Comment on volume factors (what does $c^2_{imp} \ll c_{imp}$ really mean?)

Dis14

Write $\mathrm{Vol} = v_0 N_\square$ (1)

$N_\square$: # of unit cells; v_0: volume of one unit cell

Total # of electrons: $N_e = z N_\square$ (2)

z: # delocalized electrons per unit cell per spin

per spin $= \sum_{|k|<k_F} = \mathrm{Vol} \int \frac{d^3k}{(2\pi)^3} = \mathrm{Vol}\, \frac{k_F^3}{6\pi^2}$ (3)

Density of states per spin: $\frac{1}{\mathrm{Vol}} \sum_k = \int_0^\infty dk\, k^2 \frac{4\pi}{(2\pi)^3} \int \frac{d\hat{\Omega}_k}{4\pi} = \left(\int \frac{d\Omega_k}{4\pi}\right) \int d\varepsilon\, \nu(\varepsilon)$ (4)

with $\nu(\varepsilon) \overset{(PT\,73.1)}{=} \frac{m^{3/2}\sqrt{2\varepsilon}}{2\pi^2}$ $\qquad \nu(0) k_F^2 = 3\pi\bar{n}$ (5)

$\nu(0) \overset{(5)}{=} \frac{m^{3/2}}{2\pi^2}\sqrt{2\varepsilon_F} = \frac{m k_F}{2\pi^2} = \left(\frac{N_{el}}{\mathrm{Vol}}\right) \frac{3}{2} \frac{1}{\varepsilon_F} \overset{(1,2)}{=} \frac{z N_\square}{v_0 N_\square} \frac{3}{2} \frac{1}{\varepsilon_F} = \frac{3z}{2 v_0 \varepsilon_F}$ (6)

units: [volume · energy]$^{-1}$

What are units of impurity potential?

Dis15

$\sum_i U(\vec{r} - \vec{R}_i)$

$\hat{H}_{imp} = \sum_\sigma \int d\vec{r}\, \hat{\psi}^\dagger_\sigma(\vec{r})\, \hat{\psi}_\sigma(\vec{r})\, U_{imp}(\vec{r})$ (1)

units: energy; volume; 1/volume; energy (2)

$U(\vec{r}) \overset{(2.3)}{=} U_0\, \delta(\vec{r})$, (3)

units: [energy] [energy × volume] [1/volume], (4)

$\hat{U}(\vec{p}) = \int d\vec{r}\, U(\vec{r})\, e^{-i\vec{p}\cdot\vec{r}} = U_0 \equiv v_0 \cdot U_0'$ (5)

units: volume; energy; volume; energy (6)

So, n-th order contribution to $G(i\omega_n, \vec{p})$ (units: energy^{-1}) has the form:

$\frac{1}{t^n} \int d\tau_1 \ldots d\tau_n \int d\vec{r}_1 \ldots d\vec{r}_n \langle U_{imp}(\vec{r}_1) \ldots U_{imp}(\vec{r}_n) \rangle_{imp} \langle (\psi^\dagger\psi)_1 (\psi^\dagger\psi)_2 \ldots (\psi^\dagger\psi)_n \rangle \int \frac{dz}{t} \int d\vec{r} \langle \psi\psi^\dagger \rangle$

[energy]$^{-n}$ [volume]^n [energy]^n [volume]$^{-n}$ [energy]$^{-1}$ [1].

time and volume integrals are used for Matsubara & Fourier transforms of GF: Dis16

$$\frac{1}{(Vol)^n}\sum_{p_1\dots p_n}\tilde{u}(p_1)\dots\tilde{u}(p_n)\left(G_0(i\omega_n,\vec{p})\right)^{n+1} \quad (1)$$

$[\text{volume}]^{-n}$ $[\text{volume}\times\text{energy}]^{n}$ $[\text{energy}]^{-n+1}$ $\sim$ energy^{-1} $\sim$ (2)

