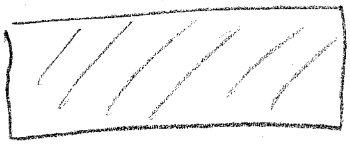
Homogeneous Electron Gas

→ Understanding weak coupling ...



constant density $n(r) = n$

↳ does not mean the system is trivial in terms of
- wave func
- corr. func
- ...

Completely specified by
- density n
- spin density $n_\uparrow - n_\downarrow$

[or polarisation $\zeta = \frac{1}{n}(n_\uparrow - n_\downarrow)$]

· How can we actually realize the system?

↳ there are electrons interaction.

↓

N repels each other (coulomb)

↓

explode !

→ We want to mimick a solide
- nucleides
- compensation of nucleides and e^- charge

charge neutrality is a prerequisite for stability ! → we need to add something that mimics nucleides

→ Replace nuclei by some uniform positiv charged background locally, the system is neutral

→ Both ground states and excitation stays nontrivial.

Definition of r_s : to introduce new expr. n.

$$\boxed{\frac{4\pi}{3}\bar{r}_s^{\,3} = \underbrace{\frac{V}{N}}_{\text{volume/part}}} \longrightarrow r_s = \left(\frac{3}{4\pi n}\right)^{1/3}$$

↳ volume available to each individual electron

→ define a dimensionless qt

$\bar{r}_s = r_s a_B$ ← Bohr radius

↓

Large r_s = low density

Low r_s = large density

unity

ex : C : $r_s = 1.31$

- Diamond = covalent insulator, e^- likely to form covalent bonds

· If I increase the density of e^- gas ? → No more interactions because of Pauli Principle! e^- have to go to higher energy

El. gas : $E_F \sim n^{2/3} \sim \left(\frac{1}{r_s^3}\right)^{2/3} \sim \frac{1}{r_s^2}$

Interactions $\sim \frac{e^2}{r_s}$ $\Rightarrow$ $\frac{\text{Kinetic energy}}{\text{Interactions}} \sim \frac{1}{r_s^2}\frac{r_s}{e^2} \sim \frac{1}{r_s}$

High density $\Rightarrow$ r_s small $\Rightarrow$ kinetic energy dominates over interactions

→ Interactions does increase, but E_c ↑ more

⟹ weak coupling limit!

Hamiltonian $H = \underbrace{-\frac{1}{2m}\sum \nabla_i^2}_{\text{Kinetic nrj}} + \frac{1}{2}\Big[\underbrace{\sum_{i\neq j}\frac{e^2}{|r_i - r_j|}}_{\text{Coulomb}} - \underbrace{\int dr\,dr' \frac{e^2 n^2}{|r-r'|}}_{\text{positive background}}\Big]$

n = density e^- (= density backgr.)

$\hbar = 1$

$m = e = \frac{4\pi}{\varepsilon_0} = 1$

$[r] = a_B$

Energy $\langle H\rangle = \langle T\rangle + \underbrace{\langle V_{ee}\rangle - \frac{1}{2}\iint \frac{n^2}{|r-r'|}}_{\text{not divergent thanks to cancellations}}$

Rescale : $\tilde{\vec{r}} = \frac{\vec{r}}{r_s}$

$$\Rightarrow \underbrace{H}_{\substack{\text{system with a}\\ \text{scaled energy unit}\\ \text{(dimensionless density)}}} = \left(\frac{a_B}{r_s}\right)^2 \sum_i \left[-\frac{1}{2}\tilde{\nabla}_i^2 + \frac{1}{2}\frac{r_s}{a_B}\left(\sum_{i\neq j}\frac{1}{|\tilde{r}_i - \tilde{r}_j|} - \frac{3}{4\pi}\int d\tilde{r}^3 \frac{1}{\tilde{r}}\right)\right]$$

the prop. of the system are actually equivalent to a system with fixed density but rescaled interactions (everything depends on density)

- Non-interacting limit : simple plane waves

States $(\vec{k}, \sigma)$ $\qquad \psi_k(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$, $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$

Ground state for given $n_\uparrow, n_\downarrow$ = Slater det of states $(\vec{k}, \sigma) \in$ Fermi sphere of radius k_F^σ

$$k_F^\sigma = 6\pi^2 n^2$$

- Unpolarized case : $n_\uparrow = n_\downarrow = \frac{n}{2} \Rightarrow k_F^3 = 3\pi^2 n$

Property (Luttinger) = unless you have a phase transition, you will continue to have a system of same Fermi surface

⟹ k_F^σ stays the same with interactions.

