TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

SFB 1143

Solid State Theory (SS2020)

Lecture 8: Interacting electron gas

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§ 2.4 Interacting electron gas

- Jellium model:
  - Develop a perturbative expansion (H_0 dominant):

$$H = H_0 + H_I$$

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

$$H_I = \frac{1}{2} \sum_{\vec{p},\vec{q},\vec{k}} \frac{e^2}{\varepsilon_0 V |\vec{k}|^2} C^{+}_{\vec{p}+\vec{k},\sigma} C^{+}_{\vec{q}-\vec{k},\sigma'} C_{\vec{q},\sigma'} C_{\vec{p},\sigma}$$

  - "Zeroth"-order ground state: Fermi sphere

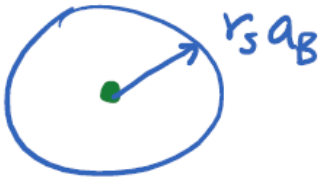
$$|Fs\rangle = \prod_{|\vec{k}|<k_F} \prod_{\sigma=\uparrow,\downarrow} C^{+}_{\vec{k},\sigma} |0\rangle$$

§ 2.4 Interacting electron gas

- Jellium model:
  - "Zeroth"-order energy:

$$E_0 = \langle F_S | H_0 | F_S \rangle$$

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



$$\begin{cases} \frac{1}{n} = \frac{V}{N_e} = \frac{4}{3}\pi (r_s a_B)^3 \\ k_F = (3\pi^2 n)^{1/3} \end{cases}$$

$$\Rightarrow \quad \frac{E_0}{N_e} = \frac{3}{5}\varepsilon_F \simeq \frac{2.21}{r_s^2} \, Ry$$

Rydberg energy unit: $1\,Ry \simeq 13.6\,eV$

§ 2.4 Interacting electron gas

- "Divergence" issue:

$$H_I = \frac{1}{2} \sum_{\vec{p},\vec{q},\vec{k}} \underbrace{\frac{e^2}{\varepsilon_0 V |\vec{k}|^2}}_{\| \; V_{\vec{k}}} c^+_{\vec{p}+\vec{k},\sigma} c^+_{\vec{q}-\vec{k},\sigma'} c_{\vec{q},\sigma'} c_{\vec{p},\sigma}$$

$\vec{k}=0$ term causes a divergence since $V_{\vec{k}=0} \to \infty$

  - Before performing the perturbative analysis, this divergence issue needs to be resolved.

§ 2.4 Interacting electron gas

- "Divergence" issue:
  - Trace back the divergence:

$\vec{k}=0$ term in H_I

$$= \frac{1}{2}\sum_{\vec{p},\vec{q}} V_{\vec{k}=0}\, C^{+}_{\vec{p},\sigma} C^{+}_{\vec{q},\sigma'} C_{\vec{q},\sigma'} C_{\vec{p},\sigma}$$

$$\simeq \frac{1}{2} V_{\vec{k}=0} \underbrace{\sum_{\vec{p},\sigma} C^{+}_{\vec{p},\sigma} C_{\vec{p},\sigma}}_{=N_e} \cdot \underbrace{\sum_{\vec{q},\sigma'} C^{+}_{\vec{q},\sigma'} C_{\vec{q},\sigma'}}_{=N_e}$$

$$= \boxed{\frac{1}{2} N_e^2 V_{\vec{k}=0}}$$

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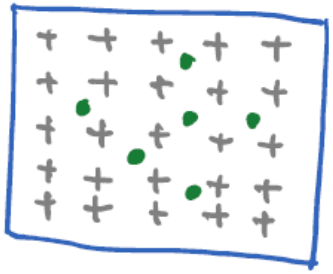
To compensate this divergence, we consider uniformly distributed positive charges (ions):

$$n(\vec{r}) = \frac{N_e}{V}$$

↓

Actually, no $\vec{r}$ dependence (uniform)



- Electrostatic potential from the "background charge":

$$\phi(\vec{r}) = \int d\vec{r}\,' \frac{+e\,n(\vec{r}\,')}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|} = \int d\vec{r}\,' \frac{e\cdot\frac{N_e}{V}}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|}$$