Term with m factors of $\langle\rangle_{imp}$:

$$\frac{(N_{imp})^m}{(Vol)^m}\left(\sum_{\vec{p}}\delta_{\vec{p}+\dots,0}\right)^m\left(\frac{1}{Vol}\sum_{p}\right)^{n-m}(\tilde{u})^n\left(G_0(i\omega_n,\vec{p})\right)^{n+1} \quad (3)$$

$$\frac{(N_{imp})^m}{(v_0 N_\square)^m}\left(N(0)\int d\varepsilon\right)^{n-m}(v_0 u_0')^n \sim \left(\frac{N_{imp}}{N_\square}\right)^m\cdot(u_0')^n$$

$\frac{3\pi}{2v_0\varepsilon_F}$ $\equiv (c_{imp})^m$

$$\hat{c}_{imp}\equiv\frac{N_{imp}}{N_\square}\overset{(14.1)}{=}c_{imp}\cdot v_0 = (\#\text{ of impurities per unit cell}) \quad (4)$$

So, $\hat{c}_{imp}\ll 1$ is the dimensionless small parameter evoked when dropping terms of order $\hat{c}_{imp}^{\,m}$, $m\geq 2$ relative to leading term $\sim\hat{c}_{imp}^{\,1}$. (5)

v_0 drops out: $\frac{\hbar}{\tau(\omega)}\overset{(12.5)}{=}2\pi c_{imp}N(\varepsilon_F)\overline{|\tilde{u}_{\vec{k}}|^2}=2\pi\left(\frac{\tilde{c}_{imp}}{v_0}\right)\overset{(4)}{\overset{(14.6)}{\left(\frac{3\pi}{2v_0\varepsilon_F}\right)}}\overset{(15.5)}{(v_0)^2}(u_0')^2$ units: energy ✓ (6)

Back to self-energy: Dis17

$$\Sigma(i\omega_n,\vec{k})\overset{(12.3)}{=}c_{imp}\int d\varepsilon_{p'}N(\varepsilon_{p'})\underbrace{\int\frac{d\Omega_{p'}}{4\pi}|\tilde{u}(\vec{k}-\vec{p}')|^2}_{\equiv\langle|\tilde{u}_k|^2\rangle_{ang}}\frac{1}{i\omega_n-\varepsilon_{\vec{p}'}} \quad (1)$$

angular average

∇ "principle value" integral

$$\left\{\begin{matrix}\text{Re}\\ \text{Im}\end{matrix}\right\}\Sigma^R(\omega,\vec{k})=c_{imp}\int d\varepsilon_{p'}N(\varepsilon_{p'})\langle|\tilde{u}_k|^2\rangle_{ang}\left\{\begin{matrix}\mathcal{P}\frac{1}{\omega-\varepsilon_{p'}}\\ -\pi\,\delta(\omega-\varepsilon_{p'})\end{matrix}\right\} \quad (2)$$

Assume short-ranged impurity potential $u(\vec{r})\overset{(2.3)}{=}u_0\,\delta(\vec{r})$ (3)

$\Rightarrow$ $\tilde{u}_k\overset{(2.4)}{=}u_0=\text{const.}\Rightarrow$ self-energy is $\vec{k}$-independent (4)

How strong is ω-dependence of retarded self-energy?

$$-\text{Im}\,\Sigma^R(\omega)=\pi c_{imp}u_0^2N(0)\left(1+\mathcal{O}(\omega/\varepsilon_F)\right) \quad (5)$$

$\sim$ negligible ...

$$\mathrm{Re}\left[\Sigma^R(\omega) - \Sigma^R(\omega')\right] = c_{imp}\, u_0^2 \int d\varepsilon_{p'}\, N(\varepsilon_{p'}) \times I(\omega, \omega', \varepsilon_{p'}) \tag{1}$$

$$I(\omega,\omega',\varepsilon_{p'}) = P\left[\frac{1}{\omega - \varepsilon_{p'}} - \frac{1}{\omega' - \varepsilon_{p'}}\right] = \frac{\omega' - \omega}{(\omega - \varepsilon_{p'})(\omega' - \varepsilon_{p'})} \sim \frac{1}{\varepsilon_{p'}^2} \quad \text{for } |\varepsilon_{p'}| \gg \omega, \omega' \tag{2}$$

