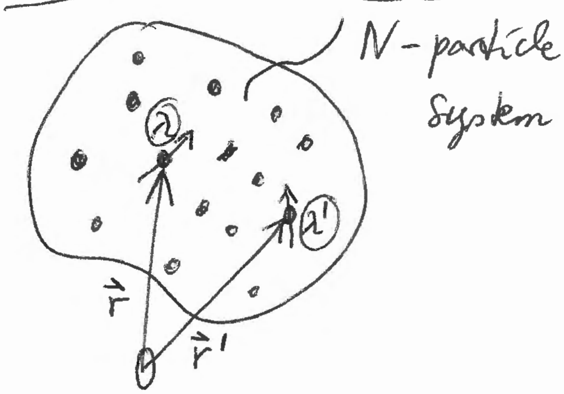
Ch. 6: Pair correlation function for $s=\frac{1}{2}$ fermions

Ref: Gordon Baym, "Lectures on QM", chapter 19



Suppose we have a $s=\frac{1}{2}$ fermion in a many-body system located at position $\vec{r}$, with spin projection $\lambda = s_z\ (=\uparrow,\downarrow)$. The quantum many-body system is in its non-interacting ground state $|\phi_0\rangle$. We may ask, what is the probability density $f_{\lambda\lambda'}(\vec{r},\vec{r}\,')$ to find another (identical) fermion with spin projection λ' at the position $\vec{r}\,'$?

The quantity

$$f_{\lambda\lambda'}(\vec{r},\vec{r}\,') \stackrel{\text{def}}{=} \langle \phi_0 | \hat{c}^+_\lambda(\vec{r})\, \hat{c}^+_{\lambda'}(\vec{r}\,')\, \hat{c}_{\lambda'}(\vec{r}\,')\, \hat{c}_\lambda(\vec{r}) | \phi_0 \rangle. \quad (1)$$

is called the pair correlation function for $s=\frac{1}{2}$ fermions.

Interpretation of eq. (1): Starting from the g.s. $|\phi_0\rangle$ of the many-body system, we first destroy a particle at $\vec{r}$ with spin projection λ, and then we destroy another particle at position $\vec{r}\,'$ with spin projection λ'. Subsequently, we re-create these particles and return to the g.s. $|\phi_0\rangle$.

Physics motivation: We will find that for $s=\frac{1}{2}$ fermions with same spin projection $(\lambda'=\lambda)$, the "Pauli correlations" arising from purely QM effects (anti-sym. of many-body WF) prevent fermions from getting close. More precisely:

$$\boxed{f_{\lambda\lambda}\left(R=|\vec{r}-\vec{r}\,'|\to 0\right) = 0.}$$

At the end of ch-6, we will briefly comment on bosonic systems and show that bosons like to be close together.

This stunning difference between fermion and boson systems manifests itself in many-body calculations (free Fermi gas, atoms, nuclei, etc.).

To calculate the pair correlation function, eq. (1), we expand the quantum field operators ($\hat{c}$, $\hat{c}^+$) in a suitable s.p.-basis

$$\varphi_{n\lambda}(\vec{r})$$

notation:

$\lambda = \pm\frac{1}{2}$ (spin projection)

n = all other quantum numbers

examples:

a) free Fermi gas: $n \equiv \vec{k}$

b) N-electron atom: $n \equiv (n, l, m_l)$

etc.

Expand the field operators in (1), e.g.

$$\left.\begin{aligned} \hat{c}_\lambda(\vec{r}) &= \sum_{n=1}^{\infty} \hat{c}_{n\lambda}\,\varphi_{n\lambda}(\vec{r}) \\ \hat{c}^+_\lambda(\vec{r}) &= \sum_{k=1}^{\infty} \hat{c}^+_{k\lambda}\,\varphi^+_{k\lambda}(\vec{r}) \end{aligned}\right\} \qquad (2)$$

Insert expansion (2) into (1):

$$f_{\lambda\lambda'}(\vec{r},\vec{r}\,') = \sum_{k,\ell,m,n=1}^{\infty} \varphi^{+}_{k\lambda}(\vec{r})\,\varphi^{+}_{\ell\lambda'}(\vec{r}\,')\,\varphi_{m\lambda'}(\vec{r}\,')\,\varphi_{n\lambda}(\vec{r})\times$$

$$\times\langle\phi_0|\,\hat{c}^{+}_{k\lambda}\,\hat{c}^{+}_{\ell\lambda'}\,\hat{c}_{m\lambda'}\,\hat{c}_{n\lambda}\,|\phi_0\rangle. \tag{3}$$

