4. Coulomb + Screening

4.1 Hartree Fock – Overview

- Drude → Free electrons $KE = \frac{p^2}{2m}$

  → Independent electrons $U_{coulomb} = 0$

  → Scattering from ions + e^- captured in τ.

- Sommerfeld → Pauli exclusion

- HF → Basis for independent e^-

  → Fails → fix with "screening"

4-2 Energy + Length Scales

- Full Hamiltonian

$$H = -\sum_i \frac{\hbar^2 \nabla^2}{2m_e} + \sum_i V(r_i) + \sum_{i<j} \frac{e^2}{4\pi\epsilon_0 r_{ij}}$$

$r_{ij} = |r_i - r_j|$

T = kinetic energy

V = potential energy

→ includes ions etc

(generically approx V = const)

U = interaction energy

→ Sommerfeld: ignores U

→ standard physics: fine if $U \ll T$ for typical states

- Kinetic Energy per e^-

$$E_{KE} = \frac{\hbar^2 k_F^2}{2m^*} \qquad N = \underbrace{\frac{V}{4\pi^3}}_{\text{states per k-space vol}} \cdot \underbrace{\frac{4}{3}\pi k_F^3}_{\text{vol of FS in k-space}}$$

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

- Interaction energy per e^-

$$\underbrace{E_c}_{\text{coulomb}} = \frac{1}{4\pi\epsilon_0} \cdot \frac{q_1 q_2}{r_{12}} = \frac{e^2}{4\pi\epsilon_0 r_s}$$

$q_1 = q_2 = -e$ $\quad r_{12} = r_s =$ typical distance between e^-

$$\text{vol per } e^- = \frac{V}{N} = \frac{4}{3}\pi r_s^3$$

$$\therefore n^{-1} = \frac{4}{3}\pi r_s^3$$

$$\therefore \frac{E_c}{E_{KE}} = \frac{e^2}{4\pi\epsilon_0 r_s} \cdot \frac{2m^*}{\hbar^2 k_F^2} \sim 2 \,!!$$

$r_s \sim 2$ Å

$m^* \sim m_e$

$r_s \rightarrow n \rightarrow k_F$

!!!

- Not at all justified in ignoring U

- Length Scales

  - $r_s = \left(\frac{4}{3}\pi n\right)^{-1/3}$ — Wigner seitz radius
    - typical $e^- - e^-$ distance
    - $r_s \sim k_F^{-1}$

  - $a_0 = \frac{4\pi\epsilon_0 \hbar^2}{me^2}$ — Bohr radius
    - Characteristic length of interactions

  - $$\frac{E_C}{E_{KE}} = \underbrace{\left(\frac{128}{81\pi^2}\right)^{1/3}}_{\simeq 0.5} \frac{r_s}{a_0} \quad \begin{matrix} \leftarrow \sim 2\mathring{A} \\ \leftarrow \sim 0.5\mathring{A} \end{matrix}$$

- Note $E_C \gg E_{KE}$ when $\underbrace{r_s \gg a_0}_{\text{low density}}$

$$E_C \sim \frac{1}{r_s} \quad E_{KE} \sim k_F^2 \sim \frac{1}{r_s^2}$$

4.3 Hartree Fock Approximation

- Why does Sommerfeld theory work so well?

  - We assumed a Fermi Gas $|GS\rangle$

Assumeds $|GS\rangle \doteq$ Slater determinant $|\Psi\rangle$

$$\langle r_1\sigma_1 \cdots r_N\sigma_N|\Psi\rangle = \Psi(r_1\sigma_1\ r_2\sigma_2 \cdots r_N\sigma_N)$$

$$= \frac{1}{\sqrt{N!}} \det\left[\psi_i(r_j\sigma_j)\right]_{ij=1}^{N}$$

$$\langle r_j\sigma_j|\psi_i\rangle = \psi_i(r_j\sigma_j) \qquad \sigma_j \in \{\uparrow, \downarrow\}$$

eigenstates of S_z

where $\langle\psi_i|\psi_j\rangle = \delta_{\sigma_i\sigma_j}\int d^3r\, \psi_i^*(r)\psi_j(r) = \delta_{ij}$

— Total Energy

$$U_s = \langle \Psi | H | \Psi \rangle$$

$$U_{KE} = \langle \Psi | T | \Psi \rangle = -\sum_i \underbrace{\frac{\hbar^2}{2m} \langle \psi_i | \nabla^2 | \psi_i \rangle}_{\text{single particle KE}}$$

$$U_{ext} = \langle \Psi | V | \Psi \rangle = \sum_i \int d^3r \, |\psi_i(r)|^2 V(r)$$

suppress spin ~~ind~~ index for brevity

$$U_c = \langle \Psi | U | \Psi \rangle$$

$$= \sum_{i<j}^{N} \Big[\underbrace{\langle \psi_i \psi_j | U | \psi_i \psi_j \rangle}_{U_H} - \underbrace{\langle \psi_i \psi_j | U | \psi_j \psi_i \rangle}_{U_x} \Big]$$

Hartree energy — Exchange/Fock energy

$$U_H = \frac{1}{4\pi\epsilon_0} \sum_{i<j}^{N} \int d^3r \int d^3r' \, \frac{|\psi_i(r)|^2 |\psi_j(r')|^2}{|r-r'|}$$

$$U_x = \frac{1}{4\pi\epsilon_0} \sum_{i<j}^{N} \int d^3r \int d^3r' \, \frac{\psi_i^*(r)\psi_j^*(r')\,\psi_i(r')\psi_j(r)}{|r-r'|}$$