$\Rightarrow$ integral is limited to the range $|\varepsilon_{p'}| \lesssim \omega, \omega'$ (3)

So, we may replace the integral in (1) by

$$\int_{-\infty}^{\infty} d\varepsilon_{p'}\, N(0)\, P\left[\frac{1}{\omega - \varepsilon_{p'}} - \frac{1}{\omega' - \varepsilon_{p'}}\right] \simeq 0 \tag{4}$$

$\Rightarrow$ $\mathrm{Re}\,\Sigma^R(\omega)$ depends only weakly on ω, i.e. is essentially constant,

$\Rightarrow$ can be absorbed into shift: $\mu \to \tilde{\mu}$ (5)

$\Rightarrow$ In practice, we can set $\Sigma^R(\omega, \vec{k}) = -i/2\tau$ (6)

$$\Rightarrow\quad g^R(\omega,\vec{k}) = \frac{1}{\omega - \varepsilon_k + i/2\tau}, \qquad g(i\omega_n, \vec{k}) = \frac{1}{i\omega_n - \varepsilon_k + \mathrm{sgn}(\omega_n)\, i/2\tau} \tag{7}$$

In real time:

$$g^R(t,\vec{k}) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \frac{1}{\omega - \varepsilon_k + i/2\tau} = -i\,\theta(t)\, e^{-i\varepsilon_k t}\, e^{-t/2\tau} \tag{1}$$

So τ = life-time of excitation with momentum $\vec{k}$

In position space:

$$g^R(\omega,\vec{r}) = \int \frac{d\vec{k}}{(2\pi)^3}\, e^{i\vec{k}\cdot\vec{r}}\, \frac{1}{\omega - \varepsilon_k + i/2\tau} \tag{2}$$

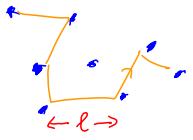
go to radial coordinates, angular integral is trivial, do radial integral by contour integration, $\Rightarrow$ pole when $\omega - \underbrace{\frac{k^2 - k_F^2}{2m}}_{\simeq (k - k_F)\cdot k_F/m} \simeq -i/2\tau$ (3)

$\Rightarrow\quad k \simeq k_F + i\,\frac{m}{k_F\tau}$ (4)

Careful calculation (homework!) gives:

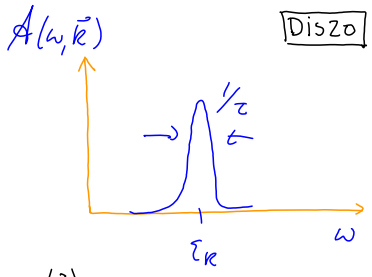
$$g^R(\omega,\vec{r}) \simeq -\frac{N(0)\,\pi}{k_F r}\, e^{i k_F r}\, \underbrace{e^{-\frac{r}{2}\frac{m}{k_F\tau}}}_{\equiv\, e^{-r/2\ell}} \tag{5}$$

$\ell \equiv \frac{\hbar k_F \tau}{m} = v_F\tau$ = mean free path



(6)

Spectral function:



$$A(\omega,\vec{k}) = -\frac{1}{\pi}\,\mathrm{Im}\,G^R(\omega,\vec{k}) \qquad (1)$$

$$\overset{(18.7)}{=} \frac{1}{(2\pi\tau)} \frac{1}{(\omega-\varepsilon_k)^2 + \left(\frac{1}{2\tau}\right)^2} = \text{Lorentzian} \qquad (2)$$

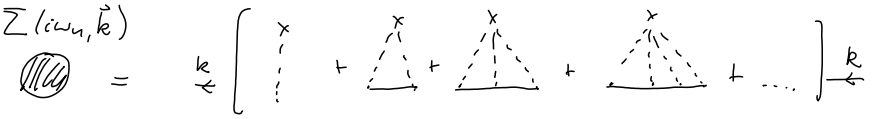
Density of states per spin:

$$N(\omega) = \frac{1}{\mathrm{Vol}} \sum_{\vec{k}} A(\omega,\vec{k}) \qquad (3)$$

