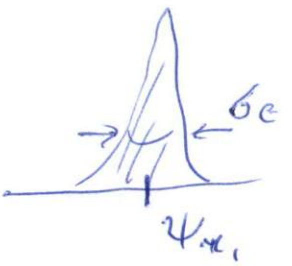
Diffusion probability

consider a wave packet , center in energy



$$|\psi_{r_1}\rangle = \underbrace{A}_{\text{normalization}} \sum_n \langle \phi_n|\vec{r}_1\rangle \underbrace{e^{-\frac{(\varepsilon_n-\varepsilon_0)^2}{4\sigma_\varepsilon^2}}}_{\text{coefficient}} |\phi_n\rangle$$

initial state at $\vec{r}_1$

The overlap with $|\vec{r}'\rangle$:

$$\langle \vec{r}'|\psi_{r_1}\rangle = A \sum_n \langle \vec{r}'|\phi_n\rangle\langle \phi_n|\vec{r}_1\rangle e^{-\frac{(\varepsilon_n-\varepsilon_0)^2}{4\sigma_\varepsilon^2}}$$

Check yourselves that $A^2 = \frac{1}{\sqrt{2\pi}\,\rho_0\,\sigma_\varepsilon}$

Evolution from $\vec{r}_1$ to $\vec{r}_2$ during t is described by

$$\underbrace{\langle r_2| e^{-i\hat{H}t}|\psi_{r_1}\rangle}_{\text{evolution operator}} \underbrace{\theta(t)}_{\text{retardation}} = \theta(t) A \sum_n \underbrace{\langle r_2| e^{-i\hat{H}t}|\phi_n\rangle}_{\langle r_2|\phi_n\rangle e^{-i\varepsilon_n t}} \langle \phi_n|\vec{r}_1\rangle \times e^{-\frac{(\varepsilon_n-\varepsilon_0)^2}{4\sigma_\varepsilon^2}}$$

Use the identity $\theta(t)\, e^{-i\varepsilon_n t} f(\varepsilon_n) \Rightarrow i\int \frac{e^{-i\varepsilon t} f(\varepsilon)}{\varepsilon-\varepsilon_n+i0}\frac{d\varepsilon}{2\pi}$

$$\Rightarrow \langle r_2| e^{-i\hat{H}t}|\psi_{r_1}\rangle \Rightarrow iA\int \frac{d\varepsilon}{2\pi} \underbrace{\sum_n \frac{\langle r_2|\phi_n\rangle\langle \phi_n|r_1\rangle}{\varepsilon-\varepsilon_n+i0}}_{G^R(r_1, r_2; \varepsilon)} e^{-\frac{(\varepsilon-\varepsilon_0)^2}{4\sigma_\varepsilon^2}} e^{-i\varepsilon t}$$

Def. the probability $r_1 \to r_2$ during t as

$$P(r_1, r_2; t) \equiv \overline{|\langle r_2| e^{-i\hat{H}t}|\psi_{r_1}\rangle \theta(t)|^2} \to \text{after renaming energy variables}$$

$$\to A^2 \int \frac{d\varepsilon\, d\omega}{(2\pi)^2} \langle G^R(\vec{r}_1, \vec{r}_2; \varepsilon+\tfrac{\omega}{2})\, G^A(r_2, r_1; \varepsilon-\tfrac{\omega}{2})\rangle_{dis} \times e^{-i\omega t} \exp\left(-[\varepsilon_+^2+\varepsilon_-^2]/4\sigma_\varepsilon^2\right)$$

with $\varepsilon_\pm = \varepsilon \pm \frac{\omega}{2} - \varepsilon_0$

Important assumption

$\langle G^R(\varepsilon+\frac{\omega}{2})\, G^A(\varepsilon-\frac{\omega}{2})\rangle_{dis}$ depends on ε very slowly, which can be justified for $\nu(\underbrace{\varepsilon_F \pm \Delta\varepsilon}_{\Delta\varepsilon \ll \varepsilon_F}) \simeq \nu(\varepsilon_F) = \text{const}$

