Lectures 19-20

Impurities in metals – screening.

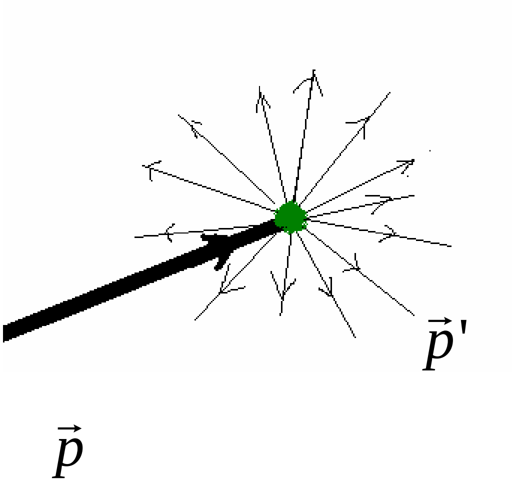
Friedel oscillations in metal.

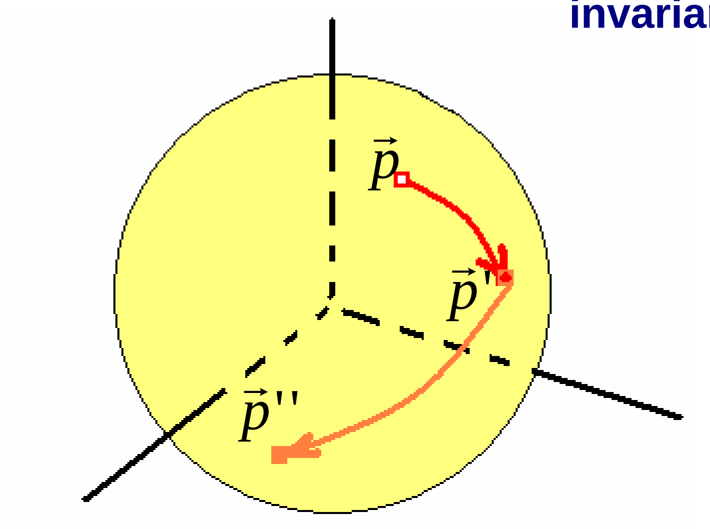
**Friedel oscillations in quantum wires;
the effect of electron-electron interaction
on the impurity scattering in a wire.**

Impurity scattering

$$H=\sum_i \frac{m}{2}\dot{\vec{r}}_i^{\,2}+\sum_{i\neq j}\frac{e^2/\chi}{2|\vec{r}_i-\vec{r}_j|}+\sum_i^{n-imp}u(\vec{r}_i-\vec{X}_n)$$

violates translational invariance





Impurity scattering may transfer the momentum taken from the electrons accelerated by an electric field to the lattice into which they are incorporated.

Quantum mechanics: Born approximation for the impurity scattering:

$$w_{\vec{p}\to\vec{p}\,'}=\frac{2\pi}{\hbar}\cdot\left|\langle\vec{p}\,|\sum_n u(\vec{r}-\vec{X}_n)\,|\,\vec{p}\,'\rangle\right|^2\delta(\varepsilon(\vec{p})-\varepsilon(\vec{p}\,'))$$

$$\left|\langle\vec{p}\,|\sum_n u(\vec{r}-\vec{X}_n)\,|\,\vec{p}\,'\rangle\right|^2=\left|\int d\vec{r}\,\frac{e^{i\vec{r}\cdot(\vec{p}-\vec{p}\,')/\hbar}}{L^d}\sum_n u(\vec{r}-\vec{X}_n)\right|^2$$

after averaging over X_n

$$=\sum_{n,m}\frac{e^{i(\vec{X}_n-\vec{X}_m)\cdot(\vec{p}-\vec{p}\,')}}{L^d}\left|\int d\vec{r}\,e^{i\vec{r}\cdot(\vec{p}-\vec{p}\,')}u(\vec{r})\right|^2\approx\frac{N_{imp}}{L^d}\,|u_{\vec{p}-\vec{p}\,'}|^2=n_{imp}\,|u_{\vec{p}-\vec{p}\,'}|^2$$

Models for impurity scattering

$$w_{\vec{p}\to\vec{p}'} = n_{imp}\frac{2\pi}{\hbar}\cdot|u_{\vec{p}-\vec{p}'}|^2\,\delta(\varepsilon(\vec{p})-\varepsilon(\vec{p}'))$$

$$u_{\vec{p}-\vec{p}'} = \int d\vec{r}\cdot e^{i\vec{r}(\vec{p}-\vec{p}')/\hbar}u(\vec{r})$$