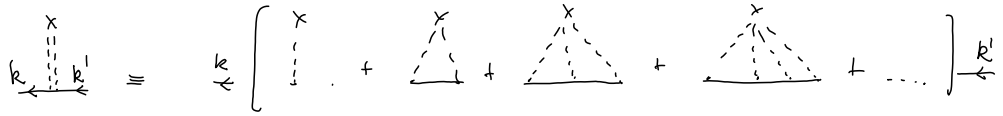
$$\overset{(2)}{=} \int d\varepsilon_k\, N(\varepsilon_k)\, A(\omega,\vec{k}) = N(0) \qquad (4)$$

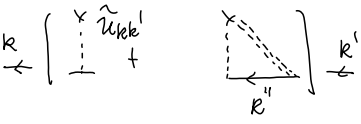
$\Rightarrow$ DOS near Fermi energy is not changed by disorder.

Higher order diagrams: Class A:

$\Sigma(i\omega_n,\vec{k})$ =  $\equiv t_{kk}(i\omega_n)$ (1)

To sum up this series, consider the so-called t-matrix:

 (2)

 (3)

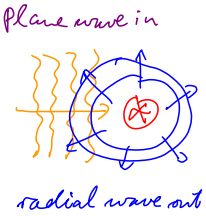
$$t_{kk'}(i\omega_n) = \tilde{u}_{kk'} + \tilde{u}_{kk''}\, g^0(i\omega_n,k'')\, t_{k''k'}(i\omega_n) \qquad (4)$$

where we defined $\tilde{u}_{kk'} \equiv \tilde{u}(\vec{k}-\vec{k}')$ (5)

For $i\omega_n \to E + i0^+$, this yields matrix version of

$$T = \tilde{u} + \tilde{u}\,\frac{1}{E - H^0 + i0^+}\,T \qquad (1)$$

This is the well-known eq. for T-matrix from scattering theory, for constructing scattering states for a single target.



Optical theorem says:

standard result ↓

Total scattering cross section for $\vec{k}' \to$ all $\vec{k}$ $= \sigma_{\vec{k}'}(\omega) = -2\,\mathrm{Im}\, t_{\vec{k}'\vec{k}'}(\omega) \overset{(21.1)}{=} -2\,\mathrm{Im}\,\Sigma^R(\omega, \vec{k}')$ (2)

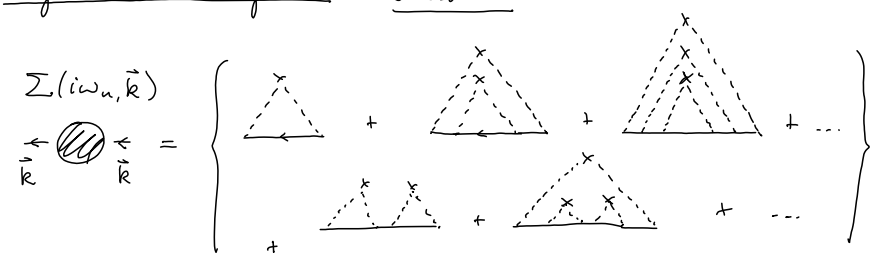
So: summation of all diagrams of class A yields

$$\frac{1}{2\tau_k(\omega)} = -\,\mathrm{Im}\, t_{kk}(\omega) \qquad (3)$$

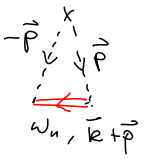
so we get the lifetime from the exact (single-scattering-site) t-matrix, instead of from the Born approximation.

Higher order diagrams: Class B:

$\Sigma(i\omega_n, \vec{k})$

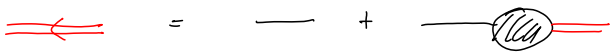


$\equiv$



(1)

where



(2)

$$\Sigma(i\omega_n, \vec{k}) \overset{(11.1)}{=} \frac{N_{imp}}{(Vol)^2} \sum_{\vec{p}} |\tilde{u}|^2\, G(i\omega_n, \vec{k}+\vec{p}) \qquad (3)$$

