- field operator:

$$\psi(\vec{x}) = \sum_{\vec{k}} \varphi_{\vec{k}}(\vec{x})\, a_{\vec{k}} = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}\, a_{\vec{k}}\,, \qquad \psi^\dagger(\vec{x}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}}\, a^\dagger_{\vec{k}}$$

- particle density:

$$n(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x}) = \frac{1}{V} \sum_{\vec{k},\vec{k}'} e^{-i(\vec{k}'-\vec{k})\cdot\vec{x}}\, a^\dagger_{\vec{k}'} a_{\vec{k}}$$

Fourier transform:

$$\tilde{n}(\vec{q}) = \int d^3x\, e^{-i\vec{q}\cdot\vec{x}}\, n(\vec{x}) = \frac{1}{V} \sum_{\vec{k},\vec{k}'} \int d^3x\, e^{-i(\vec{q}+\vec{k}'-\vec{k})\cdot\vec{x}}\, a^\dagger_{\vec{k}'} a_{\vec{k}} = \sum_{\vec{k}} a^\dagger_{\vec{k}-\vec{q}} a_{\vec{k}}$$

$$\Rightarrow \quad \tilde{n}(\vec{0}) = \sum_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} = \sum_{\vec{k}} \hat{n}_{\vec{k}} = \hat{N} \qquad \text{(total particle number operator)}$$

Including spin

- particle with spin:

  basis states additionally characterized by the z-component of the spin

  $\rightarrow$ field operators: $\psi(\vec{x}) = \sum_i \varphi_i(\vec{x})\, a_i = \sum_{\vec{k},s} \varphi_{\vec{k}}(\vec{x})\, a_{\vec{k},s} = \sum_s \psi_s(\vec{x})$

  $$\psi_s(\vec{x}) \equiv \sum_{\vec{k}} \varphi_{\vec{k}}(\vec{x})\, a_{\vec{k},s}$$

- commutator relations:

  $$\left[\psi_s(\vec{x}), \psi_{s'}(\vec{x}\,')\right]_\pm = \left[\psi_s^\dagger(\vec{x}), \psi_{s'}^\dagger(\vec{x}\,')\right]_\pm = 0, \quad \left[\psi_s(\vec{x}), \psi_{s'}^\dagger(\vec{x}\,')\right]_\pm = \delta_{ss'}\,\delta^3(\vec{x}-\vec{x}\,')$$

- replacement rule for spin independent quantities:

  $$\int d^3x \;\to\; \sum_s \int d^3x, \qquad \sum_{\vec{k}} \;\to\; \sum_{\vec{k},s}$$

- example: $\hat{N} = \int d^3x\, \psi^\dagger(\vec{x})\psi(\vec{x}) = \sum_s \int d^3x\, \psi_s^\dagger(\vec{x})\psi_s(\vec{x}) = \sum_s n_s(\vec{x}) = \tilde{n}(\vec{0})$

  $$\tilde{n}(\vec{q}) = \sum_{\vec{k},s} a^\dagger_{\vec{k}-\vec{q},s} a_{\vec{k},s}$$

4.6 Many-fermion systems: Non-interacting spin-$\frac{1}{2}$-particles

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- Ground state: Fermi sphere, filled up to the Fermi momentum $p_F = \hbar k_F$

$$|\phi_0\rangle = \prod_{\substack{\vec{k} \\ |\vec{k}| \leq k_F}} \prod_s a^\dagger_{\vec{k},s} |0\rangle$$

$\Rightarrow$ occupation numbers:

$$n_{\vec{k},s} = \langle \phi_0 | a^\dagger_{\vec{k},s} a_{\vec{k},s} | \phi_0 \rangle = \begin{cases} 1 & \text{for} \quad |\vec{k}| \leq k_F \\ 0 & \phantom{\text{for}} \quad |\vec{k}| > k_F \end{cases} = \theta(k_F - |\vec{k}|)$$

$\Rightarrow$ total particle number:

$$N = \sum_{\vec{k},s} n_{\vec{k},s} = \sum_s \sum_{\vec{k}} \theta(k_F - |\vec{k}|) = 2 \sum_{\vec{k}} \theta(k_F - |\vec{k}|)$$