- Use variational principle to find best approximate $|GS\rangle$

$$U_s = \langle \Psi | H | \Psi \rangle \geq E_{GS}$$

$\therefore$ Approximate $|GS\rangle \Longrightarrow$ minimise U_s wrt ψ_i

$\Longrightarrow$ constraint $\int d^3r |\psi_i(r)|^2 = 1$

Define a Lagrange function

$$\underbrace{\tilde{U}_s}_{\text{lagrange function}} = U_s - \sum_i \epsilon_i \int d^3r \, |\psi_i(r)|^2$$

$\nwarrow$ langauge multipliers associated to the constraint

at energy minimum

$$\frac{\delta \tilde{U}_s}{\delta \psi_i^*(r)} = 0 \quad \Longleftarrow \text{ functional derivative}$$

- Get Hartree-Fock equation

$$\underbrace{\left[-\frac{\hbar^2\nabla^2}{2m}}_{\text{KE}} + \underbrace{V(r)}_{V_{ext}} + \underbrace{U_H^i(r)}_{\text{Hartree}}\right]\psi_i(r) + \underbrace{\int d^3r' U_x^i(r,r')}_{\text{Fock/Exchange}}\psi_i(r') = \epsilon_i^{HF}\psi_i(r)$$

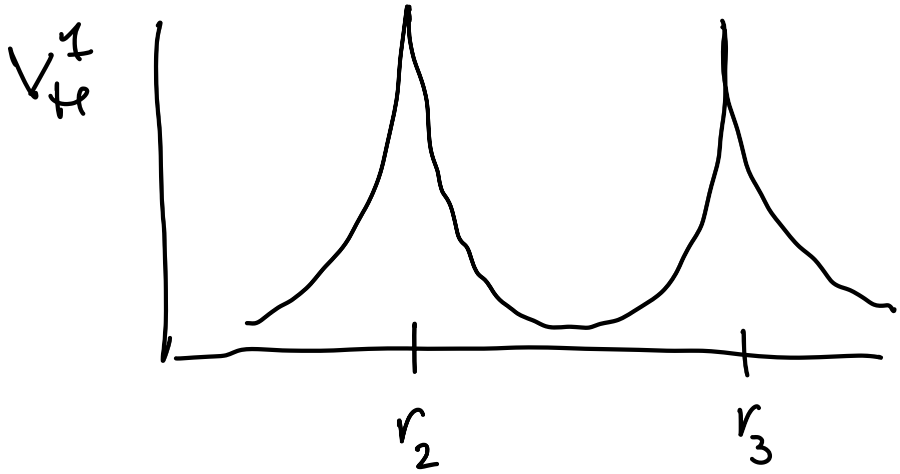
- Hartree term

$$U_H^i(r) = \frac{1}{4\pi\epsilon_0}\sum_{j\neq i}\int d^3r\,\frac{|\psi_j(r)|^2}{r}$$

→ Simple interpretation

→ Each e^- experiences a potential due to the presence of other e^-

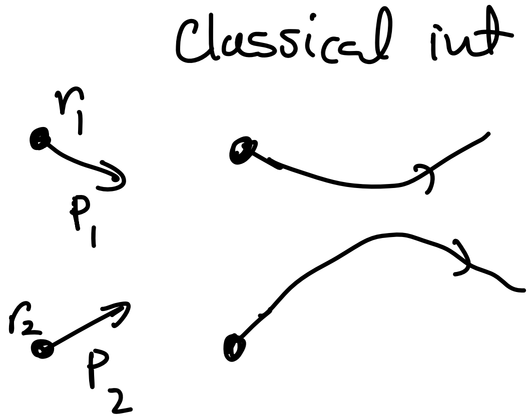
eg 3-electron universe r_1 r_2 r_3

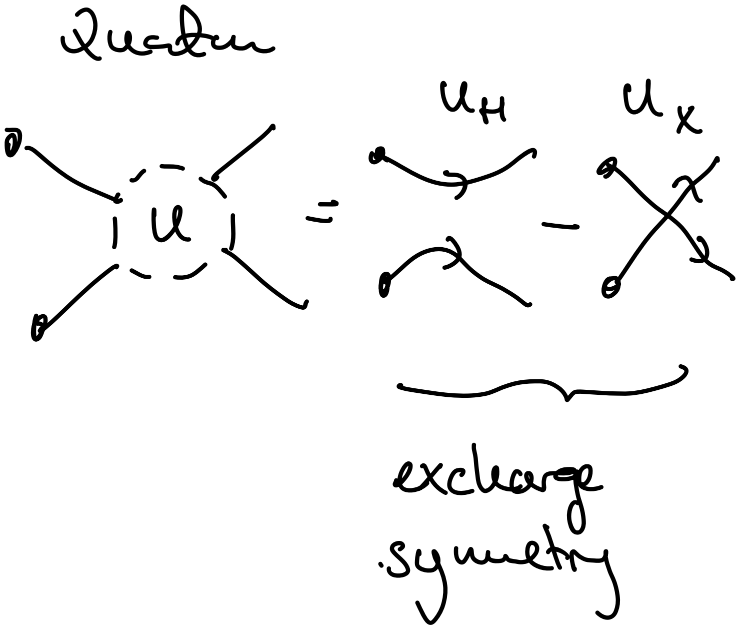


- Fock/Exchange term

$$u_x^i(r,r') = -\frac{1}{4\pi\epsilon_0}\sum_{j\neq i}\frac{\psi_j(r)\,\psi_j^*(r')}{|r-r'|}$$

