The Fermi Hole

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Some properties of Fermi gas

Particles dwell in a large but finite volume \mathcal{V} .

Periodical boundary conditions.

Restriction on values of the wave vector:

$$\mathbf{k} = 2\pi \left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z} \right) \tag{1}$$

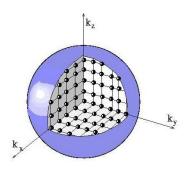
The volume of the unit cell in k-space:

$$dk_x dk_y dk_z = d^3 k = \frac{(2\pi)^3}{\mathcal{V}}$$
 (2)

Some properties of Fermi gas

Particles occupy all energy levels bellow Fermi energy. Volume in k-space:

$$V_{\mathsf{k}} = \frac{4}{3}\pi\mathsf{k}_{\mathsf{F}}^3\tag{3}$$



Some properties of Fermi gas

Particles occupy all energy levels bellow Fermi energy. Volume in k-space:

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Number of particles:

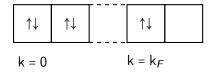
$$N = g_{\sigma} \frac{V_{k}}{d^{3}k} = \frac{2\frac{4}{3}\pi k_{F}^{3} \mathcal{V}}{8\pi^{3}} = \frac{k_{F}^{3} \mathcal{V}}{3\pi^{2}} \Longrightarrow$$

$$k_{F}^{3} = \frac{3\pi^{2} N}{\mathcal{V}}$$

$$(4)$$

Fermionic ground state

In the ground state $|g\rangle$ fermions occupy all available levels in the k-space up to k_F :



We remove a particle at **position** ${\bf x}$ with a spin σ

$$|\phi_{\sigma}(\mathbf{x})\rangle = \hat{\psi}_{\sigma}(\mathbf{x})|g\rangle$$

Particle density at this state:

$$\rho(\mathbf{x}', \sigma') = \langle \phi_{\sigma}(\mathbf{x}) | \hat{\psi}_{\sigma'}^{\dagger}(\mathbf{x}') \hat{\psi}_{\sigma'}(\mathbf{x}') | \phi_{\sigma}(\mathbf{x}) \rangle$$

We will show that the density equals to

$$\left(\frac{N}{2\mathcal{V}}\right)^2 g_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}')$$

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The state after removing a particle. In coordinate space:

$$|\phi_{\sigma}(\mathbf{x})\rangle = \hat{\psi}_{\sigma}(\mathbf{x})|g\rangle$$

But we want to use momentum space:

Fourier tranform

$$\hat{\psi}_{\sigma}(\mathbf{x}) = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k},\sigma} \psi_{\mathbf{k},\sigma}(\mathbf{x})$$

$$\psi_{\mathbf{k},\sigma}(\mathbf{x}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{x}} \, \boldsymbol{\sigma}$$

Density in momentum space

$$\rho(\mathbf{x}', \sigma') =$$

$$\langle g | \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}, \sigma}^{\dagger} \psi_{\mathbf{k}, \sigma}^{*}(\mathbf{x}) \sum_{\mathbf{l}} \hat{c}_{\mathbf{l}, \sigma'}^{\dagger} \psi_{\mathbf{l}, \sigma'}^{*}(\mathbf{x}') \sum_{\mathbf{m}} \hat{c}_{\mathbf{m}, \sigma'} \psi_{\mathbf{m}, \sigma'}(\mathbf{x}') \sum_{\mathbf{n}} \hat{c}_{\mathbf{n}, \sigma} \psi_{\mathbf{n}, \sigma}(\mathbf{x}) | g \rangle =$$

$$\sum_{\mathbf{k}, \mathbf{l}, \mathbf{m}, \mathbf{n}} \langle g | \hat{c}_{\mathbf{k}, \sigma}^{\dagger} \hat{c}_{\mathbf{l}, \sigma'}^{\dagger} \hat{c}_{\mathbf{m}, \sigma'} \hat{c}_{\mathbf{n}, \sigma} | g \rangle \psi_{\mathbf{k}, \sigma}^{*}(\mathbf{x}) \psi_{\mathbf{l}, \sigma'}^{*}(\mathbf{x}') \psi_{\mathbf{m}, \sigma'}(\mathbf{x}') \psi_{\mathbf{n}, \sigma}(\mathbf{x})$$