Thermodynamic limit

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- $N = 2\sum_{\vec{k}} \theta(k_F - |\vec{k}|)\,, \quad \sum_{\vec{k}} = \sum_{k_x}\sum_{k_y}\sum_{k_z}$
- periodic boundary conditions: $\vec{k} \in 2\pi\left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right), \quad n_i \in \mathbb{Z}$

  $\Rightarrow \quad k_i = \Delta k_i\, n_i$ with $\Delta k_i \equiv \frac{2\pi}{L_i}$

  $\Rightarrow \quad \sum_{k_i} = \frac{L_i}{2\pi}\sum_{k_i}\Delta k_i \stackrel{L_i\to\infty}{\longrightarrow} \frac{L_i}{2\pi}\int dk_i \quad \Rightarrow \quad \sum_{\vec{k}} \to V\int\frac{d^3k}{(2\pi)^3}$

$$\Rightarrow \quad N \to 2V\int\frac{d^3k}{(2\pi)^3}\,\theta(k_F - |\vec{k}|) = 2V\frac{4\pi}{(2\pi)^3}\int_0^{k_F} k^2\,dk = \frac{Vk_F^3}{3\pi^2} \;\Leftrightarrow\; k_F^3 = 3\pi^2\frac{N}{V} = 3\pi^3 n$$

- thermodynamic limit: $N, V \to \infty,\; n = \frac{N}{V} \to const. \;\Rightarrow\; k_F \to const.$
- For practical calculations it is often convenient to start with a finite volume and takes the thermodynamic limit later.

Particle density

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- $\langle n(\vec{x})\rangle = \langle \phi_0 | \psi^\dagger(\vec{x})\psi(\vec{x}) | \phi_0 \rangle$

$$= \frac{1}{V}\sum_{\vec{k}',\vec{k}}\sum_{s',s} e^{-i\vec{k}'\cdot\vec{x}} e^{i\vec{k}\cdot\vec{x}} \underbrace{\langle \phi_0 | a^\dagger_{\vec{k}',s'} a_{\vec{k},s} | \phi_0 \rangle}_{\delta_{\vec{k}',\vec{k}}\,\delta_{s',s}\,n_{\vec{k},s}} = \frac{1}{V}\sum_{\vec{k},s} n_{\vec{k},s} = \frac{N}{V} = n$$

- The density $\langle n(\vec{x})\rangle$ does not depend on the position $\vec{x}$!

  This is not a trivial consequence of the definition:
  $\langle ... \rangle$ denotes the quantum mechanical expectation value,
  not a spatial average.

  So the probablility of finding a particle is the same at any place inside the volume V.

  From a physical point of view this is of course expected, since there are no interactions and no preferred spatial points.

Pair distribution function

- Pair distribution function:

$$g_{ss'}(\vec{x},\vec{x}') = \mathcal{N}\langle\phi_0|\psi_s^\dagger(\vec{x})\psi_{s'}^\dagger(\vec{x}')\psi_{s'}(\vec{x}')\psi_s(\vec{x})|\phi_0\rangle$$

$\propto$ probability to find a particle with spin projection s' at $\vec{x}'$
if there is another particle with spin projection s at $\vec{x}$

  - $|\phi_s'(\vec{x})\rangle = \psi_s(\vec{x})|\phi_0\rangle$: state resulting from the ground state after removing a particle with spin s at position $\vec{x}$

$$\Rightarrow \; g_{ss'}(\vec{x},\vec{x}') \propto \langle\phi_s'(\vec{x})|n_{s'}(\vec{x}')|\phi_s'(\vec{x})\rangle$$