→ interpretation





- Effective 1 particle Schrodinger Eqn

$$H_i^{HF}|\psi_i\rangle = \epsilon_i^{HF}|\psi_i\rangle$$

H_i^{HF} → depends on all $\psi_{j\neq i}$

- Koopman's theorem
  - Consider $|\Psi\rangle$ and $|\Psi'_i\rangle$

let $|\Psi'_i\rangle$ be $|\Psi\rangle$ with i^{th} electron removed

$$\therefore |\Psi'_i\rangle = |\Psi\rangle + \text{single hole excitation}$$

$$\therefore U = \langle\Psi|H|\Psi\rangle = \epsilon_i^{HF} + \underbrace{\langle\Psi'_i|H|\Psi'_i\rangle}_{U'_i}$$

$$\epsilon_i^{HF} = \underbrace{U - U'_i}_{\substack{\text{energy released} \\ \text{by removing } i^{th} e^-}} \neq \underbrace{\overset{\substack{j^{th}\ e^- \\ \text{removed} \\ \downarrow}}{U'_j} - \overset{\substack{i+j^{th}\ e^- \\ \text{removed} \\ \swarrow}}{U'_{ji}}}_{\substack{\text{'' '' removing } i^{th} e^- \\ \text{after } j^{th} e^-}}$$

"ionisation energy"

$$\therefore U \neq \sum_{i=1}^{N} \epsilon_i^{HF}$$

by etension

$$U \neq \sum_i \epsilon_i^{HF} f_i \qquad f_i = \begin{cases} 1 & \text{occupied} \\ 0 & \text{unoccupied} \end{cases}$$

<u>but</u>

$$\frac{\partial U}{\partial f_i} = \epsilon_i^{HF} \quad \leftarrow \text{prove useful}$$

Still controls physics + eq heat capacity

$$C = \frac{dU}{dT}\bigg|_{n,T=0} = \sum_i \frac{\partial U}{\partial f_i} \cdot \frac{\partial f_i}{\partial T}\bigg|_{n,T=0}$$

$$= \frac{\partial}{\partial T}\bigg|_{n,T=0} \underbrace{\sum_i \epsilon_i^{HF} f_i}_{\neq U}$$

$$= \frac{\partial}{\partial T}\bigg|_{n,T=0} \int d\epsilon \, g^{HF}(\epsilon) \, \epsilon \, f_{FD}(\beta(\epsilon - \mu))\bigg|_{T=0}$$

$$= \frac{\pi^2}{2} g^{HF}(\epsilon) k_B^2 T + O(T^3)$$

4·4 HF solution to Jellium

- Jellium model
  - Coulomb Interacting electrons
  - Uniform backround charge from +ve ions

- HF solution
  - Continuous translational invariance
    - H invariant under $\vec{r}_i \rightarrow \vec{r}_i' = \vec{r}_i + \vec{a}$
    - ψ_i invariant (up to a phase)

      $\therefore$ ψ_i are plane waves

$$\psi_j = \frac{1}{\sqrt{L^3}} e^{-i\vec{k}_j \cdot \vec{r}_j} \quad \therefore \left(|\psi_j\rangle = |\vec{k}_j\rangle \right)$$

  - u_{ext}^{i} = const

    → coulomb ~~force~~ potential due to a uniform background charge

electron density

$$\rho_q^{ion} = e\, n_{ion} = e\, n$$

charge density

ion density

$- \quad u_H^i = \text{const}$

+ coulomb potential ~~due~~ due to

a uniform background

$$\rho_q^{el} = -e n$$

$$u^i_{ext} + u^i_H = \int d^3\vec{r}\left[-\frac{e}{4\pi\epsilon_0}\,\frac{1}{|\vec{r}-\vec{r}'|}\right]\left(\rho_q^{ion} + \rho_q^{el}\right)$$

- $u_x^i = -\frac{1}{4\pi\epsilon_0}\sum_{j\neq i}\frac{e^{-ik_j\cdot(r-r')}}{|r-r'|}$

- $\epsilon_i^{HF} = \langle k_i|H|k_i\rangle$

$$= \underbrace{\langle k_i|T|k_i\rangle}_{\frac{\hbar^2k_i^2}{2m}} + \underbrace{\langle k_i|u_x^i|k_i\rangle}_{\Sigma(\vec{k}_i)}$$

- $\Sigma(\vec{k}_i) = \langle k_i|u_x^i|k_i\rangle$

$$= \sum_{i\neq j}\langle k_i\, k_j|\frac{e^2}{4\pi\epsilon_0 r_{ij}}|k_j\, k_i\rangle$$

$$=' -\frac{e^2}{\epsilon_0}\int_{k'<k_F}\frac{d^3k}{(2\pi)^3}\frac{1}{|\vec{k}-\vec{k}'|^2} \qquad FT\left[\frac{1}{r}\right]\sim\frac{1}{k^2}$$

$$= -\frac{e^2k_F}{2\pi^2\epsilon_0}L\left(\frac{k}{k_F}\right)$$

$$= -e\,\frac{\hbar^2k_F^2}{2m}\cdot\frac{r_s}{a_0}L\left(\frac{k}{k_F}\right)$$

$$\uparrow$$

$$\simeq \frac{1}{3}$$

$$L(x) = \left[\frac{1}{2} + \frac{1-x^2}{4x} \log\left| \frac{1+x}{1-x} \right| \right]$$

"Lindhard function"

