \frac{1}{V^2} \Big\{ \underbrace{\sum_{\vec{k},\vec{q}} n_{\vec{k}} n_{\vec{q}}}_{= N^2} - \sum_{\vec{k}} n^2_{\vec{k}} +$$

$$+ \left| e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')} n_{\vec{k}} \right|^2 - \sum_{\vec{k}} n_{\vec{k}}^2 + \sum_{\vec{k}} (n_{\vec{k}}^2 - n_{\vec{k}}) \Big\}$$

$$= n^2 + \left| \frac{1}{V} \sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')} n_{\vec{k}} \right|^2 - \frac{1}{V^2} \sum_{\vec{k}} n_{\vec{k}} (n_{\vec{k}}+1)$$

$\Rightarrow$ positive contribution from exchange symmetry, negative from multiple occupancy.

Examples:

(i) Sharp momentum distribution: $n_{\vec{k}} = N \delta_{\vec{k},\vec{k}_0}$

(e.g. $\vec{k}_0 = 0$ for the ground state)

$$\Rightarrow \quad n^2 g^{(2)}(\vec{r}-\vec{r}\,') = n^2 + n^2 - \frac{N(N+1)}{V^2} = \frac{N(N-1)}{V^2}$$

$\Rightarrow$ no spatial dependence due to cancellation of the two contributions.

(ii) Gaussian momentum distribution:

$$n_{\vec{k}} = \frac{(2\pi)^3 n}{(\sqrt{\pi}\,\Delta)^3} \exp\left(-\frac{|\vec{k}-\vec{k}_0|^2}{\Delta^2}\right)$$

normalized such that

$$\sum_{\vec{k}} n_{\vec{k}} \simeq \left(\frac{L}{2\pi}\right)^3 \int d^3k \, n_{\vec{k}} = N$$

$$\Rightarrow \quad \frac{1}{V} \sum_{\vec{k}} e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')} n_{\vec{k}} \simeq$$

$$\simeq \frac{n}{(\sqrt{\pi}\Delta)^3}\int d^3k\, e^{-i\vec{k}\cdot(\vec{r}-\vec{r}\,')}\, e^{-\frac{|\vec{k}-\vec{k}_0|^2}{\Delta^2}} =$$

$$= \underline{n\, e^{-\frac{\Delta^2}{4}|\vec{r}-\vec{r}\,'|^2}\, e^{-i\vec{k}_0\cdot(\vec{r}-\vec{r}\,')}}$$

The multiple occupancy contribution is

$$\frac{1}{V^2}\sum_{\vec{k}} n_{\vec{k}}(n_{\vec{k}}+1) \cong \frac{N}{V^2} + \frac{1}{V}\frac{1}{(2\pi)^3}\int d^3k\,(n_{\vec{k}})^2$$

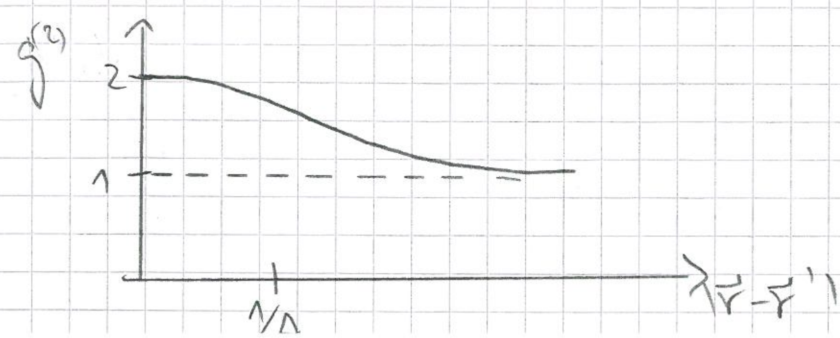
$$= \frac{N}{V^2} + \frac{1}{V}\frac{(2\pi)^3 n^2}{(\sqrt{\pi}\Delta)^6}\underbrace{\int d^3k\, e^{-\frac{2|\vec{k}-\vec{k}_0|^2}{\Delta^2}}}_{=\left(\frac{\pi}{2}\right)^{3/2}\Delta^3}$$

$$= \frac{1}{V}\left(n + \frac{(2\pi)^{3/2} n^2}{\Delta^3}\right) \longrightarrow 0$$ <u>if $N, V \to \infty$ at fixed n, Δ</u>

$$\Rightarrow \underline{g^{(2)}(\vec{r}-\vec{r}\,') = 1 + \exp\left(-\frac{\Delta^2}{2}|\vec{r}-\vec{r}\,'|^2\right)} > 1$$

