What is effect of interactions? Screening!

PT65

Mobile charges in metal move around, in such a way as to screen (reduce effect of) the external potential. Simplest treatment of this effect: Hartree approximation. External potential changes density, and therefore also $v_H(1)$. Thus, each particle feels $U(1) + v_H(1)$, where v_H includes effect of other particles, that cause screening.

Explicit derivation:

Use eq. (57.1), with $h_0(1) \to h_0(1) + U(1)$, and only Hartree term:

$$\left(-\partial_{\tau_1} - h_0(1) - U(1)\right) \underset{(\mathcal{G}^{(0)}+\mathcal{G}^{(1)})}{\mathcal{G}(1,2)} \overset{(57.1)}{=} \delta(1,2) + \underset{(\mathcal{G}^{(0)}+\mathcal{G}^{(1)})}{\mathcal{G}(1,2)} \overbrace{\int d1'\, v(1,1')\,(-\xi)\, \mathcal{G}(1',1'_+)}^{v_H(1)} \qquad (1)$$

$$(v^{(0)} + v^{(1)})$$

Since we seek linear response to $U(1)$, linearize (1) in $U(1)$, by writing:

$$\mathcal{G}(1,2) = \mathcal{G}^{(0)}(1,2) + \mathcal{G}^{(1)}(1,2) \qquad (2)$$

$$v_H(1) = \underbrace{v_H^{(0)}(1)}_{\text{0th order}} + \underbrace{v_H^{(1)}(1)}_{\text{1st order}} \quad \text{in } U(1) \qquad (3)$$

Insert (65.2,3) into (65.1): $\mathcal{G}^{(0)}$ satisfies standard Hartree equation in absence of potential:

PT66

$$\left[-\partial_{\tau_1} - h_0(1) - v_H^{(0)}(1)\right] \mathcal{G}^{(0)}(1,2) = \delta(1,2) \qquad (1)$$

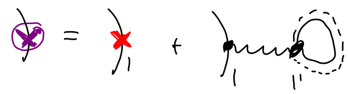
$$v_H^{(0)}(1) = \int d1'\, v(1,1')\,(-\xi)\, \mathcal{G}^{(0)}(1',1'_+) \qquad (2)$$

$\mathcal{G}^{(1)}$ satisfies:

$$\left[-\partial_{\tau_1} - h_0(1) - v_H^{(0)}(1)\right] \mathcal{G}^{(1)}(1,2) =$$

$$\mathcal{G}^{(0)}(1,2) \underbrace{\left[U(1) + \int d1'\, v(1,1')\,(-\xi)\, \mathcal{G}^{(1)}(1',1'_+) \right]}_{} \qquad (3)$$

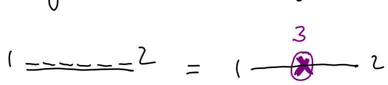
$$\equiv U_{\text{eff}}(1) = \qquad (4)$$



$\leftarrow$ denotes $\mathcal{G}^{(1)}$

Integrate (3), using solution of (2):

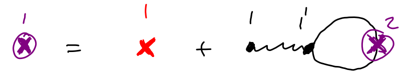
$$\mathcal{G}^{(1)}(1,2) = \int d3\, \mathcal{G}^{(0)}(1,3)\, U_{\text{eff}}(3)\, \mathcal{G}^{(0)}(3,2) \qquad (5)$$

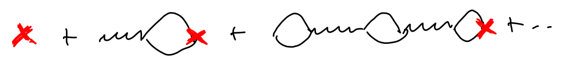


(6)

PT67

$$U_{eff}(1) \overset{(66.6)\text{ into }(66.4):}{=} U(1) + \int d1'\, v(1,1')\, \underbrace{(-\xi)\int dz\, G_0(1',2)\, G_0(2,1'^{+})\, U_{eff}(2)}_{=\,\delta\rho(1)\ \text{see (5), below}} \qquad (1)$$

U_{eff} =  (2)

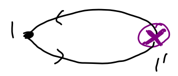
iterate: =  (3)