δ **- scatterer** $$u(\vec{r}) = u\cdot\delta(\vec{r})$$

$$u_{\vec{p}-\vec{p}'} = \int d\vec{r}\cdot e^{i\vec{r}(\vec{p}-\vec{p}')/\hbar}u\cdot\delta(\vec{r}) = u$$

results in the isotropic scattering (independent of the angle θ**)**

$$\varepsilon(\vec{p}) = \varepsilon(\vec{p}') \approx \varepsilon_F \Rightarrow p = p' \approx p_F \qquad \cos\theta = \frac{\vec{p}\cdot\vec{p}'}{p_F^2}$$

$$w_{\vec{p}\to\vec{p}'} = n_{imp}\frac{2\pi}{\hbar}\delta(\varepsilon(\vec{p})-\varepsilon_F)\cdot u^2$$

For an arbitrary scatterer

$$w_{\vec{p}\to\vec{p}'} = n_{imp}\frac{2\pi}{\hbar}\cdot|u_{\vec{p}-\vec{p}'}|^2\,\delta(\varepsilon(\vec{p})-\varepsilon(\vec{p}'))$$

$$\Downarrow$$

$$w(\theta) = n_{imp}\frac{\pi\gamma_F}{\hbar}|u(\theta)|^2$$

underlying Coulomb impurity,

$$u_C(\vec{r}) = \frac{e^2/\chi}{r} \Leftrightarrow \nabla^2 u_C = -4\pi \frac{e^2}{\chi}\delta(\vec{r})$$

(excessively charged ions: 'donors' and 'acceptors')
χ is the dielectric constant of the medium.

Actual scattering potential $u(\vec{r})$ is formed both by the charge of the ion and by the cloud of electrons attracted to that ion.

Tomas-Fermi screening in the random phase aproximation

$$\nabla^2 u = -4\pi \frac{e^2}{\chi}\left[\delta(\vec{r}) + \delta n_e(\vec{r})\right] \qquad n_e(\vec{r}) = n_e + \delta n_e(\vec{r})$$

Screening cloud is formed as the equilibrium re-distribution of electron density:

$$\varepsilon_F(\vec{r}) + u(\vec{r}) = \varepsilon_F + \delta\varepsilon_F(\vec{r}) + u(\vec{r}) = \varepsilon_F$$

$$\varepsilon_F \sim \frac{\hbar^2\, n_e^{2/d}}{m} \Rightarrow \delta\varepsilon_F(\vec{r}) \sim \frac{\hbar^2/m}{n_e^{1-2/d}}\delta n_e(\vec{r}) = \frac{\delta n_e(\vec{r})}{\gamma_F}$$

$$\gamma_F \sim \frac{m n_e^{1-2/d}}{\hbar^2}$$

$$u(\vec{r}) = -\delta\varepsilon_F(\vec{r}) = -\frac{\delta n_e(\vec{r})}{\gamma_F} \Rightarrow \underline{\delta n_e(\vec{r}) = -\gamma_F u(\vec{r})}$$

Self-consistency equation for the screened impurity potential:

$$\nabla^2 u = -4\pi \frac{e^2}{\chi}\left[\delta(\vec{r}) - \gamma_F u(\vec{r})\right]$$

$$\left[\nabla^2 - \frac{4\pi e^2}{\chi}\gamma_F\right]u(\vec{r}) = -4\pi\frac{e^2}{\chi}\delta(\vec{r})$$

Analysis in the bulk (3D) of a metal using the Fourier transform

$$u_{\vec{q}} = \int d\vec{r}e^{i\vec{q}\cdot\vec{r}}u(\vec{r})$$

$$\nabla^2 u(\vec{r}) \Rightarrow -q^2 u_{\vec{q}}$$

$$\left[q^2 + \frac{4\pi e^2\gamma_F}{\chi}\right]u_{\vec{q}} = 4\pi\frac{e^2}{\chi}$$

$$u_{\vec{q}} = \frac{4\pi\frac{e^2}{\chi}}{q^2 + \frac{4\pi e^2\gamma_F}{\chi}} = \frac{\gamma_F^{-1}}{1 + (a_{scr}q)^2}$$

$$a_{scr} \sim \sqrt{\frac{\chi}{4\pi e^2\gamma_F}} \sim \sqrt{\lambda_F a_B}$$

$$a_B = \frac{\chi\hbar^2}{e^2 m}$$

To remind: *q* is the momentum transfer from electron (to the entire crystal – via impurity) in the scattering process, so that

