Electrons

non-interacting free e^--gas.

Last time: free → scattering e-p, e-i

interacting → e-e-scattering → pauli

Non-interacting: coulomb interaction, response effect.

1. hartree-fock approach. → not now
2. screening
3. strong interactions.

Screening (Thomas-Fermi).

first page 2

~~Free~~

One electron, taking potential $\phi(\bar{r})$ into account.
let's assume a test charge $+e$ $\Rightarrow \rho(r) = \rho_t(r) + \rho^{ind}(r)$.

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(r) - e\,\phi(\bar{r})\,\psi_i(r) = \varepsilon_i\,\psi_i(r)$$

if $\phi(r)$ slowly varying then for ε_i

$$\varepsilon = \frac{\hbar^2 k^2}{2m} - e\,\phi(r).$$ (i.e. energy shifted by pot. E).

valid for spatial variation of $\phi(r)$ smaller than $1/k_F$ (which is ~ spread of wave packet @ k_F).

charge density is then.

$$\rho(r) = -e\int \frac{d\bar{k}}{4\pi^3}\cdot\frac{1}{e^{\beta[\varepsilon_k - e\phi(r) - \mu]}+1}$$

(for $\phi(r)=0 \Rightarrow \rho_0(k)$: normal charge density).

→ page 3

Screening

test charge +e ($\rho_T(r)$.) will change electron density electron gas. $\Rightarrow \rho(r) = \rho_t(r) + \rho_{ind}(r)$ A

potential of only test charge:

poisson eq. $\nabla^2 \phi_t(r) = -4\pi \rho_t(r)$. B

for total charge distr. also poisson

$$\nabla^2 \phi(r) = -4\pi \rho(r). \quad \text{C}$$

assume that $\phi_t(r)$ and "response" $\phi(r)$ are related. by diel. response like relation

$$\phi_t(r) = \int dr' \, \varepsilon(r, r') \, \phi(r') = \int dr' \, \varepsilon(r-r') \, \phi(r')$$

FT $\Rightarrow$ $\phi_t(q) = \varepsilon(q) \, \phi(q)$. (convol. theorem).

with $\varepsilon(q) = \int dr \, e^{-iqr} \varepsilon(r)$.

$\varepsilon(r) = \frac{1}{(2\pi)^3} \int dq \, e^{iqr} \varepsilon(q)$.

so total pot.

D $\quad \phi(q) = \frac{1}{\varepsilon(q)} \cdot \phi_t(q)$.

also $\rho_{ind}(q) = \chi(q) \cdot \phi(q)$. E

FT's of poisson eqn^s:

B $\quad q^2 \phi_t(q) = 4\pi \rho_t(q)$.

C $\quad q^2 \phi(q) = 4\pi \rho(q)$.

A $\quad \rho(q) = \rho_t(q) + \rho_{ind}(q)$

D $\quad \phi(q) = \frac{1}{\varepsilon(q)} \phi_t(q)$.

$$\frac{q^2}{4\pi} \left(\phi(q) - \phi_t(q) \right) = \chi(q) \phi(q)$$

or

$$\phi(q) = \frac{\phi_t(q)}{1 - \frac{4\pi}{q^2} \chi(q)}$$

and $\varepsilon(q) = \frac{\phi_t(q)}{\phi(q)} = 1 - \frac{4\pi}{q^2} \chi(q) = 1 - \frac{4\pi}{q^2} \frac{\rho_t(q)}{\phi(q)}$

induced charge density is then.

$$\rho^{ind}(r) = \rho(r) - \rho_0$$

$$= \rho_0(\mu + e\phi(r)) - \rho_0(\mu).$$

assume $\phi(r)$ small. then.

$$\rho^{ind}(r) = e\frac{\partial\rho_0}{\partial\mu}\phi(r). \qquad \text{("taylor")}.$$

from E $\chi(q) = \frac{\rho_{ind}(q)}{\phi(q)}$ $\Rightarrow$ $\chi(q) = e\frac{\partial\rho_0}{\partial\mu}$ indep of q!

using $\varepsilon(q) = 1 - \frac{4\pi}{q^2}\chi(q)$ we have.

$$\varepsilon(q) = 1 - \frac{4\pi e}{q^2}\frac{\partial\rho_0}{\partial\mu} \equiv 1 + \frac{k_0^2}{q^2}.$$

$$\left(k_0^2 = -4\pi e\frac{\partial\rho_0}{\partial\mu}\right).$$

<u>illustration</u> point charge response.

$$\phi_t(r) = \frac{Q}{r} \qquad \phi_t(q) = \frac{4\pi Q}{q^2}.$$

D total potential in metal $\phi(q) = \frac{1}{\varepsilon(q)}\cdot\phi_t(q) = \frac{4\pi Q}{q^2 + k_0^2}$

FT of $\phi(q)$:

$$\phi(r) = \int\frac{dq}{(2\pi)^3}e^{i\bar{q}\bar{r}}\frac{4\pi Q}{q^2+k_0^2} = \frac{Q}{r}e^{-k_0 r}.$$

So ~~the~~ charge is screened, potential drops faster than $\frac{1}{r}$ with length scale k_0^{-1}: thomas-fermi screening length.

plug in numbers to find that $k_0^{-1} \lesssim 1\,\text{Å}$, i.e. approx inter particle distance!!

Lindhard theory of screening

- not assuming $\phi(r)$ varies slow

then
$$\chi(q) = -e^2 \int \frac{dk}{4\pi^3} \, \frac{f_{k-\frac{1}{2}q} - f_{k+\frac{1}{2}q}}{\hbar^2 \bar{k}\cdot\bar{q}/m} \quad (F)$$

derived by calculating $\rho^{ind}(r)$ using perturbation theory (1^{st} order, calculate $\psi \to \rho = \sum_k f_k |\psi_k|^2 = \rho^0 + \rho^{ind}$).

~~q=0~~ for $q \approx 0 \Rightarrow$ Thomas Fermi result.

for $q \neq 0 \Rightarrow$ perform integral (F)

$$\text{at } T=0: \quad \chi(q) = -e^2 \left(\frac{m k_F}{\hbar^2 \pi^2}\right) \left[\frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| \right]$$

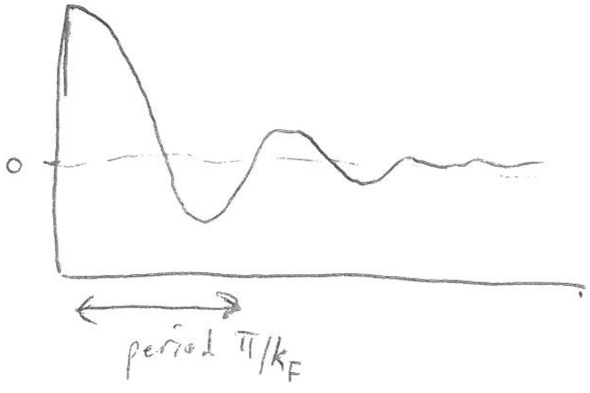
$$\text{with } x = \frac{q}{2k_F}$$

(again $x=0 \Rightarrow$ Thomas-Fermi result).

point charge response more complicated.
for large r:

$$\phi(r) \sim \frac{1}{r^3} \cos 2k_F r \quad \longrightarrow \text{friedel oscill. in charge density.}$$

decays more slowly than Thomas Fermi.



$\Rightarrow$ remember RKKY !!