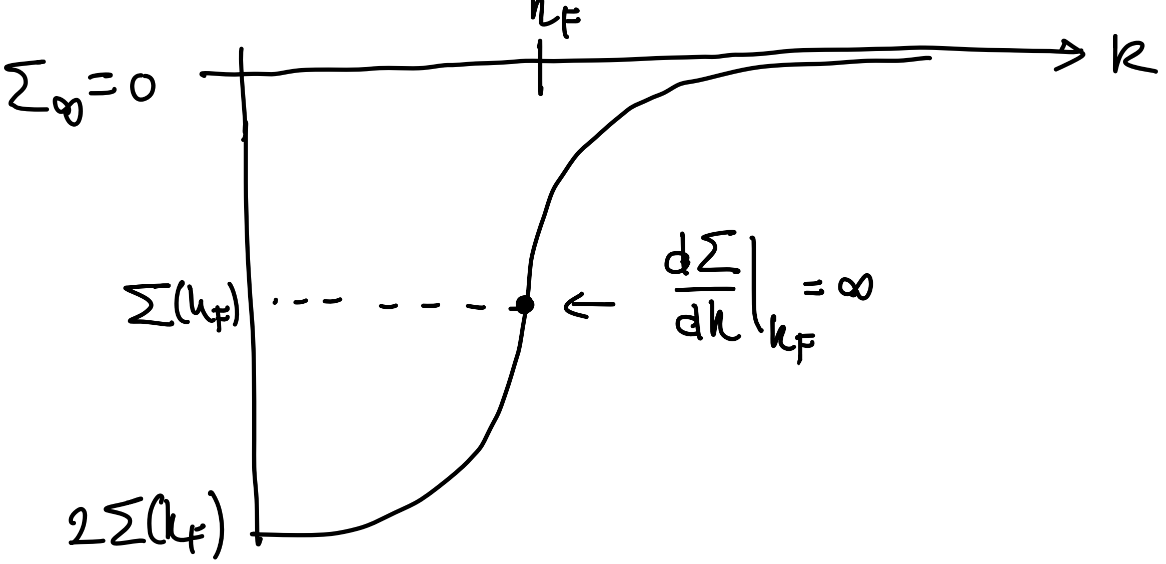
- Hartree-Fock energies

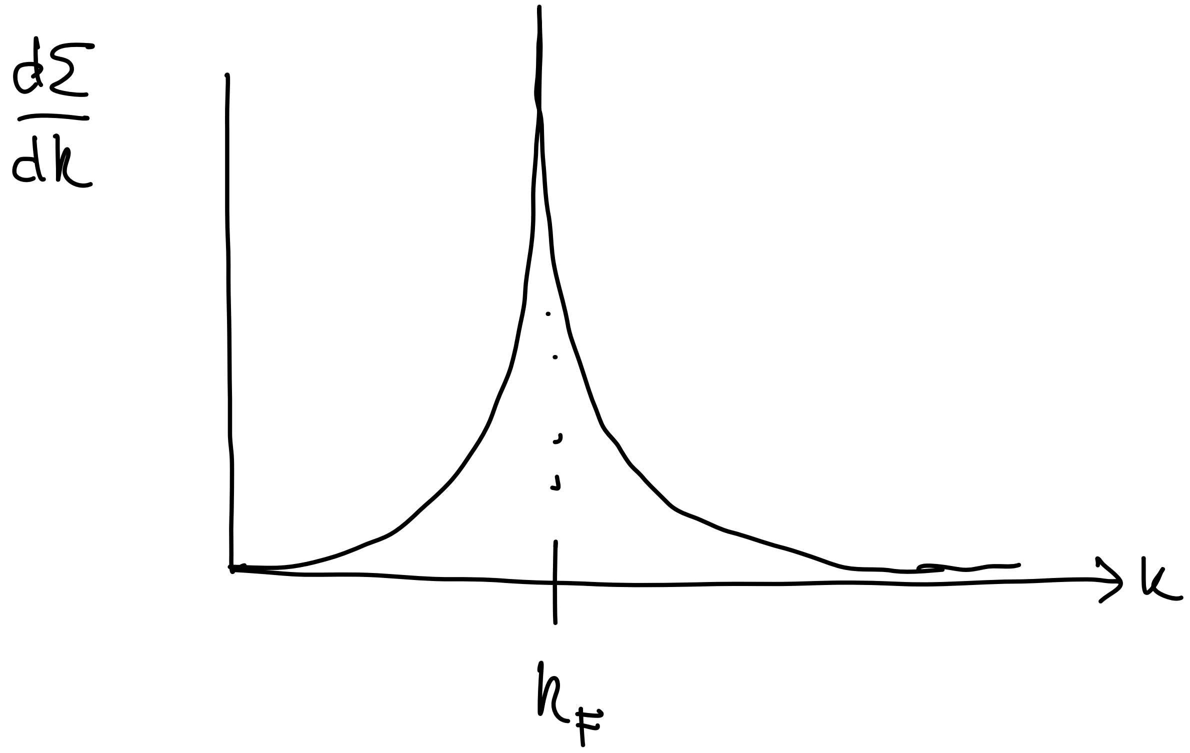
$$\epsilon^{HF}(k) = \underbrace{\epsilon^0(k)}_{\frac{\hbar^2 k^2}{2m}} + \Sigma(k)$$

- $\Sigma(\vec{k})$ = static self energy $\left(\Sigma(\vec{k},\omega)\big|_{\omega=0} \right)$

  = effective shift to single particle energies due to interactions with other particles

$$\Sigma(k_F) = -\frac{2}{3} \cdot \frac{r_s}{a_0} \cdot \frac{\hbar^2 k_F^2}{2m}$$