Now calculate the integral

$$A^2 \int \frac{d\varepsilon}{2\pi} \exp\left(-\frac{(\varepsilon+\frac{\omega}{2}-\varepsilon_0)^2+(\varepsilon-\frac{\omega}{2}-\varepsilon_0)^2}{4\sigma_\varepsilon^2}\right) \simeq A^2 \int \frac{d\varepsilon}{2\pi} \exp\left(-\frac{(\varepsilon-\varepsilon_0)^2}{2\sigma_\varepsilon^2}\right) =$$

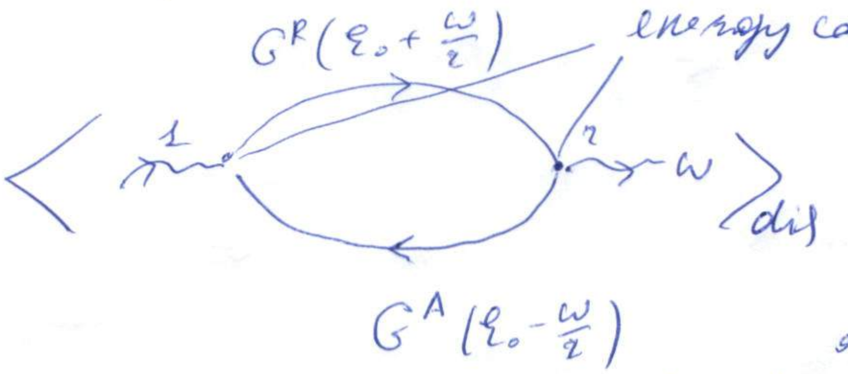
$\varepsilon_F \gg \omega$

$$= A^2 \frac{\sqrt{2\pi}\,\sigma_\varepsilon}{2\pi} = \frac{1}{\sqrt{2\pi}\,\rho_0\sigma_\varepsilon}\frac{\sigma_\varepsilon}{2\pi} = \frac{1}{2\pi\rho_0}$$

$$\Rightarrow P(1,2;t) = \int \frac{d\omega}{2\pi} P(1,2;\omega)\, e^{-i\omega t} \quad \text{where}$$

$$P(1,2;\omega) = \frac{1}{2\pi\rho_0} \left\langle G^R(1,2;\varepsilon_0+\tfrac{\omega}{2})\, G^A(2,1;\varepsilon_0-\tfrac{\omega}{2}) \right\rangle_{dis}$$

Graphic repr.



— describes the evolution of a particle at $\varepsilon_{F} = \varepsilon_0$ for long times:

$t \gg 1/\sigma_\varepsilon \Rightarrow \omega \ll \sigma_\varepsilon$ at $\nu \simeq \nu_0 = \text{const}$

Renaming energy variables:

$$P(1,2;\omega)\Big|_{\varepsilon_0 \simeq \varepsilon_F \gg \omega} = \frac{1}{2\pi\rho_0} \left\langle G^R(1,2;\varepsilon_0)\, G^A(2,1;\varepsilon_0-\omega) \right\rangle$$

Normalization of P

$$\int P(\vec{r},\vec{r}\,';\omega)\,d\vec{r}\,' = \frac{1}{2\pi\rho_0}\left\langle \sum_{m,n}\int d\vec{r}\,' \frac{\varphi_n^*(\vec{r})\varphi_n(\vec{r}\,')\varphi_m(\vec{r}\,')\varphi_m^*(\vec{r})}{(\varepsilon_0-\varepsilon_n+i0)(\varepsilon_0-\varepsilon_m-\omega-i0)}\right\rangle$$

Using the orthogonality and completeness of w/fn the definition of LDoS:

$$\Rightarrow \int P(\vec{r},\vec{r}\,';\omega)\,d\vec{r}\,' = \frac{1}{2\pi\rho_0}\int d\varepsilon \frac{\langle\rho(\vec{r},\varepsilon)\rangle \simeq \rho_0 = \text{const}}{(\underbrace{\varepsilon_0-\varepsilon}_{\tilde{\varepsilon}}+i0)(\underbrace{\varepsilon_0-\varepsilon}_{\tilde{\varepsilon}}-\underset{\omega+i0}{\underset{\uparrow}{\omega_+}})} =$$