§ 2.4 Interacting electron gas

- Interaction energy between electrons and "background charge":

$$E_{ion-el} = \int d\vec{r}\,[-e n(\vec{r})]\,\phi(\vec{r})$$

$$= -\left(\frac{N_e}{V}\right)^2 \int d\vec{r}\,d\vec{r}\,' \frac{e^2}{4\pi\varepsilon_0 |\vec{r}-\vec{r}\,'|}$$

$$= \boxed{-N_e^2 V_{\vec{k}=0}}$$

$\vec{k}=0$ Fourier component of the Coulomb potential

Last lecture: $V_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} = \frac{1}{V^2}\int d\vec{r}\,d\vec{r}\,' \frac{e^2}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|} e^{i(\vec{k}_3-\vec{k}_2)\cdot\vec{r}\,' + i(\vec{k}_4-\vec{k}_1)\cdot\vec{r}}$

$$= \delta_{\vec{k}_1+\vec{k}_2,\,\vec{k}_3+\vec{k}_4} \cdot \frac{e^2}{\varepsilon_0 V |\vec{k}_1-\vec{k}_4|^2}$$

§ 2.4 Interacting electron gas

- Similar derivation leads to a "divergent" interaction energy from the uniform "background charges":

$$E_{ion\text{-}ion} = \frac{1}{2}\int d\vec{r}\,\left[+e\,n(\vec{r})\right]\phi(\vec{r})$$

$\frac{1}{2}$: avoid double counting

$$= \boxed{\frac{1}{2} N_e^2 V_{\vec{k}=0}}$$

$\Rightarrow$ $E_{ion\text{-}el} + E_{ion\text{-}ion}$ exactly compensate the divergent $\vec{k}=0$ term in H_z !

§ 2.4 Interacting electron gas

- Jellium model:

$$H_{Jellium} = H_0 + H_I + E_{ion\text{-}el} + E_{ion\text{-}ion}$$

$$= H_0 + H_I'$$

$$H_I' = \frac{1}{2} \sum_{\vec{p},\vec{q}} \sum_{\vec{k}(\neq 0)} \frac{e^2}{\varepsilon_0 V |\vec{k}|^2} C^+_{\vec{p}+\vec{k},\sigma} C^+_{\vec{q}-\vec{k},\sigma'} C_{\vec{q},\sigma'} C_{\vec{p},\sigma}$$

➢ Divergence is removed – We are ready to perform perturbative analysis.

§ 2.4 Interacting electron gas

- Jellium model:
  - First-order correction to the ground-state energy:

$$E_I = \langle FS | H_I' | FS \rangle$$

$$= \frac{1}{2} \sum_{\vec{p},\vec{q}} \sum_{\vec{k}(\neq 0)} \frac{e^2}{\varepsilon_0 V |\vec{k}|^2} \langle FS | c^+_{\vec{p}+\vec{k},\sigma} c^+_{\vec{q}-\vec{k},\sigma'} c_{\vec{q},\sigma'} c_{\vec{p},\sigma} | FS \rangle$$

dig two holes in the FS and refill them, otherwise no overlap with $\langle FS|$!

§ 2.4 Interacting electron gas

- Jellium model:
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Case 1: $(\vec{p}+\vec{k},\sigma) = (\vec{p},\sigma)$

$(\vec{q}-\vec{k},\sigma') = (\vec{q},\sigma')$

direct term (Hartee term)

Vanishing since $\vec{k}=0$ excluded

dig two holes in the FS and refill them, otherwise no overlap with $\langle FS|$!

§ 2.4 Interacting electron gas

- Jellium model:
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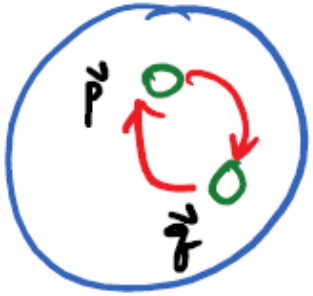


$$E_I = \langle FS | H_I' | FS \rangle$$

$$= \frac{1}{2} \sum_{\vec{p},\vec{q}} \sum_{\vec{k}(\neq 0)} \frac{e^2}{\varepsilon_0 V |\vec{k}|^2} \langle FS | c^+_{\vec{p}+\vec{k},\sigma} c^+_{\vec{q}-\vec{k},\sigma'} c_{\vec{q},\sigma'} c_{\vec{p},\sigma} | FS \rangle$$

Case 2: $(\vec{p}+\vec{k},\sigma) = (\vec{q},\sigma')$

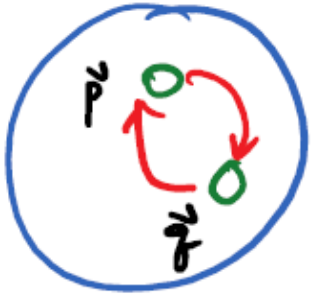
$(\vec{q}-\vec{k},\sigma') = (\vec{p},\sigma)$

exchange term (Fock term) ✓

dig two holes in the FS and refill them, otherwise no overlap with $\langle FS|$!