→ Divergence comes from $\frac{1}{k^2}$ integral

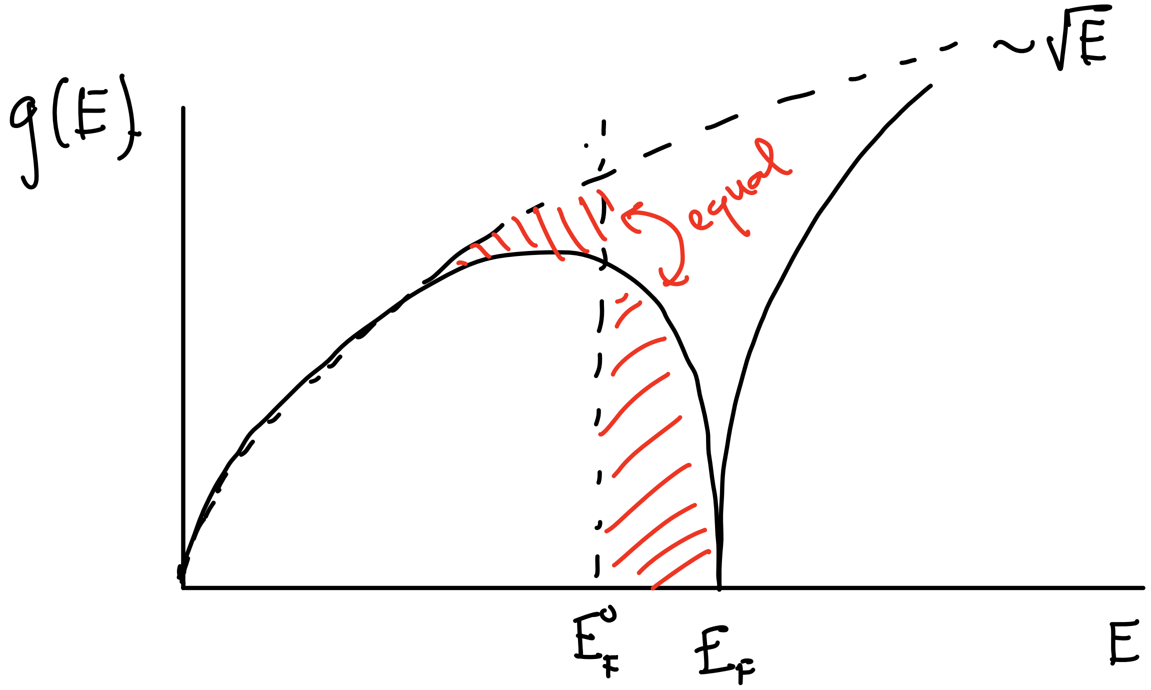
↳ i.e. because interaction is long ranged

↳ small k^2 divergence

→ Problematic

$$g(E) \sim \left| \frac{\partial \epsilon^{HF}}{\partial k} \right|^{-1} \to 0$$

$$v_F \sim \frac{1}{\hbar} \frac{\partial \epsilon^{HF}}{\partial k} \to \infty$$



Note E_F is corrected

$$E_F = \epsilon^{HF}(k_F) = \epsilon(k_F) + \Sigma(k_F)$$

k_F = unchanged

$n = \int_{-\infty}^{E_F} d\epsilon \, g^{HF}(\epsilon)$ is unchanged

$$\therefore\ C = \frac{dU}{dT} = \sum_{k\sigma} \frac{\partial f_{\sigma k}}{\partial T} \frac{\partial U}{\partial f_{k\sigma}}$$

$$= \sum_{k\sigma} \frac{\partial f_{\sigma k}}{\partial T} \epsilon^{HF}_{k\sigma}$$

$$= \frac{\partial}{\partial T} \sum_{k\sigma} f_{k\sigma} \epsilon^{HF}_{k\sigma}$$

can still use the derivatives of this form even though $\neq U$

$$= \frac{\partial}{\partial T} \underbrace{\int d\epsilon\, g^{HF}(\epsilon)\, \epsilon\, f_{FD}(\beta(\epsilon-\mu))}_{\text{sommerfeld} \sim \frac{1}{2}\gamma T^2}$$

$$= \gamma T \quad \text{where} \quad \gamma = \frac{\pi^2}{3} g(E_F)$$

→ At finite T — # accessible states

$$\sim \int_{E_F - k_B T}^{E_F + k_B T} g^{HF}(E)\, dE > 0$$

4.5 Summary of naive HF

- Particle dispersion corrected by other e^-

$$\underset{\uparrow}{\epsilon^{HF}_{k\sigma}} = \epsilon^{0}_{k\sigma} + \Sigma(k) \leftarrow \text{self energy}$$

"renormalised" or "dressed" dispersion

bare dispersion

- Many body problem reduces to effective single body problem

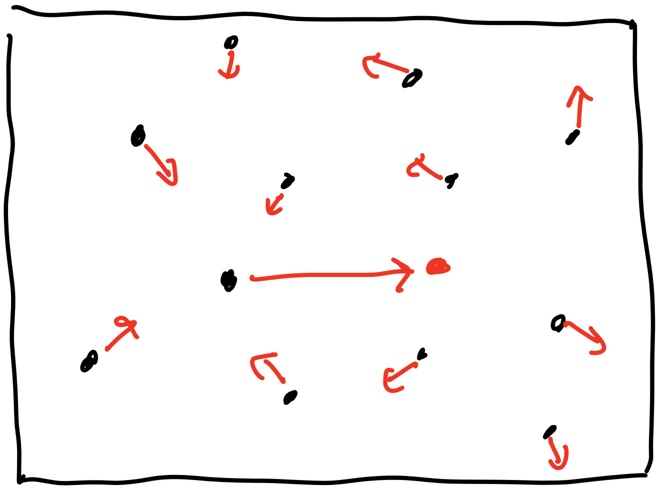
- Unphysical heat capacity

  - $C(T) \to 0$ faster than $C \sim \gamma T$

  - $C \sim \gamma T$ is robust observation in metals

4.6 Screening

- HF captures limited correlations
  - Particle statistics
    - specifically each orbital can contain only 1 fermion
  - Not interactions
- Main Idea
  - Electrons rearrang due to each others position
    - Cartoon



- move 1 electron

→ Changes eqm positions of other electrons

→ In QM electrons characterised by wavefunctions — not positions but idea still applies

