talasna funkcija sistema od N identičnih elektrona $\Psi_N(\vec r_1\sigma_1 \dots \vec r_N\sigma_N)$

$$\langle \Psi_N | \sum_i \delta(\vec r - \vec r_i)\delta_{\sigma\sigma_i} \sum_{j\neq i} \delta(\vec r' - \vec r_j)\delta_{\sigma'\sigma_j} | \Psi_N \rangle$$

$$= \sum_{i=1}^{N} \sum_{\substack{j=1 \\ (j\neq i)}}^{N} \int d\vec r_1 \sum_{\sigma_1} \dots \int d\vec r_N \sum_{\sigma_N} \Psi_N^*(\vec r_1\sigma_1 \dots \vec r_N\sigma_N)\,\delta(\vec r - \vec r_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \vec r_j)\delta_{\sigma'\sigma_j}\,\Psi_N(\vec r_1\sigma_1 \dots \vec r_N\sigma_N)$$



<u>član sa $i=1$</u> $\displaystyle \sum_{j=2}^{N} \int d\vec r_2 \sum_{\sigma_2} \dots \int d\vec r_N \sum_{\sigma_N} \Psi_N^*(\vec r\sigma, \vec r_2\sigma_2, \dots, \vec r_N\sigma_N)\,\delta_{\sigma'\sigma_j}\,\delta(\vec r' - \vec r_j)\,\Psi_N(\vec r\sigma, \vec r_2\sigma_2, \dots, \vec r_N\sigma_N)$

$$= \int d\vec r_3 \sum_{\sigma_3} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r\sigma, \vec r'\sigma', \vec r_3\sigma_3, \dots, \vec r_N\sigma_N)|^2$$

$$+ \int d\vec r_2 \sum_{\sigma_2} \int d\vec r_4 \sum_{\sigma_4} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r\sigma, \vec r_2\sigma_2, \vec r'\sigma', \vec r_4\sigma_4, \dots, \vec r_N\sigma_N)|^2$$

$$+ \dots + \int d\vec r_2 \sum_{\sigma_2} \dots \int d\vec r_{N-1} \sum_{\sigma_{N-1}} |\Psi_N(\vec r\sigma, \vec r_2\sigma_2, \dots, \vec r_{N-1}\sigma_{N-1}, \vec r'\sigma')|^2$$

imamo ukupno $N-1$ sabirak, pri čemu su svi sabirci identični

$$= (N-1) \int d\vec r_3 \sum_{\sigma_3} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r\sigma, \vec r'\sigma', \vec r_3\sigma_3, \dots, \vec r_N\sigma_N)|^2$$

takođe, članovi za svako $i$ su međusobno identični

$$\Rightarrow \boxed{\langle \Psi_N | \sum_i \delta(\vec r - \vec r_i)\delta_{\sigma\sigma_i} \sum_{j\neq i} \delta(\vec r' - \vec r_j)\delta_{\sigma'\sigma_j} | \Psi_N \rangle = N(N-1) \int d\vec r_3 \sum_{\sigma_3} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r\sigma, \vec r'\sigma', \vec r_3\sigma_3, \dots, \vec r_N\sigma_N)|^2}$$

ako je normiranje talasne funkcije $\Psi_N$ na 1: $\displaystyle \int d\vec r_1 \sum_{\sigma_1} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r_1\sigma_1 \dots \vec r_N\sigma_N)|^2 = 1$

onda je zajednička gustina verovatnoće da se elektron spina $\sigma$ nađe u tački $\vec r$, a elektron spina $\sigma'$ u tački $\vec r'$ oblika

$$\boxed{S_{\sigma\sigma'}(\vec r\vec r')} = \int d\vec r_3 \sum_{\sigma_3} \dots \int d\vec r_N \sum_{\sigma_N} |\Psi_N(\vec r\sigma, \vec r'\sigma', \vec r_3\sigma_3, \dots, \vec r_N\sigma_N)|^2$$

$$= \langle \Psi_N | \frac{1}{N(N-1)} \sum_{\substack{i,j \\ (i\neq j)}} \delta(\vec r - \vec r_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \vec r_j)\delta_{\sigma'\sigma_j} | \Psi_N \rangle$$

$$\boxed{\underset{N\gg 1}{\approx} \langle \Psi_N | \frac{1}{N^2} \sum_{\substack{i,j \\ (i\neq j)}} \delta(\vec r - \vec r_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \vec r_j)\delta_{\sigma'\sigma_j} | \Psi_N \rangle}$$

pri tome je, zbog normiranosti $\Psi_N$, $\boxed{\displaystyle \int d\vec r \sum_{\sigma} \int d\vec r' \sum_{\sigma'} S_{\sigma\sigma'}(\vec r, \vec r') = 1}$