We use now the result established in cl. 4, p. 14, with the help of Wick's theorem:

$$\langle\phi_0|\,\hat{c}_\alpha^{+}\,\hat{c}_\beta^{+}\,\hat{c}_\delta\,\hat{c}_\gamma\,|\phi_0\rangle = \rho_{\delta\beta}\cdot\rho_{\gamma\alpha} - \rho_{\delta\alpha}\cdot\rho_{\gamma\beta}$$

where the density parameters are given by

$$\rho_{\beta\alpha} = \theta(\varepsilon_F - \varepsilon_\alpha)\,\delta_{\alpha\beta}. \tag{4}$$

By comparing (3) and (4), we identify

$$\alpha \equiv (k,\lambda) \qquad \beta \equiv (\ell,\lambda') \qquad \delta \equiv (m,\lambda') \qquad \gamma \equiv (n,\lambda)$$

resulting in

$$\langle\phi_0|\,\hat{c}^{+}_{k\lambda}\,\hat{c}^{+}_{\ell\lambda'}\,\hat{c}_{m\lambda'}\,\hat{c}_{n\lambda}\,|\phi_0\rangle =$$

$$= \rho_{m\lambda',\ell\lambda'}\cdot\rho_{n\lambda,k\lambda} - \rho_{m\lambda',k\lambda}\cdot\rho_{n\lambda,\ell\lambda'} =$$

$$= \theta(\varepsilon_F - \varepsilon_\ell)\,\delta_{m\ell}\,\underbrace{\delta_{\lambda'\lambda'}}_{=1}\cdot\theta(\varepsilon_F - \varepsilon_k)\,\delta_{kn}\,\underbrace{\delta_{\lambda\lambda}}_{=1} -$$

$$- \theta(\varepsilon_F - \varepsilon_k)\,\delta_{mk}\,\delta_{\lambda\lambda'}\cdot\theta(\varepsilon_F - \varepsilon_\ell)\,\delta_{n\ell}\,\delta_{\lambda\lambda'} \tag{5}$$

Insert (5) into (3):

$$f_{\lambda\lambda'}(\vec r, \vec r') = \sum_{k,l,m,n=1}^{\infty} \varphi^+_{k\lambda}(\vec r)\,\varphi^+_{l\lambda'}(\vec r')\,\varphi_{m\lambda'}(\vec r')\,\varphi_{n\lambda}(\vec r)$$
$$\times \Big\{ \theta(\varepsilon_F - \varepsilon_l)\,\delta_{ml} \cdot \theta(\varepsilon_F - \varepsilon_k)\,\delta_{kn} - \delta_{\lambda\lambda'} \cdot \big[\theta(\varepsilon_F - \varepsilon_k)\,\delta_{mk}$$
$$\cdot\, \theta(\varepsilon_F - \varepsilon_l)\,\delta_{nl}\big] \Big\} \qquad (6)$$

The θ-functions restrict the infinite basis to states below the Fermi surface, e.g.

$$\sum_{l=1}^{\infty} \varphi^+_{l\lambda'}\,\theta(\varepsilon_F - \varepsilon_l) \rightarrow \sum_{l=1}^{F} \varphi^+_{l\lambda'}$$

and the Kronecker δ's, δ_{ml} and δ_{kn}, result in a collapse of the 4-fold sum $(k,l,m,n) \rightarrow (k,l)$.

Hence, we obtain:

$$f_{\lambda\lambda'}(\vec r, \vec r') = \sum_{k,l=1}^{F} \varphi^+_{k\lambda}(\vec r)\,\varphi^+_{l\lambda'}(\vec r')\,\varphi_{l\lambda'}(\vec r')\,\varphi_{k\lambda}(\vec r)$$
$$- \delta_{\lambda\lambda'} \cdot \sum_{k,l=1}^{F} \varphi^+_{k\lambda}(\vec r)\,\varphi^+_{l\underset{\lambda}{\underset{\parallel}{\lambda'}}}(\vec r')\,\varphi_{k\underset{\lambda}{\underset{\parallel}{\lambda'}}}(\vec r')\,\varphi_{l\lambda}(\vec r). \qquad (7)$$

Note, that in the second term, because of $\delta_{\lambda\lambda'}$, we can put $\lambda' = \lambda$ in the WF's.