Density in momentum space

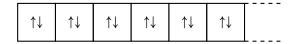
$$\begin{split} \rho(\mathbf{x}',\sigma') = \\ \langle g | \sum_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \psi^{*}_{\mathbf{k},\sigma}(\mathbf{x}) \sum_{\mathbf{l}} \hat{c}^{\dagger}_{\mathbf{l},\sigma'} \psi^{*}_{\mathbf{l},\sigma'}(\mathbf{x}') \sum_{\mathbf{m}} \hat{c}_{\mathbf{m},\sigma'} \psi_{\mathbf{m},\sigma'}(\mathbf{x}') \sum_{\mathbf{n}} \hat{c}_{\mathbf{n},\sigma} \psi_{\mathbf{n},\sigma}(\mathbf{x}) | g \rangle = \\ \sum_{\mathbf{l}} \langle g | \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}^{\dagger}_{\mathbf{l},\sigma'} \hat{c}_{\mathbf{m},\sigma'} \hat{c}_{\mathbf{n},\sigma} | g \rangle \psi^{*}_{\mathbf{k},\sigma}(\mathbf{x}) \psi^{*}_{\mathbf{l},\sigma'}(\mathbf{x}') \psi_{\mathbf{m},\sigma'}(\mathbf{x}') \psi_{\mathbf{n},\sigma}(\mathbf{x}) \end{split}$$

We will focus on the expression

$$\langle g | \, \hat{c}_{\mathbf{k},\sigma}^{\dagger} \hat{c}_{\mathbf{l},\sigma'}^{\dagger} \hat{c}_{\mathbf{m},\sigma'} \hat{c}_{\mathbf{n},\sigma} | g \rangle$$

Removing two particles:

$$|g\rangle$$

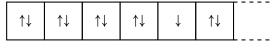


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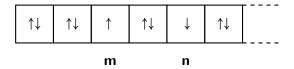
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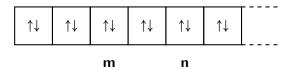


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Restoring the state:

$$\hat{c}_{\mathbf{k},\sigma}^{\dagger}\hat{c}_{\mathbf{l},\sigma'}^{\dagger}\hat{c}_{\mathbf{m},\sigma'}\hat{c}_{\mathbf{n},\sigma}\left|g\right\rangle$$



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Allowed indices

$$\begin{cases} \mathbf{k}, \sigma = \mathbf{m}, \sigma' \\ \mathbf{l}, \sigma' = \mathbf{n}, \sigma \\ \mathbf{k}, \sigma \neq \mathbf{l}, \sigma' \end{cases} \begin{cases} \mathbf{k}, \sigma = \mathbf{n}, \sigma \\ \mathbf{l}, \sigma' = \mathbf{m}, \sigma' \\ \mathbf{k}, \sigma \neq \mathbf{l}, \sigma' \end{cases}$$

If spins are different

$$\sigma \neq \sigma' \implies \text{only } \begin{cases} \mathbf{k} = \mathbf{n} \\ \mathbf{l} = \mathbf{m} \\ \mathbf{k} \neq \mathbf{l} \end{cases}$$

