

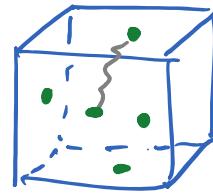
## §2. Electron gas

### \* Interacting electron gas (Jellium model)

Turn on Coulomb interactions between electrons.

$$H = H_0 + H_I$$

$$H_0 = \int d\vec{r} \psi_{\sigma}^+(\vec{r}) \left( -\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 \right) \psi_{\sigma}(\vec{r})$$



$$H_I = \frac{1}{2} \int d\vec{r} d\vec{r}' \psi_{\sigma}^+(\vec{r}) \psi_{\sigma'}^+(\vec{r}') \frac{e^2}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} \psi_{\sigma'}(\vec{r}') \psi_{\sigma}(\vec{r})$$

(summation over  $\sigma, \sigma'$  assumed if not otherwise indicated.)

Get familiar with second quantization:

$$\psi_{\sigma}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} C_{\vec{k}, \sigma} e^{i\vec{k} \cdot \vec{r}}$$

$$\begin{aligned} \Rightarrow H_0 &= \int d\vec{r} \frac{1}{V} \sum_{\vec{k}, \vec{k}'} C_{\vec{k}, \sigma}^+ C_{\vec{k}', \sigma} e^{-i\vec{k} \cdot \vec{r}} \left( -\frac{\hbar^2}{2m} \nabla_{\vec{r}}^2 \right) e^{i\vec{k}' \cdot \vec{r}} \\ &= \underbrace{\int d\vec{r} \frac{1}{V} \sum_{\vec{k}, \vec{k}'} C_{\vec{k}, \sigma}^+ C_{\vec{k}', \sigma} \frac{\hbar^2 |\vec{k}'|^2}{2m} e^{i(\vec{k}' - \vec{k}) \cdot \vec{r}}}_{\delta_{\vec{k}, \vec{k}'}} \\ &= \sum_{\vec{k}, \sigma} \frac{\hbar |\vec{k}|^2}{2m} C_{\vec{k}, \sigma}^+ C_{\vec{k}, \sigma} \end{aligned}$$

✓

kinetic term

Ground state of  $H_0$ : Fermi sphere

$$|FS\rangle = \prod_{|\vec{k}| < k_F} \prod_{\sigma=\uparrow,\downarrow} C_{\vec{k},\sigma}^+ |0\rangle$$

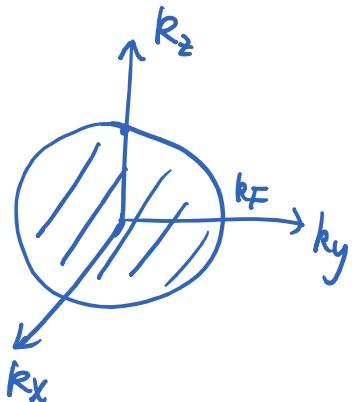
$$H_0 |FS\rangle = E_0 |FS\rangle$$

$$E_0 = 2 \sum_{|\vec{k}| < k_F} \epsilon_{\vec{k}}$$

$$\stackrel{v \rightarrow \infty}{=} \int_0^{\epsilon_F} d\varepsilon D(\varepsilon) \varepsilon$$

$$= \frac{3}{5} \epsilon_F \cdot N_e$$

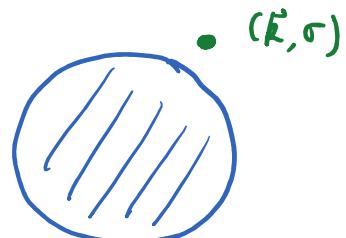
$$D(\varepsilon) = \frac{3}{2} \frac{N_e}{\epsilon_F} \left( \frac{\varepsilon}{\epsilon_F} \right)^{1/2}$$



Excited states of  $H_0$ :

