# The Fermi Hole

Ivan Kulesh Martijn Papendrecht

Delft University of Technology, The Netherlands

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:

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

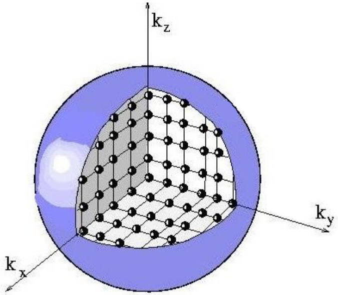
The volume of the unit cell in k-space:

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

# 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

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

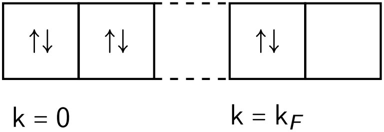
$$V_{\mathrm{k}} = \frac{4}{3}\pi \mathrm{k}_F^3 \tag{3}$$

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 $k_F$:



# Calculating sum

To continue we need to find

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

# Calculating sum

To continue we need to find

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

# Calculating sum

To continue we need to find

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

## 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

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

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

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

Change to summation inside the Fermi sphere

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

# From summation to integration

Multiply and divide by unit cell volume

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

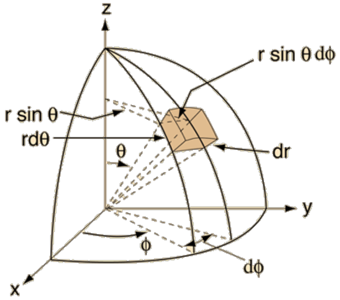
In the limit $\mathcal{V} \to \infty$

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

# Evaluation of the integral

We will integrate in spherical coordinates

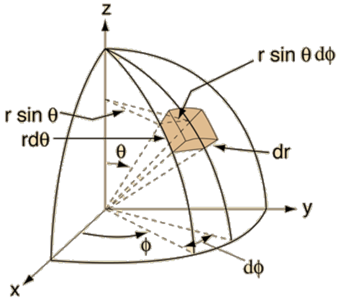
$$F(\mathrm{k}, \mathbf{r}) = \frac{1}{8\pi^3} \int_{|\mathbf{k}| \leq \mathrm{k}_F} e^{-i\mathbf{kr}} d^3\mathrm{k}$$



# 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 $\phi$

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

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

# Evaluation of the integral

Integration over $\theta$

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

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

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

# Evaluation of the integral

Integration over $\theta$

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

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

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

# 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 $\mathrm{k}_F r \to 0 \iff r \ll \lambda_F$

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

# Title

Begin with the equations.

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

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

$$\psi_k(\vec{x}) = \frac{1}{\sqrt{\mathcal{V}}}e^{-i\vec{k}\cdot\vec{x}}$$

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

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

$$\langle g|\sum_k c^\dagger_{k,\sigma}\psi^*_{k,\sigma}(\mathbf{x})\sum_l c^\dagger_{l,\sigma'}\psi^*_{l,\sigma'}(\mathbf{x}')\sum_m c_{m,\sigma'}\psi_{m,\sigma'}(\mathbf{x}')\sum_n c_{n,\sigma}\psi_{n,\sigma}(\mathbf{x})\,|g\rangle$$

Now we see two creation and two annihilation operators, but N should be conserved, so there are two cases:

$$k,\sigma = m,\sigma' \tag{5}$$