  - $\mathcal{N}$ = normalization factor
    chosen such that one gets $g_{ss'}(\vec{x},\vec{x}') = 1$ for uncorrelated particles:

$$\mathcal{N}^{-1} = \langle\phi_0|\psi_s^\dagger(\vec{x})\psi_s(\vec{x})|\phi_0\rangle\langle\phi_0|\psi_{s'}^\dagger(\vec{x}')\psi_{s'}(\vec{x}')|\phi_0\rangle = \left(\frac{n}{2}\right)^2 \;\Rightarrow\; \mathcal{N} = \left(\frac{2}{n}\right)^2$$

$$\Rightarrow \; g_{ss'}(\vec{x},\vec{x}') = \left(\frac{2}{n}\right)^2 \frac{1}{V^2}\sum_{\vec{k},\vec{k}',\vec{q},\vec{q}'} e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} e^{-i(\vec{q}-\vec{q}')\cdot\vec{x}'} \langle\phi_0|a_{\vec{k},s}^\dagger a_{\vec{q},s'}^\dagger a_{\vec{q}',s'} a_{\vec{k}',s}|\phi_0\rangle$$

- conditions for $\langle\phi_0|a^\dagger_{\vec{k},s}a^\dagger_{\vec{q},s'}a_{\vec{q}',s'}a_{\vec{k}',s}|\phi_0\rangle \neq 0$:
  1.) $|\vec{k}|,\ |\vec{k}'|,\ |\vec{q}|,\ |\vec{q}'| \leq k_F$,
  since otherwise $a_{\vec{q}',s'}a_{\vec{k}',s}|\phi_0\rangle = 0$ or $\langle\phi_0|a^\dagger_{\vec{k},s}a^\dagger_{\vec{q},s'} = 0$
  2.) For $s = s'$ we must have $\vec{k} \neq \vec{q}$ and $\vec{k}' \neq \vec{q}'$,
  because single-particle states cannot be occupied twice.
  3.) In order to get a non-vanishing product of the resulting bra and ket states, we must have
  $\left(\vec{k} = \vec{k}' \quad \text{and} \quad \vec{q} = \vec{q}'\right) \quad \text{or} \quad \left(\vec{k} = \vec{q}' \quad \text{and} \quad \vec{q} = \vec{k}' \quad \text{and} \quad s = s'\right)$

$$\Rightarrow \quad g_{ss'}(\vec{x},\vec{x}') = \left(\frac{2}{n}\right)^2 \frac{1}{V^2} \sum_{\substack{\vec{k},\vec{k}',\vec{q},\vec{q}' \\ \in \text{Fermi sphere}}} e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} e^{-i(\vec{q}-\vec{q}')\cdot\vec{x}'} \left(\delta_{\vec{k},\vec{k}'}\delta_{\vec{q},\vec{q}'} - \delta_{\vec{k},\vec{q}'}\delta_{\vec{q},\vec{k}'}\delta_{s,s'}\right)$$

$$\overset{nV=N}{=} \left(\frac{2}{N}\right)^2 \sum_{\vec{k},\vec{q}\in \text{F.s.}} \left(1 - \delta_{s,s'}\, e^{-i(\vec{k}-\vec{q})\cdot(\vec{x}-\vec{x}')}\right)$$

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- $g_{ss'}(\vec{x},\vec{x}') = \left(\frac{2}{N}\right)^2 \sum\limits_{\vec{k},\vec{q}\in\text{F.s.}} \left(1 - \delta_{s,s'}\, e^{-i(\vec{k}-\vec{q})\cdot(\vec{x}-\vec{x}')}\right)$

- $\sum\limits_{\vec{k},\vec{q}\in\text{F.s.}} 1 = \left(\sum\limits_{\vec{k}\in\text{F.s.}} 1\right)^2 = \left(\frac{N}{2}\right)^2$