"particle"-type excitations:

$$C_{\vec{k},\sigma}^+ |FS\rangle, \quad \underline{|\vec{k}| > k_F}$$



$$\text{Excitation energy } E - E_0 = \frac{\hbar^2 |\vec{k}|^2}{2m}$$

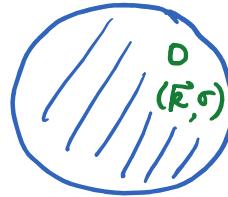
momentum  $\hbar \vec{k}$

electron #  $N_e + 1$

(forbidden if particle # conserved)

"hole"-type excitations:

$$C_{\vec{k},\sigma}^+ |FS\rangle, \quad |\vec{k}| < k_F$$



$$\text{Excitation energy } E - E_0 = - \frac{\hbar^2 |\vec{k}|^2}{2m}$$

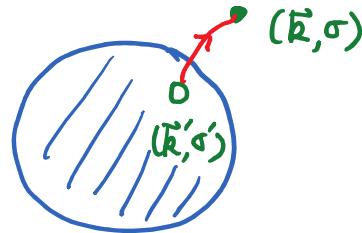
$$\text{momentum } -\hbar \vec{R}$$

$$\text{electron # } N_e - 1$$

(forbidden if particle # conserved)

particle-hole excitations:

$$C_{\vec{k},\sigma}^+ C_{\vec{k}',\sigma'}^- |FS\rangle, \quad |\vec{k}| > k_F, \\ |\vec{k}'| < k_F$$



$$\text{Excitation energy } E - E_0 = \frac{\hbar^2}{2m} (\underbrace{|\vec{k}|^2 - |\vec{k}'|^2}_{> 0}) > 0$$

( can be made arbitrarily small  
when particle & hole are close to  
the Fermi surface ! )

$$\text{momentum } \hbar(\vec{k} - \vec{k}')$$

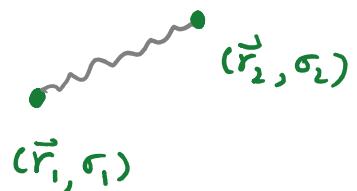
$$\text{electron # } N_e \Rightarrow \text{conserved!}$$

( Well-defined excitations for # - conserving systems )

Justification of the second-quantized form for the Coulomb interactions:

$$4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2) |0\rangle$$

↑  
two electrons at  $\vec{r}_1$  and  $\vec{r}_2$



$$\begin{aligned} H_I & 4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2) |0\rangle \\ &= \frac{1}{2} \int d\vec{r} d\vec{r}' 4_{\sigma}^+(\vec{r}) 4_{\sigma'}^+(\vec{r}') \frac{e^2}{4\pi\epsilon_0 |\vec{r}-\vec{r}'|} \underbrace{4_{\sigma'}^-(\vec{r}') 4_{\sigma}^-(\vec{r})}_{\text{---}} \\ &\quad \times \underbrace{4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2)}_{\text{---}} |0\rangle \end{aligned}$$

two cases with nonvanishing results:

$$1) (\vec{r}, \sigma) = (\vec{r}_1, \sigma_1) \text{ and } (\vec{r}', \sigma') = (\vec{r}_2, \sigma_2)$$

$$2) (\vec{r}, \sigma) = (\vec{r}_2, \sigma_2) \text{ and } (\vec{r}', \sigma') = (\vec{r}_1, \sigma_1)$$

$$\begin{aligned} &= \frac{1}{2} 4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2) \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} |0\rangle \\ &\quad + \frac{1}{2} 4_{\sigma_2}^+(\vec{r}_2) 4_{\sigma_1}^+(\vec{r}_1) \frac{e^2}{4\pi\epsilon_0 |\vec{r}_2 - \vec{r}_1|} (-1) |0\rangle \end{aligned}$$

$$\begin{aligned} & 4_1 4_2 4_1^+ 4_2^+ |0\rangle \\ &= - 4_1 4_1^+ 4_2 4_2^+ |0\rangle \\ &= - |0\rangle \end{aligned}$$

$$= \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|} 4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2) |0\rangle$$