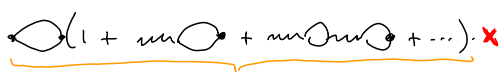
Sum of chains of bubble diagrams ≡ "RPA approximation"

Note that linear response of density can be expressed in terms of $G^{(1)}$, too:

In general: $\langle \hat\rho(1)\rangle = \langle \hat\psi^{\dagger}(1_{+})\, \hat\psi(1)\rangle = -\xi\, G(1,1^{+})$ (4)

expand to linear order in $U(1)$: $\delta\rho(1) \overset{(65.2)}{=} (-\xi) G^{(1)}(1,1^{+}) \overset{(66.5)}{=} \int dz\, G_0(1,2)\, U_{eff}(2)\, G^{0}(2,1^{+})$ (5)

$\overset{(5)}{=}$  (5)

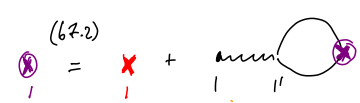
$\overset{(3)}{=}$ 

this is of the form of (63.5): $\equiv \int dz\, G^{RPA}_{\rho\rho}(1,2)\, U(2)$

"RPA for density response" is obtained by summing up chains of bubbles (6)

Explicit evaluation of U_{eff} (Rickayzen, § 5.2(6))

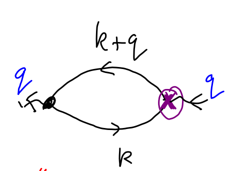
PT68

$U_{eff}(1) \overset{(67.1)}{=} U(1) + \int d1'\, v(1,1')\, \delta\rho(1')$  (1)

Fourier- and Matsubara-transform: $U(1) = U(\vec r,\tau) = \sum_{(q)} e^{-i\omega_n\tau}\, e^{i\vec q\cdot\vec r}\, U(q)$ (2)

$q \equiv (i\omega_m, \vec q)$, $\sum_{(q)} \equiv \underbrace{\frac{1}{Vol}\sum_{\vec q}\frac{1}{\beta}\sum_{\omega_n}}_{=\int d(q)}$, $x \equiv (\tau,\vec x)$, $q\cdot x = \omega_n\tau - \vec q\cdot\vec x$ (3)

$$U_{eff}(q) \overset{(1)}{=} U(q) + v(q)\,\delta\rho(q) \qquad (4)$$

$\delta\rho(q) \overset{(67.5)}{=} (-\xi) G^{(1)}(q) \overset{(66.5)}{=} \underbrace{2\sum_{(k)} G_0(k)\, G_0(k+q)}\, U_{eff}(q)$  (5)

spin sum

$\equiv \chi(q)$ = "Polarisation bubble" (6)

(5) into (4): $U_{eff}(q) = U(q) + v(q)\,\chi(q)\, U_{eff}(q)$ (7)

solve: $= \dfrac{U(q)}{1 - v(q)\chi(q)} \equiv \dfrac{U(q)}{\varepsilon(q)}$ "dielectric constant" (8)

Details of Fourier transform leading to (68.6): $\boxed{PT69}$

$$\delta\rho(q) = \int d\vec{r}_1 \int_0^\beta d\tau_1 \; \delta\rho(1)\, e^{iq\cdot x_1} \quad (1)$$

$$= \int d1 \int d2 \; \mathcal{G}_0(1,2)\, \mathcal{U}_{eff}(2)\, \mathcal{G}^0(2,1^+)\, e^{iq\cdot x_1} \quad (2)$$

$$= \sum_{(k)} \sum_{(k')} \sum_{(k'')} \mathcal{G}_0(k)\, \mathcal{U}_{eff}(k')\, \mathcal{G}_0(k'') \quad (3)$$

$$\underset{\text{spin}}{\times 2} \int d1 \int d2 \; e^{-ik\cdot(x_1-x_2)}\, e^{-ik'\cdot x_2}\, e^{-ik''(x_2-x_1)}\, e^{iq\cdot x_1} \quad (4)$$

$$\beta\cdot Vol\; \delta_{0,k-k''-q} \quad Vol\; \delta_{0,k-k'-k''} \implies k' = k-k'' = q \quad (5)$$

$$= 2 \sum_{(k'')} \mathcal{G}_0(k''+q)\, \mathcal{U}_{eff}(q)\, \mathcal{G}_0(k'') \quad (6)$$

