Beyond the Relaxation Time Approximation:

We have been using

$$\frac{\partial f}{\partial t} + \vec{v}\cdot\vec{\nabla}_r f + \vec{F}\cdot\frac{1}{\hbar}\vec{\nabla}_k f = -\frac{f - f_{eq}}{\tau} = \left(\frac{\partial f}{\partial t}\right)_{coll.}$$

A more accurate & general form uses

$W_{k,k'}$ = rate to go from k to $\frac{d^3k'}{(2\pi)^3}$.

$$\left(\frac{\partial f}{\partial t}\right)_{coll.} = -\int\frac{d^3k'}{(2\pi)^3} W_{k,k'} \underbrace{f(k)}_{occupied}\underbrace{(1-f(k'))}_{empty} \quad \ldots \text{scattering out}$$

$$+\int\frac{d^3k'}{(2\pi)} W_{k',k} \underbrace{f(k')}_{occupied}(1\underbrace{- f(k))}_{empty} \quad \ldots \text{scattering in}$$

Impurity Scattering

Fermi's Golden Rule:

$$\text{Rate}\,(i \to f) = \frac{2\pi}{\hbar}\, |\langle f | H' | i \rangle|^2 \rho$$

density of final states per unit energy

$$= \frac{2\pi}{\hbar} \sum_f |\langle f | H' | i \rangle|^2 \delta(\varepsilon_i - \varepsilon_f)$$

potential for 1 impurity

$$H'(r) = \sum_\alpha U(r - R_\alpha)$$

impurity position

For plane waves (normalized)

$$\langle k' | H' | k \rangle = \int d^3r \, \frac{e^{-ik'\cdot r}}{\sqrt{\text{Vol.}}} \sum_\alpha U(r - R_\alpha) \frac{e^{ik\cdot r}}{\sqrt{\text{Vol.}}}$$

$$= \frac{1}{\text{Vol.}} \sum_\alpha \int d^3r \, e^{i(k-k')\cdot(r - R_\alpha)} U(r - R_\alpha) e^{i(k-k')\cdot R_\alpha}$$

$$= \frac{1}{\text{Vol.}} \sum_\alpha U(k - k') \, e^{i(k-k')\cdot R_\alpha}$$

$$|\langle k' | H' | k \rangle|^2 = \frac{1}{(\text{Vol.})^2} |U(k-k')|^2 \sum_{\alpha,\beta} e^{i(k-k')\cdot(R_\alpha - R_\beta)}$$

Approximation: Neglect oscillatory terms.
Keep only $R_\alpha = R_\beta$.

$$|\langle k' | H' | k \rangle|^2 = \frac{1}{(\text{Vol.})^2} |U(k-k')|^2 N_i$$

number of impurities

$$\to \text{Rate} = \frac{2\pi}{\hbar} \left(\frac{N_i}{\text{Vol.}} \right) \overbrace{\frac{1}{\text{Vol.}} \sum_{k'}}^{\int d^3k'/(2\pi)^3} |U(k-k')|^2 \delta(\varepsilon_k - \varepsilon_{k'})$$

$$\boxed{W_{k,k'} = \frac{2\pi}{\hbar} n_i |U(k-k')|^2 \delta(\varepsilon_k - \varepsilon_{k'})}$$

The approximation makes sense provided the disorder is uncorrelated and the system is large. For small systems $e^{i(k-k')\cdot(R_\alpha - R_\beta)}$ will not average to zero.

Modern example:

Doping density $\underbrace{10^{13}}_{\text{low}}$ to $\underbrace{10^{18}}_{\text{high}}$ cm^{-3}

$$\frac{10^{13} \text{ to } 10^{18}}{(0.01m)^3}(45\times10^{-9}m)^3 \approx 0.001 \text{ to } 100$$

For impurity scattering $W_{kk'} = W_{k'k}$
(elastic)

$$\left(\frac{\partial f}{\partial t}\right)_{coll.} = -\int\frac{d^3k'}{(2\pi)^3} W_{k,k'}\left(f(k) - f(k')\right)$$

Wiedeman-Franz Law valid for elastic scattering.

Matthiessen's rule rarely correct when quantum mechanics is involved. $\left(\frac{1}{\tau} = \frac{1}{\tau^{(1)}} + \frac{1}{\tau^{(2)}}\right)$.