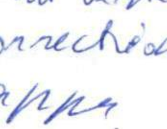
$$= \int \frac{d\tilde{\varepsilon}}{2\pi}\frac{1}{(\tilde{\varepsilon}+i0)(\tilde{\varepsilon}-\omega_+)}\Bigg|_{\text{pole integral}} = \frac{i}{\omega}$$

Calculating the FT $\omega \to t$

$$\boxed{\int P(\vec{r},\vec{r}\,';t>0)\,d\vec{r}\,' = 1}$$ – particle conservation

How to calculate P?

Step 1 (trivial) – lets decouple correlations:

$$\langle G^R G^A\rangle \to \langle G^R\rangle\langle G^A\rangle,\ \text{i.e.}$$ 

without vertex corrections

This can be called „Drude" or „Boltzmann" appr. since it allow one to find the classical (Drude) $\sigma(\omega)$.

$$P_0(1,2;\omega) \overset{\text{def}}{\equiv} \frac{1}{2\pi\rho_0}\langle G^R_\varepsilon(1,2;\omega)\rangle\langle G^A_{\varepsilon-\omega}(2,1;\omega)\rangle$$

Inserting $\langle G^{R/A}\rangle$ yields for 3d

$$P_0(1,2;\omega)\Big|_{\vec{R}=\vec{r}_1-\vec{r}_2} = \frac{1}{4\pi R^2 v_0}\, e^{i\frac{\omega R}{v_0}}\, e^{-R/l_e}$$

or in time repr.

$$\hat{FT}\left[e^{i\omega R/v_0}\right] \to \delta(R - v_0 t)$$

$$\Rightarrow P_0(1,r;t) = \frac{1}{4\pi R^2}\underbrace{\delta(R-v_0 t)}_{\text{classical ballistic propagation}} \times e^{-t/\tau_e}$$

Note, that $P_0 \to 0$ at $R > l_e$ or $t > \tau_e$ i.e., it's a short range contribution to P.

Let's check normalization

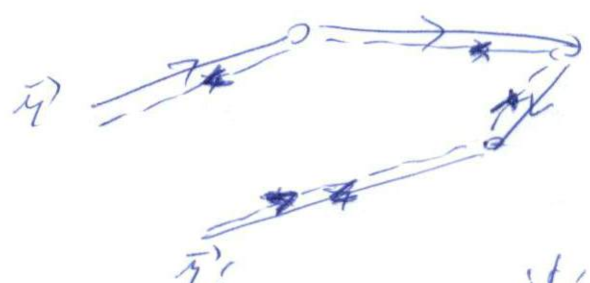
$$\int d^3R\, P(0,\vec{R};t) = \frac{\theta(t)e^{-t/\tau_e}}{4\pi}\underbrace{\int \frac{d^3R}{R^2}\,\delta(R - v_0 t)}_{4\pi} = \theta(t)\, e^{-t/\tau_e}$$

~~or in ω~~ $\neq 1$ - normalization is violated, other diagrams are needed to restore it at classical level.

Let's try to take into account diagrams without :

this is called the ladder (or the Diffuson) approximation

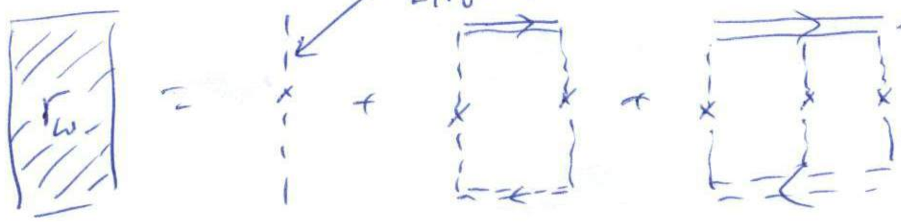
Analogy with the trajectory picture



both $G^{R/A}$ see the same impurities and explore them in the same order (up to conjugation) — it's indeed the classical contribution