$4_{\sigma_1}^+(\vec{r}_1) 4_{\sigma_2}^+(\vec{r}_2) |0\rangle$  is an eigenstate of  $H_I$  with

potential energy  $\frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$ . ✓

— Jellium model

$$H_0 = \sum_{\vec{k}} \varepsilon_{\vec{k}} C_{\vec{k},\sigma}^+ C_{\vec{k},\sigma}$$

$$H_I = \frac{1}{2} \int d\vec{r} d\vec{r}' \psi_{\sigma}^+(\vec{r}) \psi_{\sigma'}^+(\vec{r}') \frac{e^2}{4\pi\epsilon_0 |\vec{r}-\vec{r}'|} \psi_{\sigma'}(\vec{r}') \psi_{\sigma}(\vec{r})$$

$H_0$  diagonal in  $\vec{k}$ -space  $\Leftrightarrow H_I$  diagonal in  $\vec{r}$ -space

Competition of kinetic and potential terms!

(Heisenberg's uncertainty principle)

Very difficult to diagonalize  $H_0 + H_I$ ! (many-body problem)

We will have to use perturbation theory where

$H_0$  is dominant over  $H_I$  (condition to be derived),

so it's convenient to bring  $H_I$  into  $\vec{k}$ -space:

$$\begin{aligned}
 \psi_{\sigma}(\vec{r}) &= \frac{1}{N\sqrt{V}} \sum_{\vec{k}} C_{\vec{k},\sigma} e^{i\vec{k} \cdot \vec{r}} \\
 H_I &= \frac{1}{2} \underbrace{\int d\vec{r} d\vec{r}' \frac{1}{V^2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4}}_{\text{underbrace}} \underbrace{\frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}}_{\text{underbrace}} \\
 &\quad \times C_{\vec{k}_1, \sigma}^+ C_{\vec{k}_2, \sigma'}^+ C_{\vec{k}_3, \sigma'} C_{\vec{k}_4, \sigma} \underbrace{e^{i(\vec{k}_3 - \vec{k}_2) \cdot \vec{r}' + i(\vec{k}_4 - \vec{k}_1) \cdot \vec{r}}}_{\text{underbrace}} \\
 &= \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \underbrace{\sqrt{C_{\vec{k}_1, \sigma}^+ C_{\vec{k}_2, \sigma'}^+ C_{\vec{k}_3, \sigma'} C_{\vec{k}_4, \sigma}}}_{\text{underbrace}}
 \end{aligned}$$

$$V_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} = \frac{1}{V^2} \int d\vec{r} d\vec{r}' \frac{e^2}{4\pi\epsilon_0 |\vec{r} - \vec{r}'|} \quad \leftarrow \begin{cases} \vec{r} - \vec{r}' = \vec{r}_1 \\ \frac{1}{2}(\vec{r} + \vec{r}') = \vec{r}_2 \end{cases}$$

$$\times e^{i(\vec{k}_3 - \vec{k}_2) \cdot \vec{r}' + i(\vec{k}_4 - \vec{k}_1) \cdot \vec{r}}$$

$$= \underbrace{\frac{1}{V^2} \int d\vec{r}_1 d\vec{r}_2}_{\sim} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_1|} \underbrace{e^{i(\vec{k}_3 - \vec{k}_2 + \vec{k}_4 - \vec{k}_1) \cdot \vec{r}_2}}_{\sim}$$

$$\times e^{\frac{i}{2}(\vec{k}_4 - \vec{k}_1 - \vec{k}_3 + \vec{k}_2) \cdot \vec{r}_1} \quad \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}$$

$$= \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \cdot \frac{1}{V} \int d\vec{r}_1 \underbrace{\frac{e^2}{4\pi\epsilon_0 |\vec{r}_1|}}_{\sim} e^{i(\vec{k}_4 - \vec{k}_1) \cdot \vec{r}_1}$$

Fourier expansion  
of Coulomb potential:  $\frac{1}{|\vec{r}|} = \frac{1}{V} \sum_{\vec{k}} \frac{4\pi}{|\vec{k}|^2} e^{i\vec{k} \cdot \vec{r}}$  (see page 10  
for proof)