Solution for impurity scattering:

$$-e\vec{E}\cdot\frac{1}{\hbar}\vec{\nabla}_k f(k) = -\int\frac{d^3k'}{(2\pi)^3}\, W_{k,k'}\left(f(k)-f(k')\right)$$

Linear response: $f = f_{eq} + \delta f$

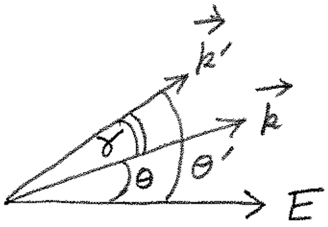
$$-e\vec{E}\cdot\frac{1}{\hbar}\vec{\nabla}_k f_{eq} = -\int\frac{d^3k'}{(2\pi)^3}\, W_{k,k'}\left(\delta f(k)-\delta f(k')\right)$$

$$= -e\vec{E}\cdot\vec{v}\,\frac{\partial f_{eq}}{\partial\mathcal{E}}$$

Take $\mathcal{E}(|k|)$ — basically free electrons. By symmetry:

$$W_{k,k'} = W(\mathcal{E},\hat{k}\cdot\hat{k}')\,\delta(\mathcal{E}_k-\mathcal{E}_{k'})$$

$$\delta f(k) = \delta f(\mathcal{E},\hat{k}\cdot\vec{E})$$



$$-eEv\,\frac{\partial f_{eq}}{\partial\mathcal{E}}\cos\theta = -\overset{\text{density of states}}{N(\varepsilon)}\int\frac{d\Omega'}{4\pi}\,W(\varepsilon,\gamma)\left(\delta f(\varepsilon,\theta)-\delta f(\varepsilon,\theta')\right)$$

Solve for a given energy, ε.

Angle addition:

$$W(\varepsilon,\gamma) = \sum_{\ell} W_\ell(\varepsilon)\,Y_{\ell 0}(\gamma) = \sum_{\ell,m} W_\ell(\varepsilon)\sqrt{\frac{4\pi}{2\ell+1}}\;Y^*_{\ell m}(\theta',\varphi')\,Y_{\ell m}(\theta,\varphi)$$

$$\delta f(\varepsilon,\theta') = \sum_{\ell}\delta f_\ell(\varepsilon)\,Y_{\ell 0}(\theta')$$

$$\int d\Omega' \, W(\varepsilon,\gamma)\, \delta f(\varepsilon,\theta') = \sum_{\ell} W_\ell(\varepsilon) \sqrt{\frac{4\pi}{2\ell+1}}\, \delta f_\ell(\varepsilon)\, Y_{\ell 0}(\theta)$$

$$\int d\Omega' \, W(\varepsilon,\gamma) \delta f(\varepsilon,\theta) = \sum_{\ell} W_0(\varepsilon) \sqrt{4\pi}\, \delta f_\ell(\varepsilon)\, Y_{\ell 0}(\theta)$$

Since the LHS has only $\ell = 1$ term,

$$RHS = \frac{N(\varepsilon)}{4\pi} \left\{ W_1(\varepsilon) \sqrt{\frac{4\pi}{3}} - W_0(\varepsilon)\sqrt{4\pi} \right\} \underbrace{\delta f_1(\varepsilon) Y_{10}(\theta)}_{\delta f(\varepsilon,\theta)}$$

$$LHS = -eEv \frac{\partial f_{eq}}{\partial \varepsilon} \cos\theta$$

$$= \delta f(\varepsilon,\theta) \frac{N(\varepsilon)}{4\pi} \int d\Omega_\gamma\, W(\varepsilon,\gamma) \left[\sqrt{\frac{4\pi}{3}}\, Y^*_{10}(\gamma) - \sqrt{4\pi}\, Y^*_{00}(\gamma) \right]$$

$$= \delta f(\varepsilon,\theta) \frac{N(\varepsilon)}{4\pi} \int d\Omega_\gamma\, W(\varepsilon,\gamma) \left[\cos\gamma - 1 \right)$$

$$= \delta f(\varepsilon,\theta) \frac{N(\varepsilon)}{4\pi} \int d\Omega_\gamma\, W(\varepsilon,\gamma) (\hat{k}\cdot\hat{k}' - 1)$$

$$= \delta f(\varepsilon,\theta) \int \frac{d^3k'}{(2\pi)^3} W_{k,k'} (\hat{k}\cdot\hat{k}' - 1)$$

$$= \frac{-1}{\tau(\varepsilon)} \delta f(\varepsilon,\theta)$$

$$\boxed{\delta f = +e \vec{E}\cdot\vec{v}\, \tau \frac{\partial f_{eq}}{\partial \varepsilon}}$$

transport lifetime

$$\boxed{\frac{1}{\tau} = \int \frac{d^3k'}{(2\pi)^3} W_{k,k'} (1 - \hat{k}\cdot\hat{k}')}$$

$$j = -2e \int \frac{d^3k'}{(2\pi)^3} \vec{v} f = \boxed{e^2 \int \frac{d^3k'}{4\pi^3} \tau\, \vec{v}\, \vec{v}\cdot\vec{E} \left(-\frac{\partial f_{eq}}{\partial \varepsilon} \right) = j}$$

Forward scattering: $1 - \hat{k}\cdot\hat{k}' = 0$

Backward scattering: $1 - \hat{k}\cdot\hat{k}' = 2$.