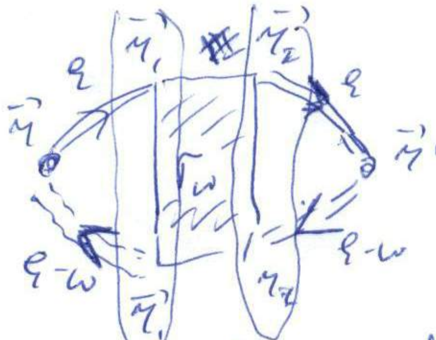
Let's introduce the vertex function Γ_ω:

$\frac{1}{2\pi\rho_0\tau_e}\delta(\vec r\,' - \vec r\,'')$ $\qquad$ $\bar{e}$-h^+ channel



$= \ldots$ – the ladder diagrams

Then the diagram we need can be drawn as

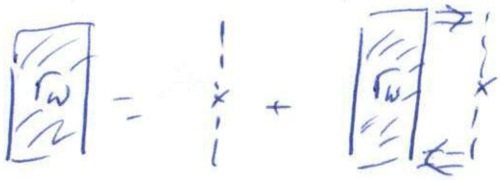
P_d 

$=$

because of the white-noise disorder

$$= \frac{1}{2\pi\rho_0}\int d\vec r_1\, d\vec r_2\; \underbrace{\bar G^R_\varepsilon(\vec r, \vec r_1)\, \bar G^R(\vec r_2, \vec r\,')}_{2\pi\rho_0 P_0}\, \Gamma_\omega(\vec r_1, \vec r_2)\, \underbrace{\bar G^A_{\varepsilon-\omega}(\vec r\,', \vec r_2)\, \bar G^A_{\varepsilon-\omega}(\vec r_1, \vec r)}_{2\pi\rho_0 P_0}$$

Γ_ω can be found by resumming:



– check yourselves $\Rightarrow$

$$\Gamma_\omega(\vec r_1, \vec r_2) = \frac{1}{2\pi\rho_0\tau_e}\Big(\delta(\vec r_1 - \vec r_2) + \int d\vec r\,''\, \Gamma(\vec r_1, \vec r\,'') \times$$

$$\times \underbrace{\bar G^R_\varepsilon(\vec r\,'', \vec r_2)\, \bar G^A_{\varepsilon-\omega}(\vec r_2, \vec r\,'')}_{2\pi\rho_0 P_0(\vec r\,'', \vec r_2;\, \omega)}\Big).$$

$$\Rightarrow \boxed{\Gamma_\omega(\vec r_1, \vec r_2) = \frac{1}{2\pi\rho_0\tau_e}\delta(\vec r_1 - \vec r_2) + \frac{1}{\tau_e}\int d\vec r\,''\, \Gamma_\omega(\vec r_1, \vec r\,'')\, P_0(\vec r\,'', \vec r_2; \omega)}$$

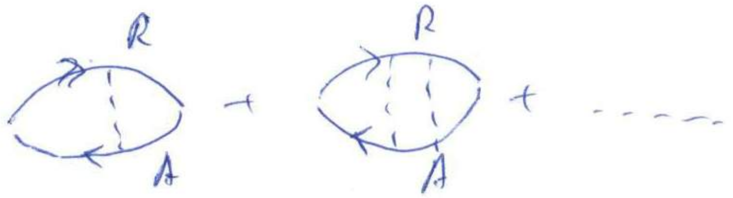
insert

$$\boxed{P_d(\vec r, \vec r\,'; \omega) = 2\pi\rho_0 \int d\vec r_1\, d\vec r_2\; P_0(\vec r, \vec r_1; \omega)\, \Gamma_\omega(\vec r_1, \vec r_2)\, P_0(\vec r_2, \vec r\,')}$$