For Coulomb potential: $v(q) = v(i\omega_n,\vec{q}) = \int d\vec{r}_1 \int d\tau_1\, e^{iq\cdot x_1} \dfrac{e^2}{|\vec{r}_1|\varepsilon_0}\, \delta(\tau_1)$ (7) {bare dielectric constant

$$= \frac{e^2}{q^2\varepsilon_0} \quad \text{(check yourself)} \quad (8)$$

<u>Evaluation of Polarisation bubble</u> (Rickayzen, §5.2) $\boxed{PT70}$

$$\chi(q) \overset{(68.6)}{=} 2\sum_{(k)} \mathcal{G}_0(k)\, \mathcal{G}_0(k+q) \qquad \begin{aligned} q &\equiv (i\omega_m, \vec{q}) \\ k &\equiv (i\omega_n, \vec{k}) \end{aligned} \quad (1)$$

$$= 2 \int d(k)\, \frac{1}{\beta}\sum_m \frac{1}{i\omega_n - \varepsilon_{\vec{k}}} \; \frac{1}{i\omega_m + i\omega_n - \varepsilon_{\vec{k}+\vec{q}}} \quad (2)$$

(GF68.7) with $\omega \to \varepsilon_{\vec{k}}$, $\omega' \to \varepsilon_{\vec{k}+\vec{q}}$

$$\chi(q) = (-\zeta)\, 2\int d(k)\, \frac{n_\zeta(\varepsilon_{\vec{k}}) - n_\zeta(\varepsilon_{\vec{k}+\vec{q}})}{i\omega_m - \varepsilon_{\vec{k}+\vec{q}} + \varepsilon_{\vec{k}}} \quad (3)$$

= { "Lindhardt-Formula for polarizability"

[see also problem set 4 on "density response"]

Analytic continuation: $i\omega_m \to \omega + i0^+$:

$\vec{k} \leftrightarrow -(\vec{k}+\vec{q})$

$$\chi^R(\omega,\vec{q}) = (-\zeta)\int d(k) \left[\frac{n_\zeta(\varepsilon_{\vec{k}}) - n_\zeta(\varepsilon_{\vec{k}+\vec{q}})}{\omega + i0^+ - \underbrace{(\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}})}_{\equiv \Delta_{\vec{k},\vec{q}}}} + \frac{n_\zeta(\varepsilon_{\vec{k}+\vec{q}}) - n_\zeta(\varepsilon_{\vec{k}})}{\omega + i0^+ \underbrace{- \varepsilon_{\vec{k}} + \varepsilon_{\vec{k}+\vec{q}}}_{\equiv \Delta_{\vec{k},\vec{q}}}} \right] \quad (4)$$

$$\frac{1}{\omega-\Delta} - \frac{1}{\omega+\Delta} = \frac{2\Delta}{\omega^2-\Delta^2}$$

$$= \underbrace{(-\zeta)}_{=1 \text{ for fermions, hence forth}} \int d(k) \left[n_\zeta(\varepsilon_{\vec{k}}) - n_\zeta(\varepsilon_{\vec{k}+\vec{q}}) \right] \left\{ \frac{2\Delta_{\vec{k},\vec{q}}}{\omega^2 - \Delta_{k,q}^2} \right\} \quad (5)$$