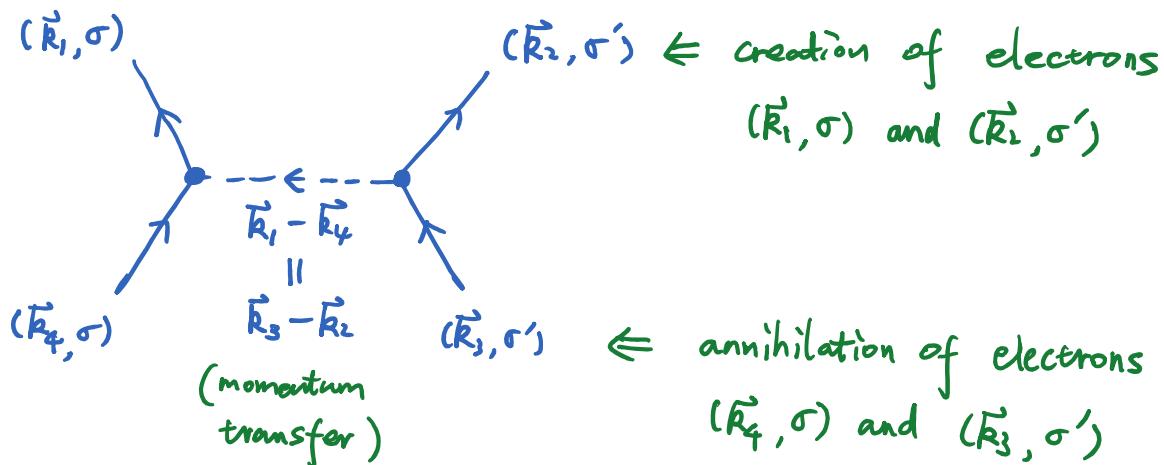
$$= \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \cdot \underbrace{\frac{e^2}{\epsilon_0 V^2} \int d\vec{r}_1}_{\sim} \sum_{\vec{k}} \frac{1}{|\vec{k}|^2} \underbrace{e^{i(\vec{k} + \vec{k}_4 - \vec{k}_1) \cdot \vec{r}_1}}_{\sim}$$

$$= \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \cdot \frac{e^2}{\epsilon_0 V |\vec{k}_1 - \vec{k}_4|^2} \quad \delta_{\vec{k}, \vec{k}_1 - \vec{k}_4}$$

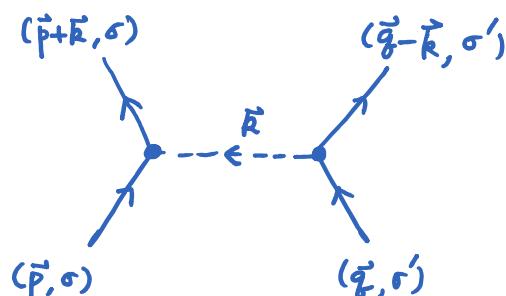
$$\Rightarrow H_I = \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \frac{e^2}{\epsilon_0 V |\vec{k}_1 - \vec{k}_4|^2}$$

$$\times C_{\vec{k}_1, \sigma}^+ C_{\vec{k}_2, \sigma'}^+ C_{\vec{k}_3, \sigma'}^- C_{\vec{k}_4, \sigma}^-$$

Graphical representation of  $H_I$ :



We could use the momentum conservation  $\delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4}$   
to eliminate one momentum:



$$H_I = \frac{1}{2} \sum_{\vec{p}, \vec{q}, \vec{k}} \frac{e^2}{\epsilon_0 V |\vec{k}|^2} C_{\vec{p} + \vec{k}, \sigma}^+ C_{\vec{q} - \vec{k}, \sigma'}^+ C_{\vec{q}, \sigma'} C_{\vec{p}, \sigma}$$

It's now obvious why  $|FS\rangle$  is not ground/eigenstate  
state of  $H_0 + H_I$ :

$$H_I |FS\rangle =$$

$\vec{p} + \vec{k}$

$\vec{p}$

$\vec{q}$

$\vec{q} - \vec{k}$

+ other particle-hole excitations

— Perturbation theory

Q: Under which condition is  $H_0$  dominant over  $H_I$ ?