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$$\rho(\mathbf{x}', \sigma') = \sum_{\mathbf{k}, \mathbf{l}} \left\langle g | \, \hat{c}_{\mathbf{k}, \sigma}^{\dagger} \hat{c}_{\mathbf{l}, \sigma'}^{\dagger} \hat{c}_{\mathbf{l}, \sigma'} \hat{c}_{\mathbf{k}, \sigma} | g \right\rangle \psi_{\mathbf{k}, \sigma}^{*}(\mathbf{x}) \psi_{\mathbf{l}, \sigma'}^{*}(\mathbf{x}') \psi_{\mathbf{l}, \sigma'}(\mathbf{x}') \psi_{\mathbf{k}, \sigma}(\mathbf{x})$$

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Wave functions

$$\psi_{\mathbf{l},\sigma'}(\mathbf{x}') = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{l}\cdot\mathbf{x}'} \sigma'$$

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$$\{\hat{c}_{\mathbf{l},\sigma'}\hat{c}_{\mathbf{k},\sigma}\} = 0 \implies \hat{c}_{\mathbf{l},\sigma'}\hat{c}_{\mathbf{k},\sigma} = -\hat{c}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{l},\sigma'}$$

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Insert identity operator:

$$\rho(\mathbf{x}', \sigma') = \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}, \mathbf{l}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{k}, \sigma} \hat{c}_{\mathbf{k}, \sigma} \, \hat{\mathcal{I}} \, \hat{c}^{\dagger}_{\mathbf{l}, \sigma'} \hat{c}_{\mathbf{l}, \sigma'} | g \rangle$$

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Identity

$$\hat{\mathcal{I}} = \sum_{n} |n\rangle \langle n|$$

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Fock space

$$\langle n|g\rangle = \delta_{n,g}$$

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Number of particles operator

$$\hat{c}_{\mathbf{k}\sigma}^{\dagger}\hat{c}_{\mathbf{k}\sigma}=\hat{n}_{\mathbf{k}\sigma}$$

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If spins are equal

$$\sigma = \sigma' \implies \begin{cases} \mathbf{k} = \mathbf{n} \\ \mathbf{l} = \mathbf{m} \end{cases}$$
 or $\begin{cases} \mathbf{k} = \mathbf{m} \\ \mathbf{l} = \mathbf{n} \end{cases}$ and $\mathbf{k} \neq \mathbf{l}$

We can simplify expression for density:

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Wave functions

$$\psi_{\mathbf{k}\sigma}(\mathbf{x}') = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{x}'} \sigma$$

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Insert identity operator:

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Fock space

$$\langle n|g\rangle=\delta_{n,g}$$

Density for equal spin

$$\begin{split} &\rho(\mathbf{x}',\sigma) = \\ &= -\frac{1}{\mathcal{V}^2} \left[\sum_{\mathbf{k}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} | g \rangle \, e^{-i\mathbf{k}(\mathbf{x}'-\mathbf{x})} \right] \left[\sum_{\mathbf{l}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{l}\sigma} \hat{c}_{\mathbf{l}\sigma} | g \rangle \, e^{-i\mathbf{l}(\mathbf{x}'-\mathbf{x})} \right] + \left(\frac{N}{2\mathcal{V}} \right)^2 \end{split}$$

To continue we need to find

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} | g \rangle$$

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Number of particles operator

$$\hat{c}_{\mathbf{k}\sigma}^{\dagger}\hat{c}_{\mathbf{k}\sigma}=\hat{n}_{\mathbf{k}\sigma}$$

$$\langle g | \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} | g \rangle = \langle g | \hat{n}_{\mathbf{k}\sigma} | g \rangle = \begin{cases} 1 & \mathbf{k} \leq \mathbf{k}_{F} \\ 0 & \mathbf{k} > \mathbf{k}_{F} \end{cases}$$

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Heaviside step function

$$\langle g | \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} | g \rangle = H(\mathbf{k}_F - |\mathbf{k}|)$$

To continue we need to find

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \langle g | \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} | g \rangle$$

Change to summation inside the Fermi sphere

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{|\mathbf{k}| \le \mathbf{k}_F} e^{-i\mathbf{k}\mathbf{r}}$$