PT71

In limit $\vec{q} \to 0$, $\Delta_{\vec{k},\vec{q}} \ll \omega$:

rewrite: $\vec{k}+\vec{q} \to \vec{k}$, to get factor 2

$$\chi(\omega,\vec{q}) \simeq \frac{2}{\omega^2}\int d(k) \left[n_\xi(\varepsilon_{\vec{k}}) - n_\xi(\varepsilon_{\vec{k}+\vec{q}})\right]\left[\varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}\right] \quad (1)$$

$$= \frac{2}{\omega^2}\int d(k)\, n_\xi(\varepsilon_{\vec{k}})\left[\frac{1}{2m}\left[(\vec{k}+\vec{q})^2 - \vec{k}^2\right] + \frac{1}{2}\left[(\vec{k}-\vec{q})^2 - \vec{k}^2\right]\right] \quad (2)$$

$$= \frac{2}{\omega^2}\frac{\vec{q}^2}{2m}\, 2 \underbrace{\int d(k)\, n_\xi(\varepsilon_k)}_{\rho_0 = \text{density per spin species.}} \quad (3)$$

So, dielectric constant $$\varepsilon(\omega,\vec{q}) \overset{(68.8)}{=} 1 - \underbrace{v(q)}_{(69.8)\ =\ \frac{e^2}{\varepsilon_0 \vec{q}^2}} \chi(\omega,\vec{q}) \quad (4)$$

reduces to $$\varepsilon(\omega,0) = 1 - \left(\frac{e^2}{\varepsilon_0 \cancel{\vec{q}^2}}\right)\left(\frac{2\cancel{\vec{q}^2}}{m\omega^2}\rho_0\right) \equiv 1 - \left(\frac{\omega_{p0}}{\omega}\right)^2 \quad (5)$$

with plasma frequency: $$\omega_{p,0} \equiv \left(\frac{e^2 \cdot 2\rho_0}{\varepsilon_0 m}\right)^{1/2} \quad (6)$$

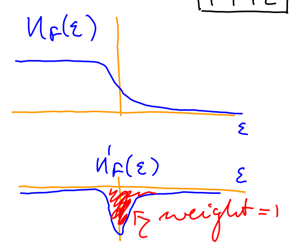
At $\omega = \omega_{p,0}$, $\varepsilon(\omega,0)$ vanishes, hence response diverges: $$U_{eff}(\omega,0) \overset{(68.8)}{=} \frac{U(\omega,0)}{\varepsilon(\omega,0)} \to \infty \quad (7)$$

Divergent response at $\omega = \omega_{p,0}$, $\vec{q} \to 0$, is called "plasma resonance".

PT72

Static limit at long wavelengths: ($\omega = 0$, $q \to 0$)

$$\chi(0,\vec{q}) \overset{(70.5)}{=} 2 \underbrace{\int d(k)}_{\int d\varepsilon_k N(\varepsilon_k)} \underbrace{\frac{n_\xi(\varepsilon_{\vec{k}}) - n_\xi(\varepsilon_{\vec{k}+\vec{q}})}{\varepsilon_{\vec{k}} - \varepsilon_{\vec{k}+\vec{q}}}}_{\xrightarrow{\vec{q}\to 0}\ \frac{\partial n(\varepsilon_{\vec{k}})}{\partial \varepsilon_{\vec{k}}}} = -2 \underbrace{N(\mu)}_{\text{density of states per spin at } \varepsilon=\mu=\varepsilon_F} \quad (1)$$



since $$\frac{\partial n_F(\varepsilon_k)}{\partial \varepsilon_k} \simeq \frac{\partial}{\partial \varepsilon_k}\left(\frac{1}{e^{\beta(\varepsilon_k-\mu)}+1}\right) = -\beta\frac{e^{\beta(\varepsilon_k-\mu)}}{(e^{\beta(\varepsilon_k-\mu)}+1)} \simeq -\delta(\varepsilon_k-\mu) \quad (2)$$

for $T \ll \mu$

$$\varepsilon(\omega=0,\vec{q}\to 0) \overset{(68.8)}{=} 1 - v(q)\,\chi(\omega=0,\vec{q}\to 0) = 1 + 2\underbrace{v(q)}_{(69.8)}\underbrace{N(\mu)}_{(73.3)} \quad (3)$$

$$\xrightarrow{q\to 0} 1 + \frac{1}{\vec{q}^2}\underbrace{\left(\frac{e^2 m k_F}{\varepsilon_0 \pi^2}\right)}_{\equiv k_0^2} = 1 + \frac{k_0^2}{\vec{q}^2} \quad (4)$$