Only parameter in the problem: density of electrons

$$n = \frac{N_e}{V}$$

Naive expectation:

In the low-density limit, electrons are far from each other, so that interactions are "minimized".

However, kinetic energy

$$\frac{E_0}{N_e} = \frac{3}{5} \varepsilon_F = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 = \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}$$

$\downarrow$

$$k_F = (3\pi^2 n)^{1/3}$$

also decreases when  $n$  decreases.

We need a careful comparison!

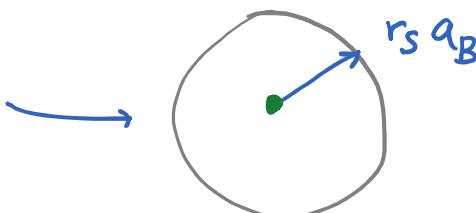
In fact,  $H_0$  is dominant at the high density limit.

We will justify this argument by using  $|FS\rangle$  as a trial wave function.

Introduce a dimensionless parameter :  
 (to control the perturbative expansion)

$$\frac{1}{n} = \frac{V}{N_e} \equiv \frac{4}{3} \pi (r_s a_B)^3$$

↑  
 average volume  
 of an electron



length unit : Bohr radius  $a_B = \frac{4\pi\epsilon_0\hbar^2}{me^2}$

( "most probable distance of electron & nucleus  
 in a hydrogen atom" )

$$\Rightarrow n = \frac{3}{4\pi} \frac{1}{(r_s a_B)^3} \quad (\text{high density : } r_s \rightarrow 0)$$

$$k_F = (3\pi^2 n)^{1/3} = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s a_B}$$

$$\frac{E_0}{N_e} = \frac{3}{5} \epsilon_F = \frac{3}{5} \frac{\hbar^2 k_F^2}{2m} = \frac{3}{5} \left(\frac{9\pi}{4}\right)^{2/3} \frac{1}{r_s^2} \cdot \frac{\hbar^2}{2m a_B^2}$$

Rydberg unit of energy: ||

key result:  $\frac{E_0}{N_e} \approx \frac{2.21}{r_s^2} Ry$

$$1 Ry = \frac{me^4}{8\epsilon_0^2 h^2} = \frac{me^4}{32\pi^2 \epsilon_0^2 h^2}$$

13.6 eV (Ionization energy  
 of hydrogen atom)

Appendix : Fourier transformation of the Coulomb potential

$$\frac{1}{|\vec{r}|} = \frac{1}{V} \sum_{\vec{k}} \frac{4\pi}{|\vec{k}|^2} e^{i\vec{k} \cdot \vec{r}}$$

Proof : RHS  $\stackrel{V \rightarrow \infty}{=} \frac{1}{(2\pi)^3} \int d\vec{k} \frac{4\pi}{|\vec{k}|^2} e^{i\vec{k} \cdot \vec{r}}$

$$= \frac{1}{2\pi^2} \underbrace{\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta}_{2\pi} \int_0^\infty dk e^{ikr \cos\theta}$$

$$= \underbrace{-\frac{1}{\pi} \int_{-1}^1 d\cos\theta}_{2\pi} \int_0^\infty dk e^{ikr \cos\theta}$$

$$= \frac{1}{\pi} \int_0^\infty dk \frac{1}{ikr} (e^{ikr} - e^{-ikr})$$

$$= \frac{1}{i\pi r} \int_0^\infty dk \frac{1}{k} (e^{ikr} - e^{-ikr}) \quad \text{||}$$

$$= \frac{2}{\pi} \int_0^\infty dk \frac{\sin(kr)}{kr} \quad 2i \sin(kr)$$

define  $x = kr$

$$= \frac{2}{\pi r} \int_0^\infty dx \frac{\sin x}{x} \quad \text{||} \frac{\pi}{2}$$

$$= \frac{1}{r} \quad \text{||} \frac{\pi}{2}$$

$$= \text{LHS} \quad \text{Q.E.D.}$$