Regrouping these expressions, we obtain

$$f_{\lambda\lambda'}(\vec{r},\vec{r}\,') = \Bigg[\left(\sum_{k=1}^{F} \varphi^{+}_{k\lambda}(\vec{r})\, \varphi_{k\lambda}(\vec{r}) \right) \left(\sum_{l=1}^{F} \varphi^{+}_{l\lambda'}(\vec{r}\,')\, \varphi_{l\lambda'}(\vec{r}\,') \right)$$

$$- \delta_{\lambda\lambda'} \cdot \left(\sum_{k=1}^{F} \varphi^{+}_{k\lambda}(\vec{r})\, \varphi_{k\lambda'}(\vec{r}\,') \right) \left(\sum_{l=1}^{F} \varphi^{+}_{l\lambda'}(\vec{r}\,')\, \varphi_{l\lambda}(\vec{r}) \right) \Bigg] \qquad (8)$$

Using the result for the g.s. density (see ch. 3, p. 9) ch. 2, p. 30

$$\rho_{\lambda}(\vec{r}) \overset{\text{def}}{=} \langle \Phi_0 | \hat{c}^{+}_{\lambda}(\vec{r})\, \hat{c}_{\lambda}(\vec{r}) | \Phi_0 \rangle = \sum_{k=1}^{F} \varphi^{+}_{k\lambda}(\vec{r})\, \varphi_{k\lambda}(\vec{r}) \qquad (9a)$$

and with the definition of the g.s. density matrix

$$\rho_{\lambda\lambda'}(\vec{r},\vec{r}\,') \overset{\text{def}}{=} \langle \Phi_0 | \hat{c}^{+}_{\lambda'}(\vec{r}\,')\, \hat{c}_{\lambda}(\vec{r}) | \Phi_0 \rangle =$$

$$= \sum_{i,j=1}^{\infty} \varphi^{+}_{j\lambda'}(\vec{r}\,')\, \varphi_{i\lambda}(\vec{r})\, \underbrace{\rho_{ij}}_{=\theta(\varepsilon_F - \varepsilon_i)\,\delta_{ij}}$$

$$= \sum_{i=1}^{F} \varphi^{+}_{i\lambda'}(\vec{r}\,')\, \varphi_{i\lambda}(\vec{r}) \qquad (9b)$$

which is obviously a generalization of the density, we can write the fermion pair correlation function as

$$f_{\lambda\lambda'}(\vec{r},\vec{r}\,') = \rho_{\lambda}(\vec{r}) \cdot \rho_{\lambda'}(\vec{r}\,') - \delta_{\lambda\lambda'} \underbrace{\rho^{+}_{\lambda\lambda'}(\vec{r},\vec{r}\,')\, \rho_{\lambda\lambda'}(\vec{r},\vec{r}\,')}_{= |\rho_{\lambda\lambda'}(\vec{r},\vec{r}\,')|^2}$$

Summary: The pair correlation function for $s=\frac{1}{2}$ fermions depends on the densities $\rho_\lambda(\vec{r})$, $\rho_{\lambda'}(\vec{r}')$ and on the density matrix $\rho_{\lambda\lambda'}(\vec{r},\vec{r}')$:

$$\boxed{f_{\lambda\lambda'}(\vec{r},\vec{r}') = \rho_\lambda(\vec{r})\cdot\rho_{\lambda'}(\vec{r}') - \delta_{\lambda\lambda'}\left|\rho_{\lambda\lambda'}(\vec{r},\vec{r}')\right|^2} \qquad (10)$$

Case a): different spin projections $(\lambda'\neq\lambda)$

$$\boxed{f_{\lambda\lambda'}(\vec{r},\vec{r}') = \rho_\lambda(\vec{r})\cdot\rho_{\lambda'}(\vec{r}')} \qquad (11)$$

this means, the probability density to find a fermion pair at positions $\vec{r}$ and $\vec{r}'$ (with spin projections $\lambda'\neq\lambda$) is simply the product of the individual probability densities, i.e. there is no correlation between these particles (same result as in classical statistical mechanics).

Case b): same spin projections $(\lambda'=\lambda)$

$$\boxed{f_{\lambda\lambda}(\vec{r},\vec{r}') = \rho_\lambda(\vec{r})\rho_\lambda(\vec{r}') - \left|\rho_{\lambda\lambda}(\vec{r},\vec{r}')\right|^2} \qquad (12)$$

The second term describes a correlation between the fermions. We will now examine its properties by considering a free Fermi gas.

g.s. density matrix $\rho_{\lambda\lambda}(\vec{r},\vec{r}\,')$ for free Fermi gas

Starting from p. 5: $\rho_{\lambda\lambda}(\vec{r},\vec{r}\,') = \sum_{i=1}^{F} \varphi^{+}_{i\lambda}(\vec{r}\,')\,\varphi_{i\lambda}(\vec{r})$. $\underline{(13)}$