- $\sum\limits_{\vec{k},\vec{q}\in\text{F.s.}} e^{-i(\vec{k}-\vec{q})\cdot(\vec{x}-\vec{x}')} = \left(\sum\limits_{\vec{k}\in\text{F.s.}} e^{-i\vec{k}\cdot(\vec{x}-\vec{x}')}\right)\left(\sum\limits_{\vec{q}\in\text{F.s.}} e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}\right)$

$$= \left(\sum_{\vec{k}\in\text{F.s.}} e^{+i\vec{k}\cdot(\vec{x}-\vec{x}')}\right)^2, \quad \text{since the sum contains } \pm\vec{k}.$$

$$\sum_{\vec{k}\in\text{F.s.}} e^{i\vec{k}\cdot\vec{y}} \longrightarrow V\int \frac{d^3k}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{y}}\theta(k_F - |\vec{k}|)$$

$$= \frac{V}{(2\pi)^2}\int_0^{k_F} k^2\, dk \int_{-1}^{1} d\cos\theta\, e^{iky\cos\theta} = \frac{V}{(2\pi)^2}\,\frac{1}{y}\int_0^{k_F} dk\, 2k\, \sin(ky)$$

$$
\begin{aligned}
\frac{V}{(2\pi)^2}\,\frac{1}{y}\int_0^{k_F} dk\, 2k\, \sin(ky) \overset{u=ky}{=}& \frac{V}{2\pi^2}\,\frac{1}{y^3}\int_0^{k_F y} du\, u\, \sin u \\
=& \frac{V}{2\pi^2}\,\frac{1}{y^3}\int_0^{k_F y} du\, u \left(-\frac{d}{du}\cos u\right) \\
=& \frac{V}{2\pi^2}\,\frac{1}{y^3}\left(-k_F y\cos(k_F y) + \sin(k_F y)\right) \\
=& \frac{k_F^3 V}{2\pi^2}\,\frac{1}{\alpha^3}\left(\sin\alpha - \alpha\cos\alpha\right), \quad \alpha \equiv k_F y \\
=& \frac{3N}{2}\,\frac{\sin\alpha - \alpha\cos\alpha}{\alpha^3}, \quad \text{since} \quad V k_F^3 = 3\pi^2 N
\end{aligned}
$$

- $g_{ss'}(\vec{x},\vec{x}') = \left(\frac{2}{N}\right)^2 \sum_{\vec{k},\vec{q}\in\text{F.s.}} \left(1 - \delta_{s,s'}\, e^{-i(\vec{k}-\vec{q})\cdot(\vec{x}-\vec{x}')}\right)$
  - $\sum_{\vec{k},\vec{q}\in\text{F.s.}} 1 = \left(\frac{N}{2}\right)^2$
  - $\sum_{\vec{k},\vec{q}\in\text{F.s.}} e^{-i(\vec{k}-\vec{q})\cdot(\vec{x}-\vec{x}')} = \left(\sum_{\vec{k}\in\text{F.s.}} e^{+i\vec{k}\cdot(\vec{x}-\vec{x}')}\right)^2 \longrightarrow \left(\frac{3N}{2}\,\frac{\sin\alpha - \alpha\cos\alpha}{\alpha^3}\right)^2,$

    $\alpha = k_F|\vec{x}-\vec{x}'|$

$$\Rightarrow\; g_{ss'}(\vec{x},\vec{x}') \;=\; 1 - \delta_{s,s'}\,\frac{9}{\alpha^6}\left(\sin\alpha - \alpha\cos\alpha\right)^2 \;\equiv\; g_{ss'}(\vec{x}-\vec{x}')$$

$$g_{ss'}(\vec{x} - \vec{x}') = 1 - \delta_{s,s'} \frac{9}{\alpha^6} \left(\sin\alpha - \alpha \cos\alpha \right)^2, \qquad \alpha \equiv k_F |\vec{x} - \vec{x}'|$$

Interpretation:

$\underline{s \neq s'}$: $g_{ss'} = 1 \quad \Rightarrow$ The particles are uncorrelated.

$\underline{s = s'}$: The probability to find the second particle close to the first one is suppressed.

$\alpha \ll 1$:

$$\sin\alpha - \alpha\cos\alpha$$
$$\approx (\alpha - \tfrac{1}{3!}\alpha^3) - \alpha(1 - \tfrac{1}{2!}\alpha^2) = \frac{\alpha^3}{3}$$

$\Rightarrow \quad g_{ss} = \mathcal{O}(\alpha^2)$

$\Rightarrow \quad g_{ss}(0) = 0 \quad$ (Pauli principle)