→ Captured by screening length k_{TF}^{-1}

$$U_{eff}(r_{12}) \sim \underset{\uparrow}{U_c}(r_{12})\, \underset{\nwarrow}{e^{-k_{TF} r_{12}}}$$

$$U_c(r) = \frac{e^2}{4\pi\epsilon_0 r}$$

k_{TF}^{-1} = screening length

→ Thomas Fermi Screening

$$k_{TF}^{-1} \sim \sqrt{r_s a_0} \sim 1\ \text{Å}$$

$r_s \sim 2\ \text{Å}$

$a_0 \sim 1\ \text{Å}$

∴ microscopic length scale

→ interaction become v. short range

4·7 – Screening of an External potential

Thomas Fermi Screening

Idea: Response of system to electron moving (4·8) = response to external coulomb pot. (4·7)

Consider response to external potential $V = -e\phi$

$$n(r) = e^- \text{ density}$$

$$U_{tot} = U_{int} + U_{ext}$$

$$U_{ext} = -e\int d^3r\, n(r)\,\phi_{ext}(r)$$

- In $|GS\rangle$ system is at an energy minimum

$$0 = \frac{\delta U_{tot}}{\delta n(r)} = \frac{\delta U_{int}}{\delta n(r)} - e\phi_{ext}(r)$$

- Expand to leading order in $\delta n(r)$

$$\frac{\delta U_{int}}{\delta n(r)} = \int d^3r' \, \frac{\delta^2 U_{int}}{\delta n(r)\,\delta n(r')} \, \delta n(r') + O(\delta n^2)$$

- define $\chi(r', r)$ as inverse

$$-\int d^3r' \, \underbrace{\frac{\delta^2 U_{int}}{\delta n(r)\,\delta n(r')}}_{-\chi^{-1}(r,r')} \, \chi(r', r'') = \delta^3(r-r'')$$

- density response to weak potential

$$\delta n(r) = -e\int d^3r' \, \chi(r,r') \, \phi_{ext}(r) + O(\phi^2)$$

- potential generated by density response

$$\delta\phi(r) = \frac{-e}{4\pi\epsilon_0} \int d^3r' \, \frac{\delta n(r')}{|r-r'|}$$