<u>u drugoj kvantizaciji</u>: operator koji treba usrednjiti po mnogočestičnom stanju da bi se dobilo $S_{\sigma\sigma'}(\vec r\vec r')$ je

$$\hat S_{\sigma\sigma'}(\vec r\vec r') = \frac{1}{N^2} \sum_{\substack{i,j \\ (i\neq j)}} \delta(\vec r - \hat{\vec r}_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \hat{\vec r}_j)\delta_{\sigma'\sigma_j}$$

$$= \frac{1}{N^2}\left( \sum_{i,j} \delta(\vec r - \hat{\vec r}_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \hat{\vec r}_j)\delta_{\sigma'\sigma_j} - \sum_i \delta(\vec r - \hat{\vec r}_i)\delta_{\sigma\sigma_i}\,\delta(\vec r' - \hat{\vec r}_i)\delta_{\sigma'\sigma_i} \right)$$

$$= \frac{1}{N^2}\left( \left(\sum_i \delta(\vec r - \hat{\vec r}_i)\delta_{\sigma\sigma_i}\right)\left(\sum_j \delta(\vec r' - \hat{\vec r}_j)\delta_{\sigma'\sigma_j}\right) - \delta(\vec r - \vec r')\delta_{\sigma\sigma'} \sum_i \delta(\vec r - \hat{\vec r}_i)\delta_{\sigma\sigma_i} \right)$$

$$= \frac{1}{N^2}\left( \hat\psi_\sigma^\dagger(\vec r)\,\hat\psi_\sigma(\vec r)\,\hat\psi_{\sigma'}^\dagger(\vec r')\,\hat\psi_{\sigma'}(\vec r') - \delta(\vec r - \vec r')\delta_{\sigma\sigma'}\,\hat\psi_\sigma^\dagger(\vec r)\,\hat\psi_\sigma(\vec r) \right)$$

$$= \dots = \boxed{\frac{1}{N^2}\,\hat\psi_\sigma^\dagger(\vec r)\,\hat\psi_{\sigma'}^\dagger(\vec r')\,\hat\psi_{\sigma'}(\vec r')\,\hat\psi_\sigma(\vec r) = \hat S_{\sigma\sigma'}(\vec r, \vec r')}$$

ove smo korake kompletirali na vežbama.

$\langle \hat S_{\sigma\sigma'}(\vec r\vec r')\rangle \equiv S_{\sigma\sigma'}(\vec r\vec r')$ ćemo izračunati za 3D idealni Fermi gas na $T=0$

$$\psi_\sigma(\vec r) = \frac{1}{\sqrt{\Omega}} \sum_{\vec k} e^{i\vec k \vec r}\, \hat c_{\vec k\sigma} \quad , \quad \psi^\dagger_\sigma(\vec r) = \sum_{\vec k} \frac{1}{\sqrt{\Omega}} e^{-i\vec k\vec r}\, \hat c^\dagger_{\vec k\sigma}$$

$$N^2 S_{\sigma\sigma'}(\vec r\vec r') = \frac{1}{\Omega^2} \sum_{\substack{\vec k_2 \vec k_2' \\ \vec k_1' \vec k_1}} e^{-i\vec k_2 \vec r} e^{-i\vec k_2'\vec r'} e^{+i\vec k_1'\vec r'} e^{+i\vec k_1 \vec r} \langle \hat c^\dagger_{\vec k_2\sigma} \hat c^\dagger_{\vec k_2'\sigma'} \hat c_{\vec k_1'\sigma'} \hat c_{\vec k_1\sigma}\rangle_0 \longrightarrow \text{usredujavanje po velikom kanonskom ansamblu za idealni gas}$$