For free Fermi gas, the quantum numbers are

$$(i,\lambda) \to (\vec{k},\lambda)$$

and the s.p. WF's have the structure (ch. 2, p. 7)

$$\varphi_{i\lambda}(\vec{r}) \equiv \varphi_{\vec{k}\lambda}(\vec{r}) = L^{-3/2}\, e^{i\vec{k}\cdot\vec{r}}\,\chi_{\lambda}^{s=\frac{1}{2}} \qquad \underline{(14)}$$

Insert (14) into (13):

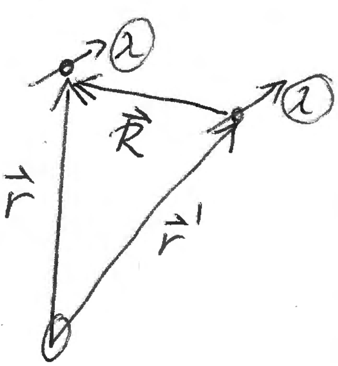
$$\rho_{\lambda\lambda}(\vec{r},\vec{r}\,') = \sum_{\vec{k}}^{k_F} \varphi^{+}_{\vec{k}\lambda}(\vec{r}\,')\,\varphi_{\vec{k}\lambda}(\vec{r}) = \sum_{\vec{k}}^{k_F} L^{-3} e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}\underbrace{\chi^{+}\chi}_{=1}$$

Taking the <u>large-L limit</u> (which is appropriate for a gas with large # particles) and using result from <u>ch. 3, p. 12</u>:

$$\frac{1}{L^3}\sum_{\vec{k}} f(\vec{k}) \to \frac{1}{(2\pi)^3}\int d^3k\, f(\vec{k})$$

we obtain

$$\rho_{\lambda\lambda}(\vec{r},\vec{r}\,') = \left(\frac{1}{2\pi}\right)^3 \int_0^{k_F} d^3k\; e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}$$

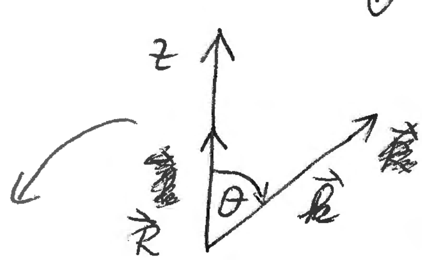


Define distance vector between fermions

$$\boxed{\vec{R} \overset{\text{def}}{=} \vec{r} - \vec{r}\,'}$$

and write

$$\vec{k}\cdot\vec{R} = kR\cos\theta$$



In k-space, vector $\vec{R}$ is constant (put it in z-direction)

$$\vec{R} = R\,\vec{e}_z$$

resulting in

$$\rho_{\lambda\lambda}(R) = \frac{1}{(2\pi)^3} \int_0^{k_F} k^2 dk \underbrace{\int_0^{2\pi} d\varphi}_{=2\pi} \int_0^{\pi} \sin\theta \, d\theta \, e^{ikR\cos\theta}$$

Substitute variable $u = \cos\theta$ and use $\sin\theta \, d\theta = -d(\cos\theta)$:

$$\rho_{\lambda\lambda}(R) = \frac{1}{(2\pi)^2} \int_0^{k_F} dk\, k^2 \int_{-1}^{+1} du \, e^{ikRu} =$$

$$= \frac{1}{(2\pi)^2} \int_0^{k_F} dk\, k^{\cancel{2}} \frac{1}{i\cancel{k}R} \, e^{ikRu} \Big|_{u=-1}^{u=+1} =$$

$$= \frac{1}{(2\pi)^2} \int_0^{k_F} dk \, \frac{k}{R} \underbrace{\left(\frac{e^{ikR} - e^{-ikR}}{i} \right)}_{=2\sin(kR)} = \frac{2}{(2\pi)^2} \int_0^{k_F} dk \frac{k}{R} \sin(kR)$$

$$= \frac{1}{2\pi^2} \left[\frac{\sin(k_F R)}{R^3} - \frac{(k_F R)\cos(k_F R)}{R^3} \right]$$

Introduce the dimensionless variable

$$x \stackrel{\text{def}}{=} k_F R$$

$$\rightsquigarrow \rho_{\lambda\lambda}(\cancel{R}x) = \frac{k_F^3}{2\pi^2} \underbrace{\left(\frac{\sin x - x\cos x}{x^3} \right)}_{= \frac{j_1(x)}{x} = \text{spherical Bessel function}}$$

Use relation between Fermi momentum, $p_F = \hbar k_F$, and density ρ_0 (see ch. 3, p.12):

$$k_F^3 = 3\pi^2 \rho_0$$

we obtain the final result

$$\boxed{\rho_{\lambda\lambda}(x) = \frac{3}{2}\rho_0 \frac{j_1(x)}{x}} \qquad (15)$$

with
ρ_0 = density
$x = k_F |\vec{r} - \vec{r}\,'|$

density matrix for free Fermi gas, same spin projection λ.