$\Rightarrow$ clustering of bosons on a length scale determined by the uncertainty relation:

$\underline{l \sim \frac{1}{\Delta} \simeq \frac{\hbar}{\Delta p}}$, since $\Delta p = \hbar\Delta$



<u>Note:</u> Limits $\Delta \to 0$, $N, V \to \infty$ do not commute

2° Weakly interacting bosons

Consider spinless bosons interacting through a general pair potential $v^{(2)}(\vec{r}-\vec{r}\,')$. The Hamiltonian reads

$$H = \sum_{\vec{k}} \frac{\hbar^2 |\vec{k}|^2}{2m} a^{+}_{\vec{k}} a_{\vec{k}} + \frac{1}{2V} \sum_{\vec{k},\vec{p},\vec{q}} \hat{v}^{(2)}(\vec{p})\, a^{+}_{\vec{k}+\vec{p}}\, a^{+}_{\vec{q}-\vec{p}}\, a_{\vec{q}}\, a_{\vec{k}}$$

with $\hat{v}^{(2)}(\vec{p}) = \int d^3r\, e^{-i\vec{p}\cdot\vec{r}}\, v^{(2)}(\vec{r})$

Strategy: Approximate by an effective non-interacting system, i.e. by an effective Hamiltonian that is quadratic in creation and annihilation operators.

---

a) Reduction of the Hamiltonian

We are looking for the ground state of H.

In the absence of interactions, all particles are in the state of zero momentum:

$$n_{\vec{k}} = N\,\delta_{\vec{k},0} \qquad (v^{(2)} = 0)$$

For weak interactions we expect most particles to remain in the ground state:

$$\begin{cases} N_0 = \langle \Phi_0 | a_0^+ a_0 | \Phi_0 \rangle & \text{condensate fraction} \\ \qquad \uparrow \text{ ground state of } H & \\ N' = \sum_{\vec{k} \neq 0} \langle \Phi_0 | a_{\vec{k}}^+ a_{\vec{k}} | \Phi_0 \rangle = N - N_0 \ll N & \text{excited fraction} \end{cases}$$

Then we can neglect interactions between particles of nonzero momentum and only consider processes where at least two of the four momenta are zero:

$$H \cong \sum_{\vec{k}} \frac{\hbar^2 |\vec{k}|^2}{2m} a_{\vec{k}}^+ a_{\vec{k}} + \underbrace{\frac{\hat{v}^{(2)}(0)}{2V} a_0^+ a_0^+ a_0 a_0}_{\text{interaction within the condensate}} +$$

$$+ \frac{1}{2V} \sum_{\vec{p} \neq 0} \hat{v}^{(2)}(\vec{p}) \underbrace{\left(a_{\vec{p}}^+ a_{-\vec{p}}^+ a_0 a_0 + a_0^+ a_0^+ a_{\vec{p}} a_{-\vec{p}} \right)}_{\text{annihilation and creation of condensate particles}}$$

scattering of excited particles by the condensate

$$\left. \begin{aligned} &+ \frac{1}{2V} \sum_{\vec{p} \neq 0} \hat{v}^{(2)}(\vec{p}) \left(a_0^+ a_{-\vec{p}}^+ a_0 a_{-\vec{p}} + a_{\vec{p}}^+ a_0^+ a_{\vec{p}} a_0 \right) + \\ &+ \frac{1}{2V} \sum_{\vec{q} \neq 0} \hat{v}^{(2)}(0) a_0^+ a_{\vec{q}}^+ a_{\vec{q}} a_0 + \frac{1}{2V} \sum_{\vec{k} \neq 0} \hat{v}^{(2)}(0) a_{\vec{k}}^+ a_0^+ a_0 a_{\vec{k}} = \end{aligned} \right.$$