$$= \frac{1}{\Omega^2} \sum_{\substack{\vec k_2 \vec k_2' \\ \vec k_1' \vec k_1}} e^{-i\vec k_2 \vec r} e^{-i\vec k_2'\vec r'} e^{i\vec k_1'\vec r'} e^{i\vec k_1 \vec r} \Big( \underbrace{-\delta_{\sigma\sigma'}\, \delta_{\vec k_2 \vec k_1'}\, \delta_{\vec k_2' \vec k_1}\, \bar n_{\vec k_2\sigma}\, \bar n_{\vec k_1\sigma}}_{\text{IZMENSKI ČLAN}} \; \underbrace{+\,\delta_{\vec k_2\vec k_1}\, \delta_{\vec k_2'\vec k_1'}\, \bar n_{\vec k_1\sigma}\, \bar n_{\vec k_1'\sigma'}}_{\text{DIREKTNI ČLAN}} \Big)$$

$$= -\delta_{\sigma\sigma'} \frac{1}{\Omega} \sum_{\vec k_1} e^{i\vec k_1(\vec r-\vec r')}\, \bar n_{\vec k_1\sigma}\; \frac{1}{\Omega}\sum_{\vec k_2} e^{-i\vec k_2(\vec r-\vec r')}\, \bar n_{\vec k_2\sigma}$$

$$+ \frac{1}{\Omega}\sum_{\vec k_1} \bar n_{\vec k_1\sigma}\; \frac{1}{\Omega}\sum_{\vec k_1'} \bar n_{\vec k_1'\sigma'}$$

2

$$\sum_{\vec k} \bar n_{\vec k\sigma} = \frac{1}{2} N \quad (\text{fiksirana vrednost spina})$$

$$\frac{1}{\Omega}\sum_{\vec k_1} e^{i\vec k_1(\vec r-\vec r')}\, \bar n_{\vec k_1\sigma} = \int \frac{d^3\vec k}{(2\pi)^3} e^{i\vec k(\vec r-\vec r')}\, \bar n_{\vec k\sigma} = \left\{ \begin{array}{l} \vec R = \vec r - \vec r' = R\vec e_z \\ \vec k\cdot\vec R = kR\cos\theta \end{array} \right\}$$

$$= \frac{1}{(2\pi)^3} \int_0^{+\infty} dk\, k^2 \int_0^\pi d\theta\, \sin\theta \int_0^{2\pi} d\varphi\, e^{ikR\cos\theta}\, \frac{1}{e^{\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}+1}$$

$\underline{\text{na } T=0}$ $\quad \bar n_{\vec k\sigma} = \left(e^{\beta\left(\frac{\hbar^2k^2}{2m}-\mu\right)}+1\right)^{-1} \longrightarrow \theta(k_F-k)$ , gde je $k_F$ Fermijev talasni vektor

$$\frac{1}{\Omega}\sum_{\vec k} e^{i\vec k(\vec r-\vec r')}\, \bar n_{\vec k\sigma}\Big|_{T=0} = \frac{1}{(2\pi)^2}\int_0^{k_F} dk\, k^2 \int_0^\pi d\theta\, \sin\theta\, e^{ikR\cos\theta}$$

$$= \frac{1}{(2\pi)^2}\int_0^{k_F} dk\, k^2\, \frac{2i\sin(kR)}{ikR} = \frac{1}{2\pi^2 R}\int_0^{k_F} dk\, k\, \sin(kR)$$

$$= \frac{1}{2\pi^2 R}\frac{1}{R^2}\int_0^{k_FR} dx\, x\sin x = \frac{1}{2\pi R^3}\Big(\sin(k_FR) - k_FR\cos(k_FR)\Big)$$

$$N = 2\frac{\Omega}{(2\pi)^3}\frac{4\pi}{3}k_F^3 = \frac{k_F^3}{3\pi^2}\Omega$$

$$N^2 S_{\sigma\sigma'}(\vec r\vec r') = \left(\frac{N}{2}\right)^2\frac{1}{\Omega^2} - \delta_{\sigma\sigma'}\frac{1}{4\pi^2}\left(\frac{\sin(k_FR)-k_FR\cos(k_FR)}{(k_FR)^3}\right)^2 k_F^6$$

$$= \left(\frac{N}{2}\right)^2\frac{1}{\Omega^2} - \delta_{\sigma\sigma'}\frac{1}{4\cancel{\pi^2}}\, 9\cancel{\pi^2}\,\frac{N^2}{\Omega^2}\left(\frac{\sin(k_FR)-k_FR\cos(k_FR)}{(k_FR)^3}\right)^2$$

$$\boxed{S_{\sigma\sigma'}(\vec r\vec r') = \frac{1}{4\Omega^2}\left(1 - 9\,\delta_{\sigma\sigma'}\left(\frac{\sin(k_FR)-k_FR\cos(k_FR)}{(k_FR)^3}\right)^2\right)}$$

formula iz teorije verovatnoće za presek događaja $P(AB) = P(A)\cdot \overbrace{P(B|A)}^{\text{uslovna verovatnoća događaja B ako se desio događaj A}}$