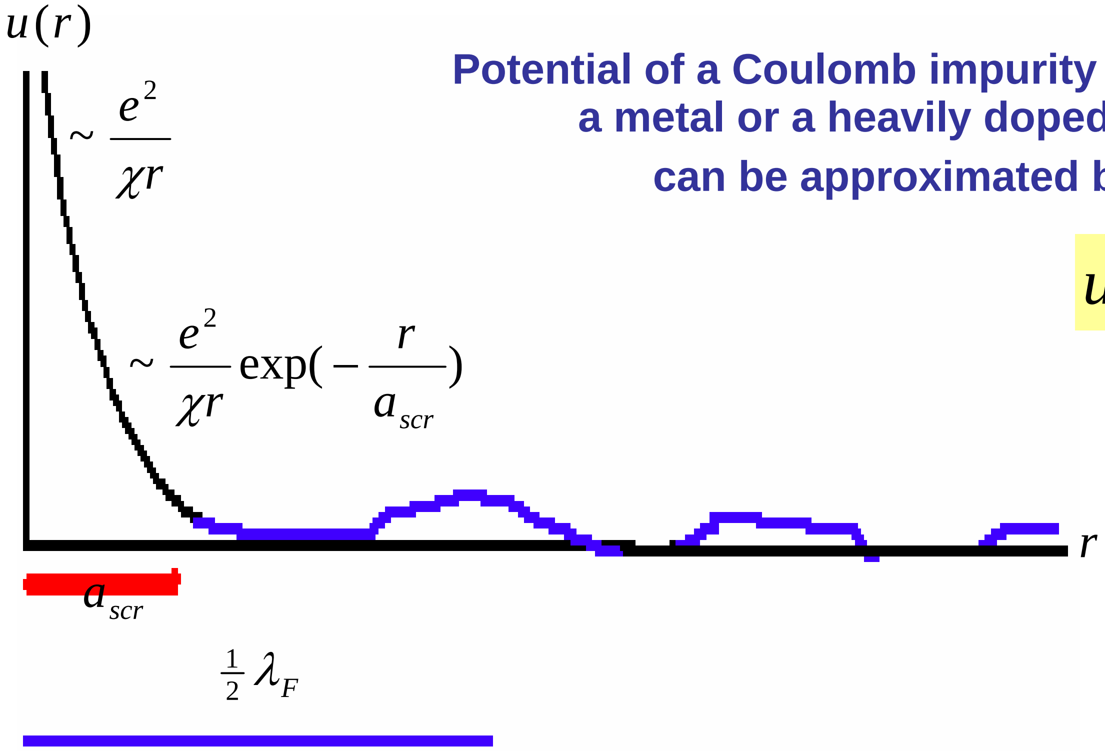
$$q = |\vec{p} - \vec{p}'| = \sqrt{\vec{p}^2 - 2\vec{p}'\vec{p} + \vec{p}'^2} = \sqrt{2p_F^2 - 2p_F^2\cos\theta} = p_F\sin\frac{\theta}{2}$$

For not very high densities, $\lambda_F \sim n_e^{-1/3} << a_B$

$$\frac{p_F^2 a_{scr}^2}{\hbar^2} \sim \frac{1}{\lambda_F^2}\lambda_F a_B = \frac{a_B}{\lambda_F} << 1 \qquad \Rightarrow \qquad u_{\vec{p}-\vec{p}'} \approx \gamma_F^{-1}$$

Potential of a Coulomb impurity (charged ion) in a metal or a heavily doped semiconductor can be approximated by a δ - function

$$u(\vec{r}) \approx \gamma_F^{-1}\delta(\vec{r})$$



Friedel oscillations of screening electron density

Electrons involved into screening are standing waves with zeros at the position of impurity.

$$\lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{p}$$

Therefore, the electron density around impurity slightly oscillates (as the function of the distance to it) with the wave number $2k_F$, so that the screened potential oscillates, too:

$$n_{Friedel}(r) = \frac{\sin(2k_F r)}{r^d}$$

$$u(\vec{r}) \approx \gamma_F^{-1}\left[\delta(\vec{r}) + u_{\text{int}}\, n_{Friedel}(r)\right]$$

d **- dimensionality (1,2, or 3)**

'Fermi liquid interaction constant'