§ 2.4 Interacting electron gas

- Jellium model:
  - First-order correction to the ground-state energy:



$$E_I = \langle FS | H_I' | FS \rangle$$

$$= \frac{1}{2} \sum_{\vec{p},\vec{q}} \sum_{\vec{k}(\neq 0)} \frac{e^2}{\varepsilon_0 V |\vec{k}|^2} \langle FS | c^+_{\vec{p}+\vec{k},\sigma} c^+_{\vec{q}-\vec{k},\sigma'} c_{\vec{q},\sigma'} c_{\vec{p},\sigma} | FS \rangle$$

$$= \frac{1}{2} \sum_{\vec{p},\vec{q}} \sum_{\sigma} \frac{e^2}{\varepsilon_0 V |\vec{q}-\vec{p}|^2} \langle FS | c^+_{\vec{q},\sigma} c^+_{\vec{p},\sigma} c_{\vec{q},\sigma} c_{\vec{p},\sigma} | FS \rangle$$

$$= -c^+_{\vec{p},\sigma} c^+_{\vec{q},\sigma}$$

within the FS

$\vec{p} \neq \vec{q}$

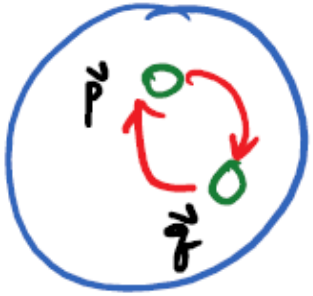
§ 2.4 Interacting electron gas

$$E_I = \frac{1}{2}\sum_{\vec{p},\vec{q}}\sum_{\sigma}\frac{e^2}{\varepsilon_0 V|\vec{q}-\vec{p}|^2}\langle Fs|\, c^+_{\vec{q},\sigma}c^+_{\vec{p},\sigma}c_{\vec{q},\sigma}c_{\vec{p},\sigma}\,|Fs\rangle$$

$$= -c^+_{\vec{p},\sigma}c^+_{\vec{q},\sigma}$$

within the FS

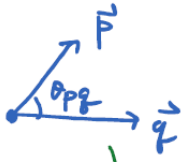
$\vec{p}\neq\vec{q}$



$$= -\frac{1}{2}\sum_{\substack{|\vec{p}|<k_F,\\ |\vec{q}|<k_F,\\ \vec{p}\neq\vec{q}}}\sum_{\sigma}\frac{e^2}{\varepsilon_0 V|\vec{q}-\vec{p}|^2}$$

$\sum_\sigma = 2$

$$= -\sum_{\substack{|\vec{p}|<k_F,\\ |\vec{q}|<k_F,\\ \vec{p}\neq\vec{q}}}\frac{e^2}{\varepsilon_0 V|\vec{q}-\vec{p}|^2}$$



$$\overset{V\to\infty}{=} -\frac{e^2}{\varepsilon_0 V}\cdot\frac{V^2}{(2\pi)^6}\int_{\substack{|\vec{p}|<k_F,\\ |\vec{q}|<k_F}} d\vec{p}\,d\vec{q}\;\frac{1}{p^2+q^2-2pq\cos\theta_{pq}}$$

Integral $= 4\pi^2 k_F^4$
(see Appendix)

§ 2.4 Interacting electron gas

$$E_I = -\frac{e^2 V}{16\pi^4 \varepsilon_0} k_F^4 \leftarrow k_F = (3\pi^2 n)^{1/3}$$

$$= -\frac{3e^2 N_e}{16\pi^2 \varepsilon_0} k_F \leftarrow \begin{cases} k_F = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s a_B} \\ a_B = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} \end{cases}$$

$$\Rightarrow \frac{E_I}{N_e} = -\frac{3}{16\pi^2}\left(\frac{9\pi}{4}\right)^{1/3} \cdot \frac{1}{r_s} \underbrace{\frac{me^4}{4\pi\varepsilon_0^2\hbar^2}}_{= 8\pi R_y}$$

$$R_y = \frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}$$

$$= -\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{r_s} R_y$$

$$\simeq -\frac{0.916}{r_s} R_y$$

(Minus sign means total energy is lowered after turning on H_I'.)

§ 2.4 Interacting electron gas

- Jellium model:
  - Justification of the perturbative analysis:

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

$$\frac{E_I}{N_e} \approx -\frac{0.916}{r_s} Ry$$

$E_I \ll E_0$ if $r_s \to 0$ high density limit !