$A$ = elektron se nalazi u tački $\vec r$ i ima spin $\sigma$

$B$ = elektron se nalazi u tački $\vec r'$ i ima spin $\sigma'$

gustina verovatnoće za događaj A je $\frac{1}{2\Omega}$, tako da je gustina uslovne verovatnoće da se elektron spina $\sigma'$ nađe u tački $\vec r'$ ako znamo da se elektron spina $\sigma$ nalazi u tački $\vec r$ :

$$\boxed{S(\vec r'\sigma'|\vec r\sigma) = \frac{1}{2\Omega}\left(1 - 9\,\delta_{\sigma\sigma'}\left(\frac{\sin(k_FR)-k_FR\cos(k_FR)}{(k_FR)^3}\right)^2\right)}$$

ako je $\sigma \neq \sigma'$ $\quad S(\bar r'\sigma'|\bar r\sigma) = \frac{1}{2\Omega}$ a to je isto kao i verovatnoća da se elektron spina $\sigma$ nađe u tački $\vec r$

dakle, elektroni suprotnih spinova se međusobno "ne vide", nema nikakve korelacije među njihovim položajima

ako je $\sigma = \sigma'$

$$S(\bar r'\sigma|\bar r\sigma) = \frac{1}{2\Omega}\left(1 - 9\left(\frac{\sin(k_F R) - k_F R\cos(k_F R)}{(k_F R)^3}\right)^2\right)$$

- $R = |\bar r - \bar r'|$ tdj. $k_F R \ll 1$ (prostorno bliski)

$$\frac{\sin(k_F R) - k_F R\cos(k_F R)}{(k_F R)^3} = \frac{1}{(k_F R)^3}\left[k_F R - \frac{1}{6}(k_F R)^3 + \frac{1}{120}(k_F R)^5 - \dots - k_F R + \frac{1}{2}(k_F R)^3 - \frac{1}{24}(k_F R)^5 + \dots\right]$$

$$= \frac{1}{(k_F R)^3}\left[\frac{1}{3}(k_F R)^3 - \left(\frac{1}{24} - \frac{1}{5\cdot 24}\right)(k_F R)^5 + \dots\right]$$

$$= \frac{1}{3}\left[1 - 3\,\frac{4}{5}\,\frac{1}{24}(k_F R)^2 + \dots\right] = \frac{1}{3}\left[1 - \frac{1}{10}(k_F R)^2 + \dots\right]$$

$$\boxed{S(\bar r'\sigma|\bar r\sigma)} = \frac{1}{2\Omega}\left(1 - 9\,\frac{1}{9}\left(1 - \frac{2}{10}(k_F R)^2 + \dots\right)\right) = \boxed{\frac{1}{2\Omega}\cdot\frac{1}{5}(k_F R)^2 + \dots}$$

kada $R \to 0$, $S(\bar r'\sigma|\bar r\sigma) \to 0$, u blizini datog elektrona ne može se naći elektron istog spina (Paulijev princip); uočeni elektron kao da se "okruži" oblašću u kojoj se ne mogu naći drugi elektroni istog spina $\longrightarrow$ exchange hole (izmenska šupljina)

- $R = |\bar r - \bar r'|$ tdj. $k_F R \gg 1$ (prostorno udaljeni)

$$S(\bar r'\sigma|\bar r\sigma) \xrightarrow[R\to+\infty]{} \frac{1}{2\Omega}$$ (elektroni istog spina, a na velikom međusobnom rastojanju, nisu korelisani)

$$\boxed{S(\bar r'\sigma|\bar r\sigma) \simeq \frac{1}{2\Omega}\left(1 - 9\,\frac{\cos^2(k_F R)}{(k_F R)^4}\right)}$$