← full Green's function

$$\Sigma^R(\omega, \vec{k}) = c_{imp}\, N(0) \int d\varepsilon_p \langle |\tilde{u}|^2 \rangle_{ang} \left[\frac{1}{\omega - \varepsilon_{\vec{k}+\vec{p}} - \Sigma^R(\omega, \vec{k}+\vec{p})} \right] \qquad (4)$$

shift in chem. potential $\equiv \delta\mu - i/2\tau$

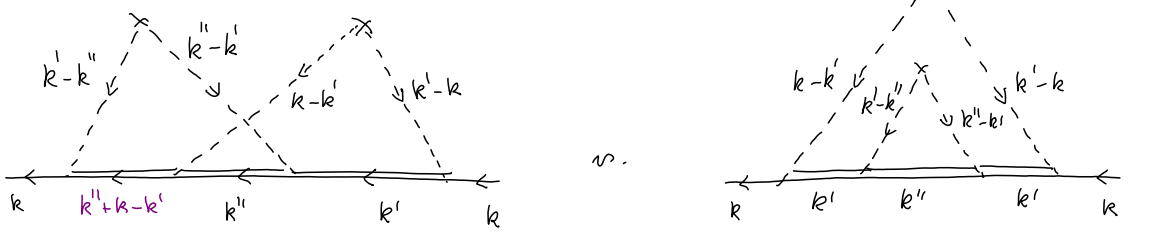
$$\frac{1}{2\tau} = -\,\mathrm{Im}\,\Sigma^R = c_{imp}\, N(0) \langle |\tilde{u}|^2 \rangle_{ang} \int d\varepsilon' \frac{1/2\tau}{(\omega - \varepsilon')^2 + (1/2\tau)^2} = c_{imp}\, N(0) \langle |\tilde{u}|^2 \rangle \qquad (5)$$

$= \pi$

↑ should be solved self-consistently

We obtain same result as before, so self-consistency did not yield anything new.

Higher order diagrams: Class C:



contribution to $\Sigma^R(\omega)$:

$$\sum_{k'k''} \frac{1}{\omega - \varepsilon_{k'} + i/2\tau} \frac{1}{\omega - \varepsilon_{k''} + i/2\tau} \left[\frac{1}{\omega - \varepsilon_{k''+k-k'} + i/2\tau} \text{ vs. } \frac{1}{\omega - \varepsilon_{k'} + i/2\tau} \right] \quad (1)$$

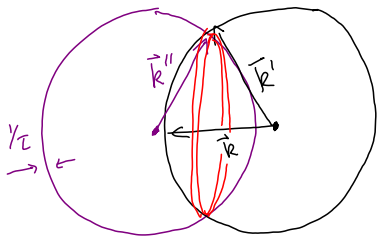
(take $i\omega_n \to \omega + i0^+$, with $\omega \lesssim 1/2\tau$)

Dominant contribution to $\sum_{kk'}$ comes from the regions:

$|\varepsilon_{k'}| \lesssim \frac{1}{2\tau}$, $|\varepsilon_{k''}| \lesssim \frac{1}{2\tau}$ and $\left[|\varepsilon_{k''+k-k'}| \lesssim \frac{1}{2\tau} \text{ vs. no new condition} \right]$

$\Rightarrow \vec{k}'' \simeq \vec{k}' - \vec{k}$

moreover $|k| \sim k_F$



$\vec{k}'' \simeq \vec{k}' - \vec{k}$ must lie on a narrow "ring"

vs. no extra limitation on $\vec{k}''$

Phase space is reduced by a factor: $\sim \frac{1/\tau}{\varepsilon_F} = \frac{1}{\varepsilon_F \tau} = \frac{2m}{k_F^2 \tau} \overset{(19.6)}{\sim} \frac{2}{k_F \ell}$ (1)

But $\frac{1}{k_F \ell} \sim \frac{\text{lattice constant}}{\ell} \sim \frac{(\text{Vol}/N_\square)^{1/3}}{(\text{Vol}/N_{imp})^{1/3}} \sim \left(\frac{N_{imp}}{N_\square}\right)^{1/3} \sim c_{imp}^{1/3} \ll 1$ (2)

so: contributions from "crossed impurity lines are negligible" (3)

$\Leftarrow O\left(\frac{1}{k_F \ell}\right)$