§ 2.4 Interacting electron gas

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

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$E_I \ll E_0$ if $r_s \to 0$ high density limit !

$$\frac{E}{N_e} \simeq Ry \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \underbrace{0.622 \ln r_s - 0.096}_{\text{"RPA"}} + O(r_s) \right]$$

See Wikipedia "Jellium"

§ 2.4 Interacting electron gas

- Jellium model:
  - Justification of the perturbative analysis:

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

$$\frac{E_I}{N_e} \approx -\frac{0.916}{r_s} Ry$$

$E_I \ll E_0$ if $r_s \to 0$ high density limit !

In neutron stars, $r_s \to 0$ is a good starting point.

However, for metals, $r_s = 2 \sim 6$!

(perturbative treatment is problematic.)

§ 2.4 Interacting electron gas

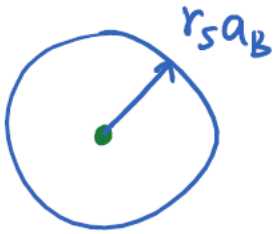
- Jellium model:
  - Simple argument why H_0 is dominant for $r_s \to 0$:

$$\frac{E_0}{N_e} \sim \frac{\hbar^2 k_F^2}{2m}$$

$$\sim \frac{\hbar^2}{2m a_B^2} \cdot \frac{1}{r_s^2}$$

$$\frac{\hbar^2}{2m a_B^2} = 1\,\mathrm{Ry}$$

$$\sim \frac{1}{r_s^2}\,\mathrm{Ry}$$



Heisenberg's uncertainty principle:

$$k_F \sim \frac{1}{r_s a_B}$$

$$\frac{E_I}{N_e} \sim \frac{e^2}{4\pi\varepsilon_0 \cdot r_s a_B} \sim \frac{1}{r_s}\,\mathrm{Ry}$$

The minus sign in E_I cannot be obtained, but the scalings with r_s are correct!

§ 2.4 Interacting electron gas

- Appendix: Evaluating an integral (see page 14):

$$I = \int_{\substack{|\vec{p}|<k_F,\\ |\vec{q}|<k_F}} d\vec{p}\, d\vec{q}\ \frac{1}{p^2+q^2-2pq\cos\theta_{pq}}$$

We first evaluate the integration over $\vec{p}$ in spherical coordinate (with $\vec{q}$ as $\hat{z}$ direction $\Rightarrow \theta_{pq} = \theta$):

$$\int_{|\vec{p}|<k_F} d\vec{p}\ \frac{1}{p^2+q^2-2pq\cos\theta_{pq}}$$

$$= \int_0^{k_F} dp\cdot p^2 \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\ \frac{1}{p^2+q^2-2pq\cos\theta}$$

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$$\int_{|\vec{p}|<k_F} d\vec{p}\ \frac{1}{p^2+q^2-2pq\cos\theta_{pq}}$$

$$= \int_0^{k_F} dp\cdot p^2 \underbrace{\int_0^{2\pi} d\phi}_{=\,2\pi} \underbrace{\int_0^{\pi} \sin\theta\, d\theta\ \frac{1}{p^2+q^2-2pq\cos\theta}}$$

$$= -2\pi \int_0^{k_F} dp\ \frac{p}{q}\ln\left|\frac{p-q}{p+q}\right|$$

$$\int_{-1}^{1} d\cos\theta\ \frac{1}{p^2+q^2-2pq\cos\theta}$$

$$= -\frac{1}{2pq}\ln(p^2+q^2-2pqx)\Big|_{-1}^{1}$$

$$= -\frac{1}{pq}\ln\left|\frac{p-q}{p+q}\right|$$

§ 2.4 Interacting electron gas

The integration over $\vec{q}$ is also done in spherical coordinate.

The integration over angles is $\int_0^{\pi} \sin\theta_q \, d\theta_q \int_0^{2\pi} d\phi_q = 4\pi$

$$I = -2\pi \int_0^{k_F} dq \; 4\pi q^2 \int_0^{k_F} dp \; \frac{p}{q} \ln\left|\frac{p-q}{p+q}\right|$$

$$= -8\pi^2 \int_0^{k_F} dp \int_0^{k_F} dq \; pq \ln\left|\frac{p-q}{p+q}\right|$$

$p = k_F x$

$q = k_F y$

$$= -8\pi^2 k_F^4 \underbrace{\int_0^1 dx \int_0^1 dy \; xy \ln\left|\frac{x-y}{x+y}\right|}_{= -\frac{1}{2}}$$

$$= 4\pi^2 k_F^4$$