The Fermi Hole

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Title

Begin with the equations.

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:

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

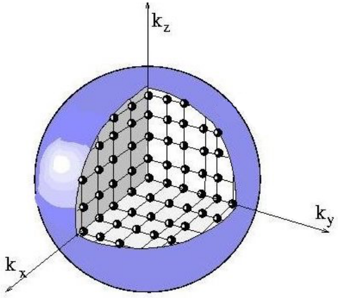
The volume of the unit cell in k-space:

$$d\mathrm{k}_x d\mathrm{k}_y d\mathrm{k}_z = d^3\mathrm{k} = \frac{(2\pi)^3}{\mathcal{V}} \tag{2}$$

Some properties of Fermi gas

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

$$V_{\mathrm{k}} = \frac{4}{3}\pi \mathrm{k}_F^3 \tag{3}$$



Some properties of Fermi gas

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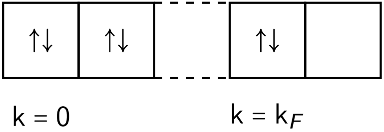
$$V_{\mathrm{k}} = \frac{4}{3}\pi \mathrm{k}_F^3 \tag{3}$$

Number of particles:

$$\begin{gathered} N = g_\sigma \frac{V_{\mathrm{k}}}{d^3\mathrm{k}} = \frac{2\frac{4}{3}\pi \mathrm{k}_F^3 \mathcal{V}}{8\pi^3} = \frac{\mathrm{k}_F^3 \mathcal{V}}{3\pi^2} \implies \\ \mathrm{k}_F^3 = \frac{3\pi^2 N}{\mathcal{V}} \end{gathered} \tag{4}$$

Fermionic ground state

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



Removing particle

We remove a particle at **position x** with a spin σ

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

Particle density at this state:

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

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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Removing particle

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:

Furie tranform

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

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

Density in momentum space

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

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

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

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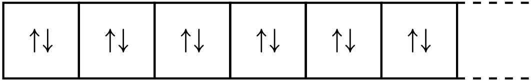
Allowed operators

We will focus on the expression

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

Removing two particles:

$$|g\rangle$$



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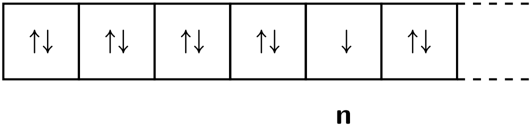
Removing two particles:

$$\hat{c}_{\mathbf{n},\sigma} \, | g \rangle$$



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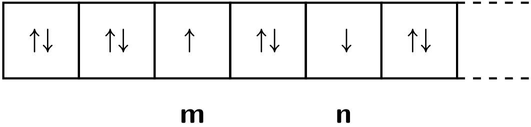
Removing two particles:

$$\hat{c}_{\mathbf{m},\sigma'} \hat{c}_{\mathbf{n},\sigma} |g\rangle$$



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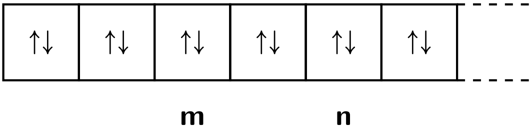
Restoring the state:

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



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

Allowed indices

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

Density for different spin

If spins are different

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

We can simplify expression for density:

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

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Wave functions

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

$$\psi^*_{\mathbf{l},\sigma'}(\mathbf{x}') = \frac{1}{\sqrt{\mathcal{V}}} e^{-i\mathbf{l}\cdot\mathbf{x}'} \boldsymbol{\sigma}'$$

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Commutation for fermions

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

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$$\{\hat{c}^\dagger_{\mathbf{l},\sigma'} \hat{c}_{\mathbf{k},\sigma}\} = \delta_{k,l} \implies \hat{c}^\dagger_{\mathbf{l},\sigma'} \hat{c}_{\mathbf{k},\sigma} = -\hat{c}_{\mathbf{k},\sigma} \hat{c}^\dagger_{\mathbf{l},\sigma'} + \delta_{k,l}$$

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Density for different spin

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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Identuty

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

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Fock space

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

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Fock space

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

Number of particles operator

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

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Number of particles operator

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

$$\rho(\mathbf{x}', \sigma') = \frac{1}{\mathcal{V}^2} \left[\sum_{\mathbf{k}} \langle g| \hat{n}_{\mathbf{k}\sigma} |g\rangle \right] \cdot \left[\sum_{textbfl} \langle g| \hat{n}_{\mathbf{l}\sigma'} |g\rangle \right] = \left(\frac{N}{2\mathcal{V}} \right)^2$$

Calculating sum

To continue we need to find

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

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Number of particles operator

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

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

Calculating sum

To continue we need to find

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

Heaviside step function

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

Calculating sum

To continue we need to find

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

Change to summation inside the Fermi sphere

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

From summation to integration

Multiply and divide by unit cell volume

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

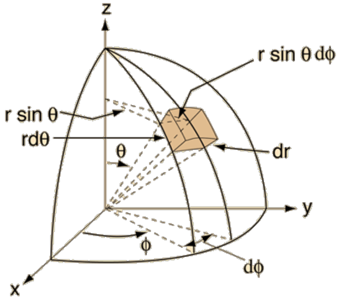
In the limit $\mathcal{V} \to \infty$

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

Evaluation of the integral

We will integrate in spherical coordinates

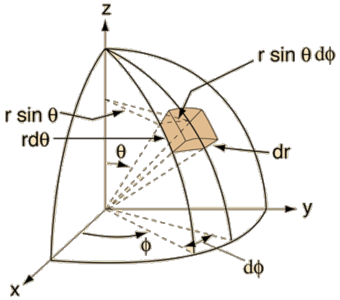
$$F(\mathrm{k},\mathbf{r}) = \frac{1}{8\pi^3}\int_{|\mathbf{k}|\leq \mathrm{k}_F} e^{-i\mathbf{kr}} d^3\mathrm{k}$$



Evaluation of the integral

We will integrate in spherical coordinates

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



Evaluation of the integral

Integration over ϕ

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

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

Evaluation of the integral

Integration over θ

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

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

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

Evaluation of the integral

Integration over θ

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

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

Evaluation of the integral

Integration over k

$$F(\mathrm{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathrm{k}=0}^{\mathrm{k}_F} \frac{2}{\mathrm{k}r} \sin(\mathrm{k}r)\, \mathrm{k}^2\, d\mathrm{k} = \frac{1}{2\pi^2 r^3} \int_{\mathrm{k}=0}^{\mathrm{k}_F} \sin(\mathrm{k}r)\, \mathrm{k}r\, d\mathrm{k}r$$

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

Evaluation of the integral

Integration over k

$$F(\mathrm{k}, \mathbf{r}) = \frac{1}{4\pi^2} \int_{\mathrm{k}=0}^{\mathrm{k}_F} \frac{2}{\mathrm{k}r} \sin(\mathrm{k}r)\, \mathrm{k}^2\, d\mathrm{k} = \frac{1}{2\pi^2 r^3} \int_{\mathrm{k}=0}^{\mathrm{k}_F} \sin(\mathrm{k}r)\, \mathrm{k}r\, d\mathrm{k}r$$

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

Fermi wavenumber

$$\mathrm{k}_F^3 = \frac{3\pi^2 N}{\mathcal{V}}$$

Evaluation of the integral

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

No divergence at zero: at $\mathrm{k}_F r \to 0 \iff r \ll \lambda_F$

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