

The Fermi Hole

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March 3, 2018

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:

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

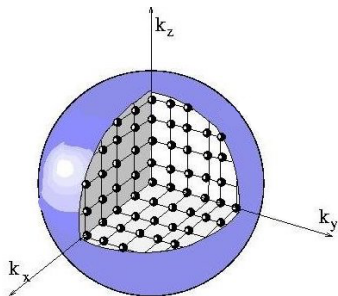
The volume of the unit cell in k-space:

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

Some properties of Fermi gas

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

$$V_k = \frac{4}{3}\pi k_F^3 \quad (3)$$



Some properties of Fermi gas

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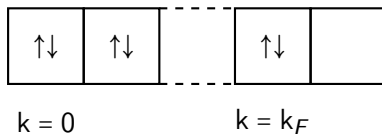
$$V_k = \frac{4}{3}\pi k_F^3 \quad (3)$$

Number of particles:

$$N = g_\sigma \frac{V_k}{d^3k} = \frac{2 \frac{4}{3}\pi k_F^3 \mathcal{V}}{8\pi^3} = \frac{k_F^3 \mathcal{V}}{3\pi^2} \implies \quad (4)$$
$$k_F^3 = \frac{3\pi^2 N}{\mathcal{V}}$$

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** \mathbf{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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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:

Fourier tranform

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

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

Density in momentum space

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

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

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

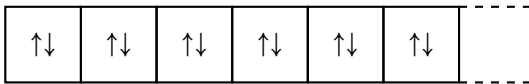
Allowed operators

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:

$$|g\rangle$$



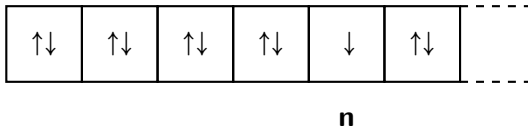
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Removing two particles:

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



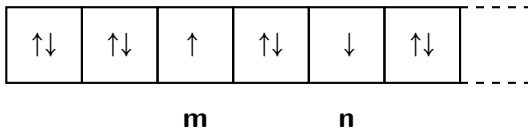
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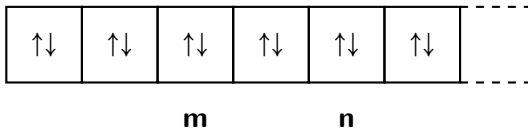
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Restoring the state:

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



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Allowed indices

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

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:

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

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Wave functions

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

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

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Commutation for fermions

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

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

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Calculating sum

To continue we need to find

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

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Number of particles operator

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

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

Calculating sum

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Heaviside step function

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

Calculating sum

To continue we need to find

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

Change to summation inside the Fermi sphere

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

From summation to integration

Multiply and divide by unit cell volume

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

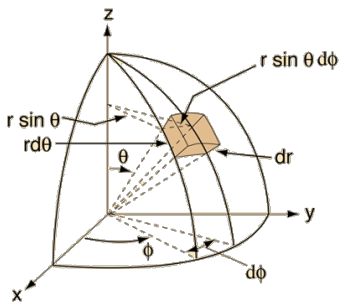
In the limit $\mathcal{V} \rightarrow \infty$

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

Evaluation of the integral

We will integrate in spherical coordinates

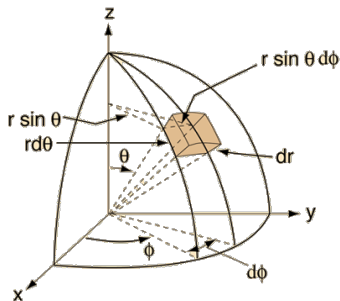
$$F(\mathbf{k}, \mathbf{r}) = \frac{1}{8\pi^3} \int_{|\mathbf{k}| \leq k_F} e^{-i\mathbf{k}\mathbf{r}} d^3k$$



Evaluation of the integral

We will integrate in spherical coordinates

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



Evaluation of the integral

Integration over ϕ

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

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

Evaluation of the integral

Integration over θ

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

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

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

Evaluation of the integral

Integration over θ

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

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

Evaluation of the integral

Integration over k

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

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

Evaluation of the integral

Integration over k

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

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

Fermi wavenumber

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

Evaluation of the integral

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

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

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

Bringing it together

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

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

Visualization