$$= \sum_{\vec{k}} \frac{\hbar^2 |\vec{k}|^2}{2m} a^+_{\vec{k}} a_{\vec{k}} + \frac{\hat{v}^{(2)}(0)}{2V} a^+_0 a^+_0 a_0 a_0 +$$

$$+ \frac{1}{2V} \sum_{\vec{p} \neq 0} \hat{v}^{(2)}(\vec{p}) \left(a^+_{\vec{p}} a^+_{-\vec{p}} a_0 a_0 + a^+_0 a^+_0 a_{\vec{p}} a_{-\vec{p}} \right) +$$

$$+ \frac{1}{V} \sum_{\vec{p} \neq 0} \left(\hat{v}^{(2)}(0) + \hat{v}^{(2)}(\vec{p}) \right) a^+_0 a_0 a^+_{\vec{p}} a_{\vec{p}}$$

by commuting and relabeling operators.

The action of a^+_0 and a_0 on a state with $n_0 = N_0 \gg 1$ is

$$\left.\begin{aligned} a_0 |\ldots N_0 \ldots\rangle &= \sqrt{N_0}\, |\ldots N_0 - 1 \ldots\rangle \simeq \\ &\simeq \sqrt{N_0}\, |\ldots N_0 \ldots\rangle \\ a^+_0 |\ldots N_0 \ldots\rangle &= \sqrt{N_0 + 1}\, |\ldots N_0 + 1 \ldots\rangle \simeq \\ &\simeq \sqrt{N_0}\, |\ldots N_0 \ldots\rangle \end{aligned}\right\}$$

$\Rightarrow$ we can replace a^+_0 and a_0 by multiplication with $\sqrt{N_0}$:

$$H \simeq \sum_{\vec{k}} \frac{\hbar^2 |\vec{k}|^2}{2m} a^+_{\vec{k}} a_{\vec{k}} + \frac{1}{2} \hat{v}^{(2)}(0) \frac{N_0^2}{V} +$$

$$+ \frac{N_0}{V} \sum_{\vec{p} \neq 0} \Big[\left(\hat{v}^{(2)}(\vec{p}) + \hat{v}^{(2)}(0) \right) a^+_{\vec{p}} a_{\vec{p}} +$$

$$+ \frac{1}{2} \hat{v}^{(2)}(\vec{p}) \left(a^+_{\vec{p}} a^+_{-\vec{p}} + a_{\vec{p}} a_{-\vec{p}} \right) \Big]$$

To eliminate the (unknown) condensate fraction N_0, we use

$$\left. \begin{aligned} N_0 &= N - \sum_{\vec{k} \neq 0} a^+_{\vec{k}} a_{\vec{k}} \\ N_0^2 &= N^2 - 2N \sum_{\vec{k} \neq 0} a^+_{\vec{k}} a_{\vec{k}} + \text{higher order terms} \end{aligned} \right\}$$

which yields, in the quadratic approximation,

$$H = \sum_{\vec{k} \neq 0} \frac{\hbar^2 |\vec{k}|^2}{2m} a^+_{\vec{k}} a_{\vec{k}} + \frac{1}{2} \hat{v}^{(2)}(0) \frac{N^2}{V} +$$

$$+ \frac{N}{V} \sum_{\vec{p} \neq 0} \hat{v}^{(2)}(\vec{p}) a^+_{\vec{p}} a_{\vec{p}} + \frac{N}{2V} \sum_{\vec{p} \neq 0} \hat{v}^{(2)}(\vec{p}) \left(a^+_{\vec{p}} a^+_{-\vec{p}} + a_{\vec{p}} a_{-\vec{p}} \right)$$

b) Bogoliubov transformation

Goal: Diagonalize the quadratic Hamiltonian by introducing quasiparticle creation and annihilation operators $b_{\vec{k}}$, $b^+_{\vec{k}}$ such that

$$H = E_0 + \sum_{\vec{k}} \varepsilon_{\vec{k}} b^+_{\vec{k}} b_{\vec{k}}$$