From summation to integration

Multiply and divide by unit cell volume

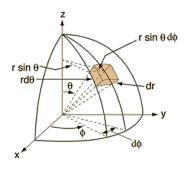
$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{|\mathbf{k}| \le k_F} e^{-i\mathbf{k}\mathbf{r}} = \frac{1}{\mathcal{V}} \frac{\mathcal{V}}{8\pi^3} \sum_{|\mathbf{k}| \le k_F} e^{-i\mathbf{k}\mathbf{r}} d^3 \mathbf{k}$$

In the limit $\mathcal{V} \to \infty$

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{8\pi^3} \sum_{|\mathbf{k}| \le \mathbf{k}_F} e^{-i\mathbf{k}\mathbf{r}} d^3 \mathbf{k} \to \frac{1}{8\pi^3} \int_{|\mathbf{k}| \le \mathbf{k}_F} e^{-i\mathbf{k}\mathbf{r}} d^3 \mathbf{k}$$

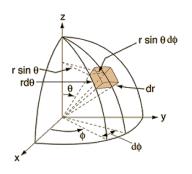
We will integrate in spherical coordinates

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{8\pi^3} \int_{|\mathbf{k}| \le \mathbf{k}_F} e^{-i\mathbf{k}\mathbf{r}} d^3 \mathbf{k}$$



We will integrate in spherical coordinates

$$F(\mathbf{k},\mathbf{r}) = \frac{1}{8\pi^3} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} \mathrm{e}^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 \sin\theta \; d\phi d\theta d\mathbf{k}$$



Integration over ϕ

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{8\pi^3} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 \sin\theta \, d\phi d\theta d\mathbf{k}$$
$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 \sin\theta \, d\theta d\mathbf{k}$$

Integration over θ

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 \sin\theta \ d\theta d\mathbf{k}$$

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 - d\cos\theta d\mathbf{k}$$

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\mathbf{n}=-1}^{1} e^{i\mathbf{k}r\eta} \mathbf{k}^2 \ d\eta d\mathbf{k}$$

Integration over θ

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 \sin\theta \ d\theta d\mathbf{k}$$

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\theta=0}^{\pi} e^{-i\mathbf{k}r\cos\theta} \mathbf{k}^2 - d\cos\theta d\mathbf{k}$$

$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \int_{\mathbf{k}=0}^{\mathbf{k}_F} \frac{2}{\mathbf{k}_F} \sin(\mathbf{k}r) \ \mathbf{k}^2 \ d\mathbf{k}$$

Integration over k

$$F(k, \mathbf{r}) = \frac{1}{4\pi^2} \int_{k=0}^{k_F} \frac{2}{kr} \sin(kr) \, k^2 \, dk = \frac{1}{2\pi^2 r^3} \int_{k=0}^{k_F} \sin(kr) \, kr \, dkr$$

$$F(k, \mathbf{r}) = \frac{1}{2\pi^2 r^3} \left\{ \sin(k_F r) - k_F r \cos(k_F r) \right\}$$

Integration over k

$$F(k, \mathbf{r}) = \frac{1}{4\pi^2} \int_{k=0}^{k_F} \frac{2}{kr} \sin(kr) k^2 dk = \frac{1}{2\pi^2 r^3} \int_{k=0}^{k_F} \sin(kr) kr dkr$$

$$F(k, \mathbf{r}) = \frac{k_F^3}{2\pi^2 r^3 k_F^3} \left\{ \sin(k_F r) - k_F r \cos(k_F r) \right\}$$

Fermi wavenumber

$$k_F^3 = \frac{3\pi^2 N}{\mathcal{V}}$$

$$\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \left\langle g \right| \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} \left| g \right\rangle = \left(\frac{N}{2\mathcal{V}} \right) \frac{3 \left\{ \sin(\mathbf{k}_{F}r) - \mathbf{k}_{F}r \cos(\mathbf{k}_{F}r) \right\}}{(k_{F}r)^{3}}$$