- At finite temperature : density operator

$$\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu\hat{N})} \Rightarrow \langle\hat{O}\rangle = \mathrm{Tr}(\hat{\rho}\hat{O}) \text{ expectation value}$$

→ single body density matrix: by expanding in SP wave f. weighted by the Fermi func,

$$\hat{\rho} = \sum_i |\psi_i^\sigma\rangle f_i^\sigma \langle\psi_i^\sigma|, \quad f_i^\sigma = \frac{1}{e^{\beta(\varepsilon_i^\sigma - \mu)} + 1}$$

$$n(r\sigma) = \rho(r\sigma, r\sigma) = \sum_i f_i^\sigma |\psi_i^\sigma(r)|^2$$

Density matrix in non-interacting case

$$\rho(\vec{r}, \vec{r}') = \rho(|\vec{r} - \vec{r}'|) = \frac{1}{(2\pi)^3} \int d\vec{k}\, f(\varepsilon(k))\, e^{ik(r-r')}$$

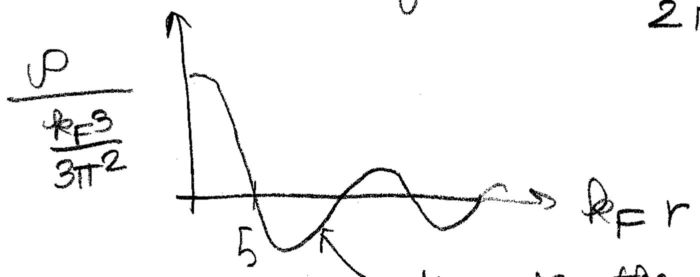
$$\boxed{\rho(r) = \frac{1}{(2\pi)^3} \int d\vec{k}\, f(\varepsilon(r))\, e^{ikr}}$$

we can show that

$$\underline{\underline{\rho(r)}} = \frac{\beta}{(2\pi)^2} \frac{1}{r} \frac{d}{dr} \frac{1}{r} \frac{d}{dr} \int_{-\infty}^{\infty} dk \cos(k-r)\, f'\left(\beta\left(\frac{k^2}{r} - \eta\right)\right)$$

At low T : $f' \to \delta$ range of $\rho \nearrow$

At $T=0$: $\rho(r) = \frac{k_F^3}{2\pi^2}\left(\frac{3\sin(k_F r) - \# \cos(k_F r)}{(k_F r)^3}\right)$



Friedel oscillations

decrease the probability of finding particles

- Hartree approximation :

$\hookrightarrow$ Rayleigh - Ritz variational principle

$\langle\psi|H|\psi\rangle \geq E_0$ $\quad\quad$ $\langle\psi|\psi\rangle = 1$

$\uparrow$ any wavefunction

Hartree : construct a N - particle wave function as a product of single particle wave functions :

$$\psi(r_1 \text{——} r_N) = \varphi_{\alpha_1}(r_1) \text{——} \varphi_{\alpha_N}(r_N)$$

Determine the choice of the particle wave function to minimize the Hamiltonian : $\langle\psi|H|\psi\rangle$

$\Rightarrow$ Eq. that determine φ_{α_1} : Hartree equation.

$$T\psi + V_{ext}\psi + \int dr' \frac{e^2 n(r')}{|r - r'|}\psi = E\psi$$

Hartree term and positive background terms cancel each other

$\to$ Hartree - Fock : trial wave function should fulfill Pauli principle $\xrightarrow{\text{planes wave}}$

$\Rightarrow$ Trial wave func = Slater det.

Hartree - Fock eq:

$$\underbrace{h\psi}_{\substack{\uparrow \\ \text{Hartree}}} - \underbrace{\text{Fock term}}_{\substack{\downarrow \\ \text{"exchange"}}} = \varepsilon\psi$$

} Plane waves stays eigenfunctions in the Electron gas case.

Eigenvalues E_k