Consider the limit that the particles are at the same position ($R \to 0$, i.e. $x \to 0$):

$$\rho_{\lambda\lambda}(x \to 0) = \frac{3}{2}\rho_0 \underbrace{\lim_{x \to 0} \frac{j_1(x)}{x}}_{=\frac{1}{3}} = \frac{3}{2}\rho_0 \cdot \frac{1}{3} = \frac{1}{2}\rho_0 \qquad (16)$$

This is correct, because the density matrix at $\vec{r}\,' = \vec{r}$ ($R = 0$) is the g.s. density $\rho_\lambda(\vec{r}) = \frac{1}{2}\rho_0$ (because of spin degeneracy). Discuss plot (separate PDF doc) on Web.

Pair correlation function for free Fermi gas (for $\lambda' = \lambda$)

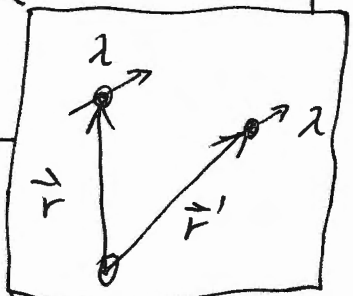
From p. 6 we obtain with $\rho_\lambda(\vec{r}) = \rho_0/2$:

$$\left.\begin{aligned} f_{\lambda\lambda}(x) &= \left(\frac{\rho_0}{2}\right)^2 - |\rho_{\lambda\lambda}(x)|^2 = \\ &= \left(\frac{\rho_0}{2}\right)^2 - \left(\frac{\rho_0}{2}\right)^2 \left(\frac{3\, j_1(x)}{x}\right)^2 \end{aligned}\right\} \qquad (17)$$

Summary: pair correlation function for free Fermi gas (for $\lambda' = \lambda$)

(18) $$f_{\lambda\lambda}(x) = \left(\frac{\rho_0}{2}\right)^2 \left[1 - \left(\frac{3\, j_1(x)}{x}\right)^2\right]$$

with ρ_0 = density
$x = k_F |\vec{r} - \vec{r}\,'|$



From (16) and (17) we obtain the important result

$$\boxed{f_{\lambda\lambda}(x \to 0) = \left(\frac{\rho_0}{2}\right)^2 - \Big|\underbrace{\rho_{\lambda\lambda}(x \to 0)}_{= \frac{\rho_0}{2}}\Big|^2 = 0} \qquad (19)$$

i.e. the probability density to find a $s = \frac{1}{2}$ fermion pair at the same position ($x = 0$), with the same spin projection ($\lambda' = \lambda$) is zero!

Discuss plot (separate PDF doc) on Website!

Observations:

1) The "Pauli exchange hole" at small particle distance ($x \to 0$) is a direct consequence of the antisymmetry of the many-body WF. Even though we considered a free Fermi gas, the "Pauli correlation" at small x prevents the fermions from getting close.

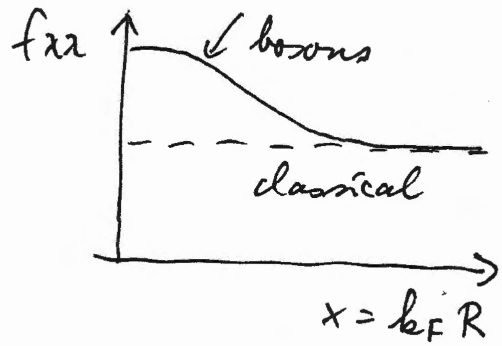
2) At "large" distances, $x \gtrsim 4$, the Pauli correlations contained in the density matrix $\rho_{\lambda\lambda}(x)$ are small, and the Pair correlation function $f_{\lambda\lambda}(x)$ approaches the "classical" limit

$$f_{\lambda\lambda}(x \gtrsim 4) \to \left(\frac{\rho_0}{2}\right)^2,$$

which is the same result as in the $\lambda' \neq \lambda$ case, see eq.(11).

A few words about pair correlation function for bosons

Ref: Gordon Baym, QM, p.429-431



In contrast to fermions, bosons like to "clump together". At small interparticle distances x, the pair correlation increases.

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exp. verification (for S=1 photons and for S=0 pions):

"Hanbury-Brown & Twiss experiment

see G. Baym, p. 431-434.