$1/k_0$ = "Thomas-Fermi screening length"

Elementary relations for free electron gas (Ashcroft & Mermin, Ch. 2) $\boxed{PT73}$

Density of states per spin, $\mathcal{N}(\varepsilon)$:

$$\int d(k) = \frac{1}{(2\pi)^3} \overbrace{\int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta)}^{=4\pi} \int_0^\infty dk\, k^2$$

$$= \int_{-\varepsilon_F}^{\infty} d\varepsilon \underbrace{\frac{1}{2\pi^2} m\sqrt{2m\varepsilon}}_{\equiv \mathcal{N}(\varepsilon)} d\varepsilon \qquad (1)$$

$$k^2 = 2m\,\varepsilon_p$$

$$2\, dk\, k = 2m\, d\varepsilon$$

$$dk\, k^2 = m\sqrt{2m\varepsilon}\, d\varepsilon$$

$$\mathcal{N}(\varepsilon_F) = \frac{m k_F}{2\pi^2} \qquad (2)$$

Density per spin: $$\rho_0 = \frac{N}{Vol} = \frac{1}{Vol}\sum_{|k|<k_F} = \int_{|k|<k_F} d(k) = \frac{4\pi}{(2\pi)^3}\int_0^{k_F} dk\, k^2 = \frac{1}{(2\pi)^3}\frac{4\pi}{3}k_F^3 = \frac{k_F^3}{6\pi^2} \qquad (3)$$

$$= \mathcal{N}(\varepsilon_F)\cdot\frac{k_F^2}{3m} = \frac{2}{3}\mathcal{N}(\varepsilon_F)\cdot\varepsilon_F \qquad (4)$$

$$\mathcal{N}(\varepsilon_F) = \frac{3}{2}\frac{\rho_0}{\varepsilon_F} = \frac{3\rho_0 m}{k_F^2} \qquad (5)$$

Suppose that the external applied potential was a Coulomb potential, $\boxed{PT74}$

$$U(1) = U(\vec{r}_1) = \frac{e^2}{\varepsilon_0|\vec{r}_1|}, \quad \text{with } \; u(\omega,\vec{q}) \overset{(69.8)}{=} \frac{e^2}{\varepsilon_0|\vec{q}|^2} \qquad (1)$$

Then the screened Coulomb potential is given by:

$$U_{eff}(\vec{q}) \overset{(68.8)}{=} \frac{u(\omega=0,\vec{q})}{\varepsilon(\omega=0, q\to 0)} \overset{(72.5)}{=} \frac{e^2}{\varepsilon_0 q^2}\,\frac{1}{1+k_0^2/q^2} = \frac{e^2/\varepsilon_0}{q^2+k_0^2} \qquad (2)$$

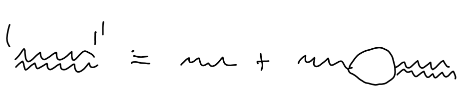
Screened Coulomb potential in real space:

$$U_{eff}(r_1) = \int (dq)\, e^{i\vec{q}\cdot\vec{r}}\, U_{eff}(\vec{q}) = \frac{e^2}{\varepsilon_0|\vec{r}|} e^{-|\vec{r}|k_0} \qquad (3)$$

← {Yukawa potential!

Thus, screening causes the range of the potential to be cut off at the Thomas-Fermi screening length.

Same will be true for Coulomb interaction!



$$= \underset{\text{screened}}{V(\vec{r}_1-\vec{r}_1')} = \frac{e^2\, e^{-|\vec{r}_1-\vec{r}_1'|k_0}}{\varepsilon_0|\vec{r}_1-\vec{r}_1'|} \qquad (4)$$