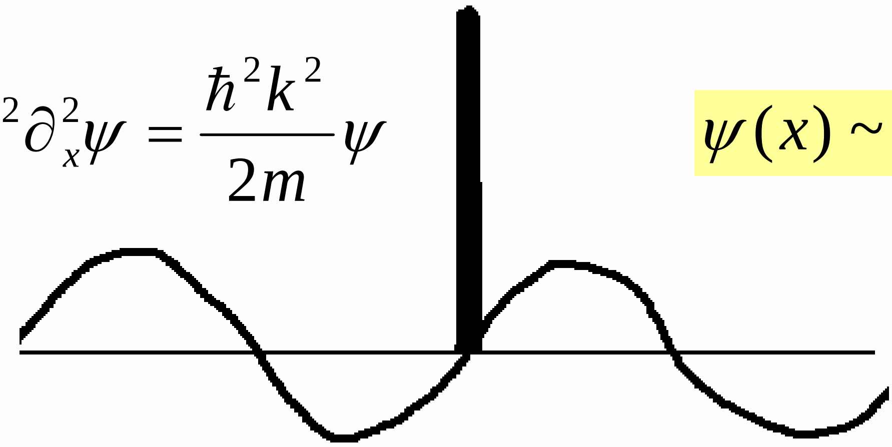
Friedel oscillations in a 1D wire

$$u(x) \approx u\delta(x)$$

$$\psi(0) = 0$$

$$-\hbar^2 \partial_x^2 \psi = \frac{\hbar^2 k^2}{2m}\psi$$

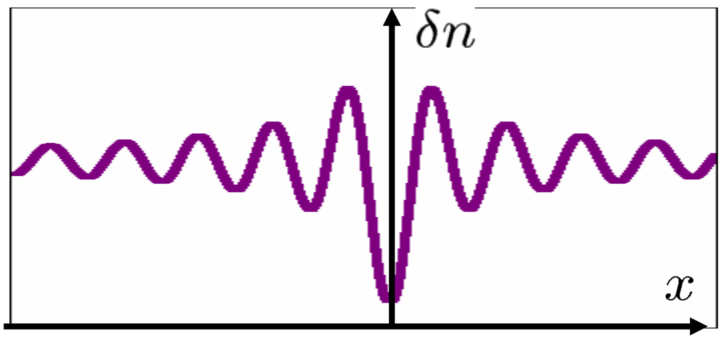
$$\psi(x) \sim \sin kx$$



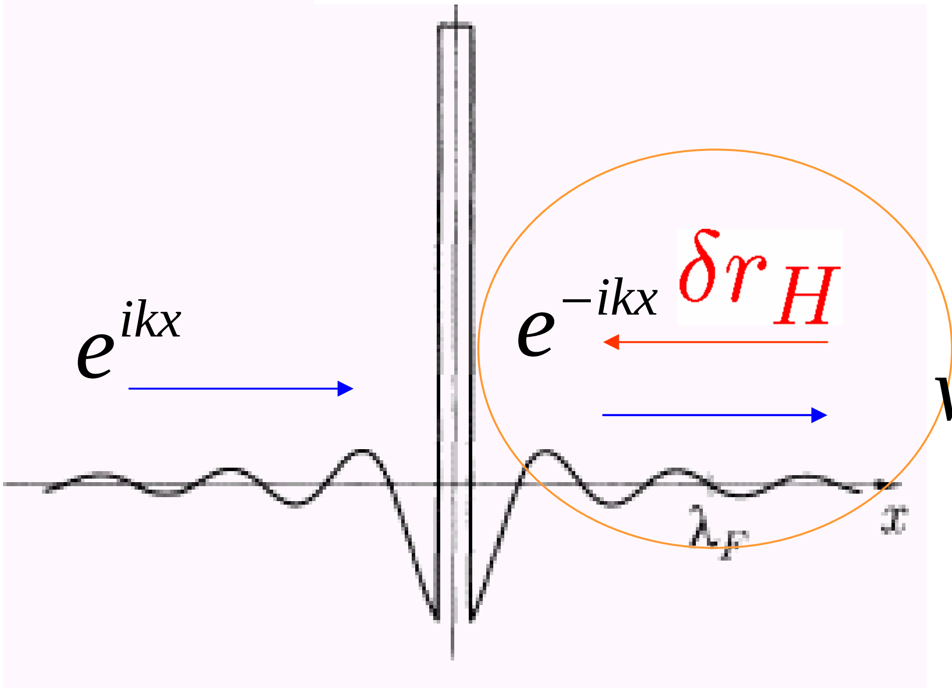
$$n_{screening}(x) = \int_0^{k_F} \frac{dk}{2\pi} \sin^2 kx = \int_0^{k_F} \frac{dk}{2\pi} \tfrac{1}{2}[1 - \cos 2kx]$$