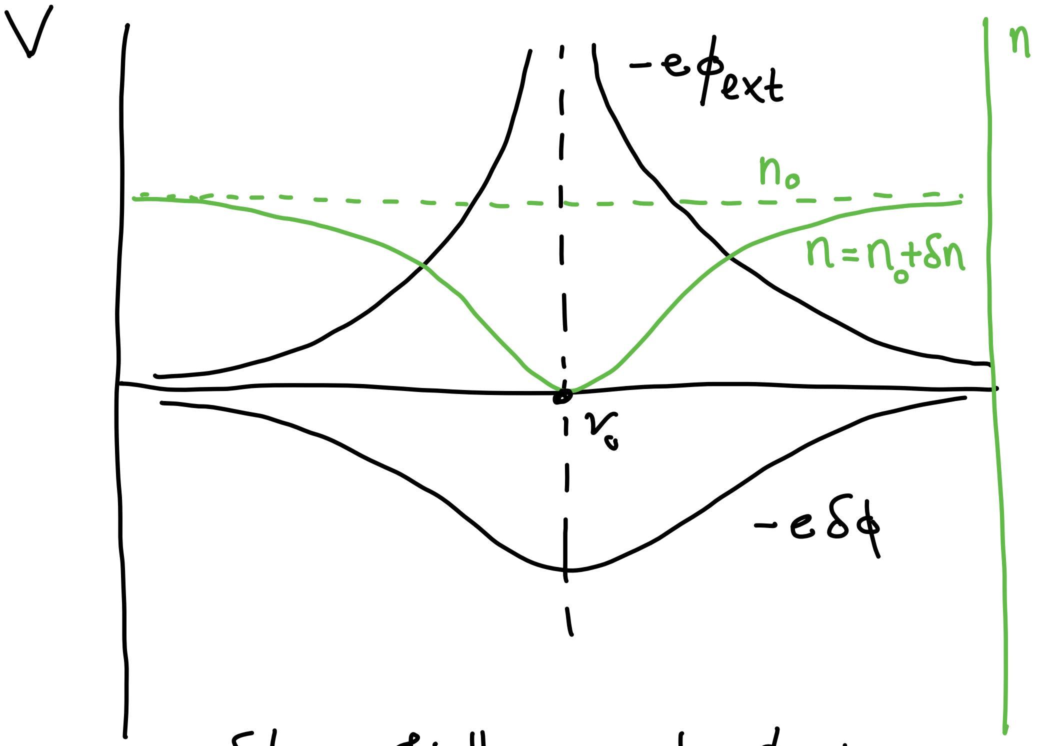
- Screened potential ϕ

$$\phi_{sc}(r) = \phi_{ext}(r) + \delta\phi(r)$$

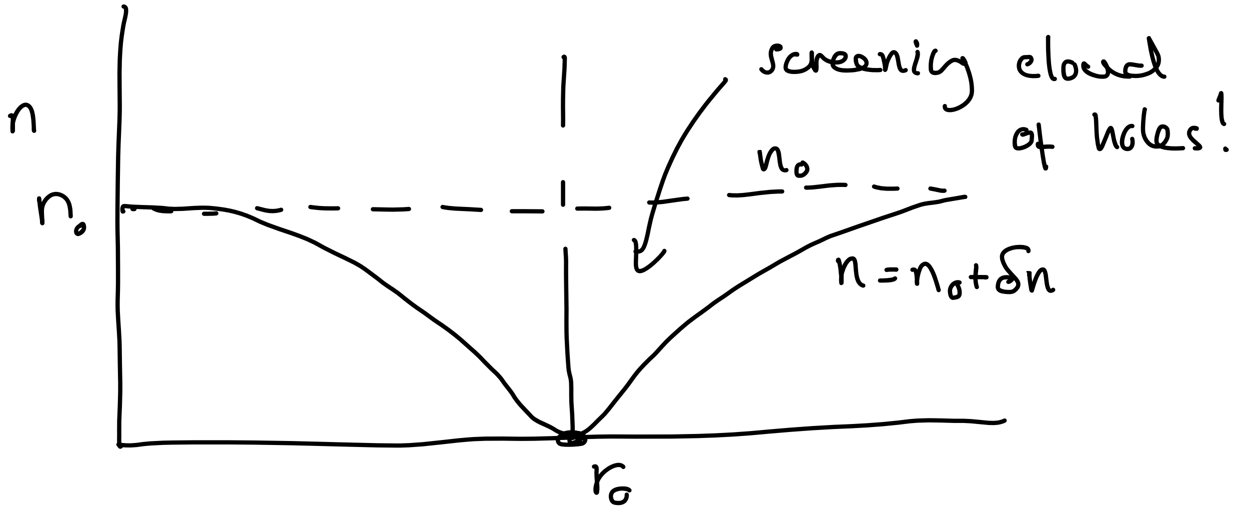
external potential

potential due to e^- response to ϕ_{ext}

– eg pin 1 electron @ r_0



$\delta\phi$ partially cancels ϕ_{ext}



- With translational invariance

$$\chi(r, r') = \chi(r+a, r'+a)$$

$$\therefore \quad = \chi(r-r')$$

in k-space

$$\delta n(k) = \int d^3r \, e^{-ik\cdot r} \delta n(r)$$

$$\chi(k, k') = (2\pi)^3 \chi(k) \, \delta^3(k-k')$$

charge response ← external potential

$$\delta n(k) = -e\chi(k)\phi_{ext}(k) + \underbrace{O(\phi_{ext}^2)}_{\text{neglect from here on}}$$

potential ← charge response

$$\delta\phi(k) = -\frac{e}{\epsilon_0 k^2} \delta n(k)$$

screened potential ⟷ sum

$$\phi_{sc}(k) = \phi_{ext}(k) + \delta\phi(k)$$

$$= \underbrace{\left(1 + \frac{e^2}{\epsilon_0 k^2}\chi(k)\right)}_{\epsilon^{-1}(k)} \phi_{ext}(k)$$

relative permittivity

$$\phi_{sc}(k) = \epsilon(k)\,\phi_{ext}(k)$$

or in r-space

$$\phi_{sc}(r) = \int d^3r'\,\epsilon(r-r)\,\phi_{ext}(r)$$

felt by e^-

accounts for reconfig of e^-

external

Obtaining $\chi(k)$

- recall $U_{int} = T_{KE} + \underbrace{\overset{\text{Hartree}}{U_H} + \overset{\text{Exchange}}{U_x}}_{U_c}$

$$U_H = \frac{1}{2}\int d^3r \int d^3r' \, n(r)\, n(r') \underbrace{\frac{\epsilon^2}{4\pi\epsilon_0} \cdot \frac{1}{|r-r'|}}_{\text{coulomb interaction}}$$

Thomas - Fermi Approx :

(1) Neglect U_x

(2) Focus on long wavelength limit

- Take 2nd derivs $\frac{\delta^2}{\delta n(r)\,\delta n(r')}$

$$-\chi^{-1}(r-r') = -\chi_0^{-1}(r-r') + \frac{e^2}{4\pi\epsilon_0}\frac{1}{|r-r'|} + \underbrace{\chi_x^{-1}(r-r')}_{\text{neglect}}$$

→ k-space

$$\underbrace{\chi^{-1}(k)}_{\text{susceptibility of interacting coulomb gas}} = \underbrace{\chi_0^{-1}(k)}_{\text{susceptibility of non interacting gass}} - \frac{e^2}{\epsilon_0 k^2}$$

$$\chi_0^{-1}(r-r') = \frac{\delta^2 U_0}{\delta n(r)\,\delta n(r')}$$

$$U_0 = T_{KE}$$
$$= \int d^3r \int d\epsilon\, g(\epsilon)\,\epsilon\, f_{FD}(\beta(\epsilon-\mu(r)))$$

→ Model: every point in space is a independent sommerfeld gas

use $$\frac{\delta U_0}{\delta n(r)} = \mu(r)$$ ← definition of chemical potential

not electro chemical as we seperated $U_{int} + U_{ext}$

$$\therefore\ \chi_0^{-1}(r-r') = \frac{\delta \mu(r)}{\delta n(r')} = \frac{\partial \mu}{\partial n}\Big|_{n_0} \delta(r-r')$$ ← local dendence assumption

$$\frac{\partial n}{\partial \mu}\Big|_{n_0} = \frac{\partial}{\partial \mu}\Big|_{n_0} \int d\epsilon\, g^{HF}(\epsilon)\, f_{FD}(\beta(\epsilon-\mu))$$

$$= \beta \int d\epsilon\, g^{HF}(\epsilon) \left(-f_{FD}'(\beta(\epsilon-\mu))\right)$$

$$= \int_{-\infty}^{-\infty} dx\, g^{HF}(\mu + k_B T x) \underbrace{\left(-f_{FD}'(x)\right)}_{\simeq \delta(x)}$$

$$= g^{HF}(\mu) \overset{T\to 0}{=} g^{HF}(E_F) + O\left(\frac{T}{T_F}\right)^2$$

$$\chi_0^{-1}(r-r') = \frac{1}{g(E_F)}\delta(r-r')$$

$$\therefore \chi_0^{-1}(k) = \frac{1}{g(E_F)}$$

$$\chi^{-1}(k) = \frac{1}{g(E_F)} - \frac{e^2}{\epsilon_0 k^2}$$

$$\epsilon(k) = \left(1 - \frac{e^2}{\epsilon_0 k^2}\chi(k)\right)^{-1}$$

$$= 1 + \frac{k_{TF}^2}{k^2} + O\left(\frac{1}{k^4}\right)$$

$$\boxed{k_{TF} = \sqrt{\frac{e^2 g(E_F)}{\epsilon_0}} \quad \text{Thomas Fermi wavenumber}} \sim \sqrt{r_s a_0}!$$

→ Set by the compressibility

$$K_T = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = \frac{1}{n^2}\left(\frac{\partial n}{\partial \mu}\right)_T = \frac{g(E_F)}{n^2}$$

- $g(E_F)$ large
- many low energy unoccupied states
- Can increas the density with low energy cost
- Highly compressible
- ∴ Charges can rearrange easily to screen
- ∴ k_{TF}^{-1} = short length scale.