No divergence at zero: at $k_F r \rightarrow 0 \iff r \ll \lambda_F$

$$3\frac{\sin(k_Fr)-k_Fr\cos(k_Fr)}{(k_Fr)^3}\approx 3\frac{x-x^3/6-x(1-x^2/2)}{x^3}=\frac{3}{3}=1$$

Bringing it together

$$\rho(\mathbf{x'},\sigma) = -\frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} | g \rangle \, e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x'})} \sum_{\mathbf{l}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{l}\sigma} \hat{c}_{\mathbf{l}\sigma} | g \rangle \, e^{i\mathbf{l}\cdot(\mathbf{x'}-\mathbf{x})}$$

 $\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \langle g | \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} | g \rangle = \left(\frac{N}{2\mathcal{V}} \right) \frac{3 \left\{ \sin(\mathbf{k}_{F}r) - \mathbf{k}_{F}r\cos(\mathbf{k}_{F}r) \right\}}{(k_{F}r)^{3}}$

Bringing it together

$$\rho(\mathbf{x'},\sigma) = -\frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} | g \rangle \, e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x'})} \sum_{\mathbf{l}} \langle g | \, \hat{c}^{\dagger}_{\mathbf{l}\sigma} \hat{c}_{\mathbf{l}\sigma} | g \rangle \, e^{i\mathbf{l}\cdot(\mathbf{x'}-\mathbf{x})}$$

$$\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \left\langle g \right| \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} \left| g \right\rangle = \left(\frac{N}{2\mathcal{V}} \right) \frac{3 \left\{ \sin(\mathbf{k}_{F}r) - \mathbf{k}_{F}r\cos(\mathbf{k}_{F}r) \right\}}{(k_{F}r)^{3}}$$

Bringing it together

$$\begin{split} &\rho(\mathbf{x}',\sigma) = -\frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}} \left\langle g \middle| \, \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} \middle| g \right\rangle e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \sum_{\mathbf{l}} \left\langle g \middle| \, \hat{c}_{\mathbf{l}\sigma}^{\dagger} \hat{c}_{\mathbf{l}\sigma} \middle| g \right\rangle e^{i\mathbf{l}\cdot(\mathbf{x}'-\mathbf{x})} \\ &\frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}} \left\langle g \middle| \, \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma} \middle| g \right\rangle = \left(\frac{N}{2\mathcal{V}}\right) \frac{3\left\{\sin(\mathbf{k}_F r) - \mathbf{k}_F r \cos(\mathbf{k}_F r)\right\}}{(k_F r)^3} \\ &\rho(\mathbf{x}',\sigma) = \left(\frac{N}{2\mathcal{V}}\right)^2 - \left(\frac{N}{2\mathcal{V}}\right)^2 \left(\frac{3\left\{\sin(\mathbf{k}_F r) - \mathbf{k}_F r \cos(\mathbf{k}_F r)\right\}}{(k_F r)^3}\right)^2 \end{split}$$

Bringing it all together

$$\left(\frac{N}{2\mathcal{V}}\right)^2 g_{\sigma\sigma}(\mathbf{x} - \mathbf{x}') = \left(\frac{N}{2\mathcal{V}}\right)^2 - \delta_{\sigma\sigma'} \left(\frac{N}{2\mathcal{V}}\right)^2 \left(\frac{3\left\{\sin(\mathsf{k}_F r) - \mathsf{k}_F r \cos(\mathsf{k}_F r)\right\}}{(k_F r)^3}\right)^2$$

Bringing it all together

$$g_{\sigma\sigma}(\mathbf{x} - \mathbf{x}') = 1 - \delta_{\sigma\sigma'} \left(\frac{3 \left\{ \sin(k_F r) - k_F r \cos(k_F r) \right\}}{(k_F r)^3} \right)^2$$

Visualization $\sigma = \sigma'$