$$= \frac{k_F}{4\pi} - \frac{\sin 2kx}{8\pi x}\Big|_0^{k_F} = \frac{k_F}{4\pi} - \frac{\sin 2k_F x}{8\pi x}$$

$$\delta n_{Friedel}(x) = -\frac{\sin 2k_F x}{8\pi x}$$



$$\delta u(x) = u_{\text{int}} \frac{\sin 2k_F x}{8\pi x}$$



Bragg scattering off a periodic potential

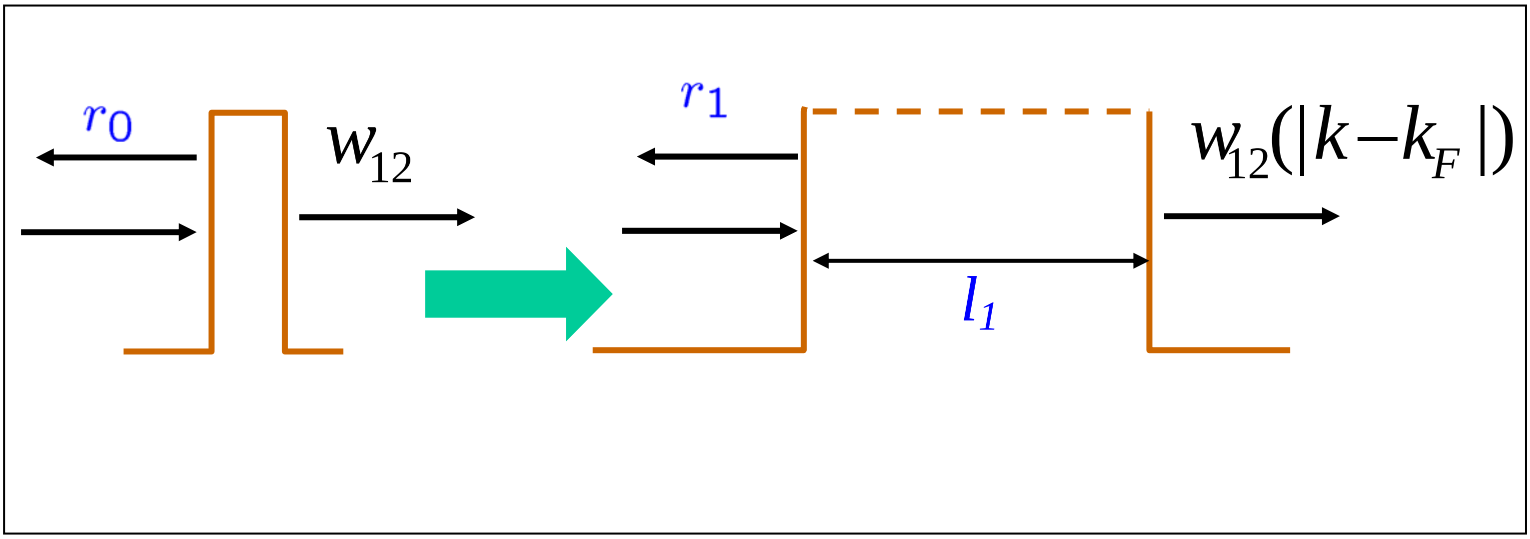
$$w_{12} = 1 - r$$

$$r = w_{k\to -k} = \frac{2\pi}{\hbar} \cdot |u_0 + \delta u_{2k}|^2 \, \delta(\varepsilon(\vec{p}) - \varepsilon(\vec{p}\,'))$$

$$\delta r = u_0 u_{\text{int}} \int dx \frac{\sin 2k_F x}{8\pi x} e^{2ikx} \sim u_0 u_{\text{int}} \ln \frac{1}{|k_F - k|\, d}$$

$$k \to k_F \;\Rightarrow\; w_{12} = 1 - r \to 0$$

Renormalisation of the transmission probability



$$G = \frac{e^2}{h} w_{12}(k \to k_F) \to 0$$

$$\varepsilon \to \varepsilon_F$$

In an infinite wire, linear conductance at zero temperature vanishes in the presence of even one single defect

$$G(T \neq 0) \sim T^{\alpha}$$

Non-linear I(V) characteristics

$$I = \int_{k(\varepsilon_F - eV/2)}^{k(\varepsilon_F - eV/2)} w_{12}(k)\ ev \frac{dk}{2\pi}$$

$$= \frac{e}{h} \int_{\varepsilon_F - eV/2}^{\varepsilon_F - eV/2} w_{12}(|\varepsilon - \varepsilon_F|)\ d\varepsilon \sim\ V^{\alpha+1}$$

Carbon nanotube – another type of 1D electron system