5.3 Screening of electronic interactions

Assume response to electron is screend in same manner

- Place a charge at $r=0$

$$\therefore \phi_{ext} \rightarrow \phi_{el}(r) = -\frac{e}{4\pi\epsilon_0} \cdot \frac{1}{|r|}$$

$$\phi_{el}(k) = -\frac{e}{\epsilon_0 k^2}$$

$$\phi_{sc}(k) = \epsilon^{-1}(k)\,\phi_{ext}$$

$$= -\frac{e}{\epsilon_0(k^2+k_{TF}^2)}$$

$$\boxed{\phi_{sc}(k) = -\frac{e}{4\pi\epsilon_0}\cdot\frac{e^{-k_{TF}r}}{r} = e^{-k_{TF}r}\,\phi_{el}(r)}$$

→ Screened electronic interaction is short range
"Yukawa potential"

→ Return to Hartree Fock — use screened coulomb

$$\underset{\text{dressed}}{\epsilon^{HF}_{k\sigma}} = \underset{\text{bare}}{\epsilon^{0}_{k\sigma}} + \underset{\text{self energy}}{\Sigma(k)}$$

find divergence is cut-off by the screening length scale

$$\left.\frac{d\Sigma}{dk}\right|_{k_F} = \frac{e^2}{2\pi^3\epsilon_0}\log\left(\frac{k_F}{k_{TF}}\right) \qquad (k_{TF} \gg k_F)$$

→ consistency check

→ recover $\left.\frac{d\Sigma}{dk}\right|_{k_F} = \infty$

→ Self consistent solution to :

Self energy correction to energy → ∴ fermi velocity

$$\epsilon_k^{HF} = \epsilon_k^0 + \Sigma_k$$

$$V_F^{HF} = \frac{1}{\hbar}\frac{\partial \epsilon^{HF}}{\partial k} = V_F^0 + \frac{1}{\hbar}\left.\frac{\partial \Sigma}{\partial k}\right|_{k_F} \quad ①$$

recall if $\epsilon = \frac{\hbar^2 k^2}{2m} \rightarrow V = \frac{1}{\hbar}\frac{\partial \epsilon}{\partial k} = \frac{\hbar k}{m} = \frac{p}{m} = v$

Self energy correction to DOS

as $g(E_F) = \frac{k_F m}{\pi^2 \hbar^2} = \frac{k_F^2}{\pi^2 \hbar V_F}$

N unchanged

∴ k_F unchanged ← k_F is just radius of ball in k-space

→ determined only by n

$$\therefore\ g^{HF}(E_F) = g^0(E_F)\,\frac{V_F^0}{V_F} \qquad ②$$

- Screening correction to Self Energy

$$\left.\frac{\partial\Sigma}{\partial k}\right|_{k_F} = \frac{e^2}{2\pi^3\epsilon_0}\log\left(\frac{k_F}{k_{TF}}\right)$$

③

$$k_{TF}^2 = \frac{e^2\,g(E_F)}{\epsilon_0}$$

- let $\tilde{r} = \left(\frac{k_{TF}}{k_F}\right)^2 = \frac{4}{\pi a_0 k_F} \sim \frac{r_s}{a_0}$ be the small parameter

- let $\eta = \frac{1}{\hbar V_F^0}\left.\frac{\partial\Sigma}{\partial k}\right|_{k_F}$ be the dimensionless correction

① $V^{HF} = V^0(1+\eta)$

② $g^{HF} = \frac{g^0}{1+\eta}$

③ $\eta = \frac{\tilde{r}}{4}\log\left(\frac{1+\eta}{\tilde{r}}\right)$

in high density limit $\tilde{r} \sim \frac{r_s}{a_0} >> 1$

$\eta << 1$

$$\eta = \frac{\tilde{r}}{4} \log\left(\frac{1}{\tilde{r}}\right) + O(\tilde{r}^2 \log \tilde{r})$$

$$\therefore \; g^{HF}(E_F) = g^{0}(E_F)\left[1 - \frac{\tilde{r}}{4}\log\left(\frac{1}{\tilde{r}}\right) + \cdots\right]$$

for typical metals

$$\frac{r_s}{a_0} \sim 2-4 \quad \therefore \; \tilde{r} = \underbrace{\frac{4}{11}\left(\frac{4}{9\pi}\right)^{1/3}}_{0.66} \frac{r_s}{a_0} \sim 1.5-2.5$$

→ $\tilde{r}$ not a small parameter in metals

→ useful toy model but not quantitative

5.4 Summary

- Toy model of screening
  - → e^- move when ϕ_{ext} applied
  - → movement generates $\delta\phi$
  - → $\delta\phi$ cancels part of ϕ_{ext}

- Screens internal e^- interactions
  - → Corrects failures of HF
  - → low energy excitations of metals are
    $$QP = e^- + \text{screening cloud}$$
- Screening most effective when $g(E_F)$ large
  - → low energy states allow charges to rearrange
  - → Screening length k_{TF}^{-1} is short
- TF model controlled for $\frac{r_s}{a_0} \lesssim \frac{3}{2}$
  - → real metals have $\frac{r_s}{a_0} \sim 2-4$
- Can be extended into more complex models
  - → Lindhard Screening

    → same basic idea