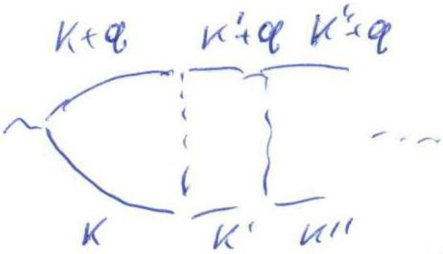
In our approximation

$$P \simeq P_0 + P_d$$

P_d can be calculated as a geometric series:

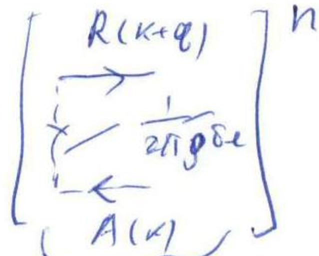


With the structure in the momentum space



– the ladder diagram

– summation of the ladder involves



P_0 up to the const factor!

$\Rightarrow$ we need

ladder block: $B = \frac{1}{2\pi\rho\tau_e} \sum_{\vec{k}} G^R_{\varepsilon}(\vec{k}+\vec{q})\, G^A_{\varepsilon-\omega}(\vec{k}) =$

$$= \frac{1}{2\pi\rho\tau_e} \sum_{\vec{k}} \frac{1}{\varepsilon - \underbrace{\xi(\vec{k}+\vec{q})}_{\text{Taylor expand}} + i/2\tau_e}\; \frac{1}{\varepsilon - \omega - \xi(\vec{k}) - i/2\tau_e} \simeq$$

$$\simeq \frac{1}{2\pi\rho\tau_e} \sum_{\vec{k}} \frac{1}{\varepsilon - \xi(\vec{k}) - \underbrace{\vec{v}\cdot\vec{q}}_{v_F \cdot \vec{n}_v} + i/2\tau_e}\; \frac{1}{\varepsilon - \xi(\vec{k}) - \omega - i/2\tau_e} \rightarrow$$

$$\rightarrow \frac{1}{2\pi\nu\tau_e} \int d\Omega_d \int d\xi\, \nu(\xi) \underbrace{\frac{1}{\varepsilon - \xi - v_F\vec{q} + i/2\tau_e}\; \frac{1}{\varepsilon - \xi - \omega - i/2\tau_e}}_{\text{Pole integral}}$$

$$= \frac{\cancel{2\pi} i}{\cancel{2\pi}\tau_e} \int d\Omega_d \frac{1}{i/\tau_e + \omega - v_F \vec{n}_v \vec{q}} =$$

$$= \int d\Omega_d \frac{1}{1 - i\omega\tau_e + i\frac{v_F\tau_e}{l_e}\vec{n}_v\vec{q}}$$

Diffusion approximation

$$\omega\tau_e \ll 1 \ \& \ l_e q \ll 1$$

- we consider only long times $\gg \tau_e$ and distances $\gg l_e$

Note that P_0 is small in this limit

$$P_0(q=0,\omega) = \int_0^\infty dt\, e^{i\omega t - t/\tau_e} =$$

$$= -\frac{1}{i\omega - 1/\tau_e} = \frac{\tau_e}{1-i\omega\tau_e} = \frac{1}{\omega}\frac{\omega\tau_e}{1-i\omega\tau_e} \text{ small}$$

because P_0 is short ranged.

P_d will be obtained after summing up the geom. series in P_0.

$$B|_{diff/appr.} \simeq \int d\Omega_0 \Big[1 + i\omega\tau_e - \underbrace{\cancel{i v_F \tau \vec{n}_v \cdot \vec{q}}}_{\text{due to angles}} - (v_F\tau)^2 \underbrace{(\vec{n}_v\vec{q})^2}_{\to q^2/d} \Big]$$

$$= 1 + i\omega\tau_e - \tau\underbrace{\frac{v_F^2\tau}{d}}_{D} q^2 = 1 + i\omega\tau_e - \tau D q^2$$

Now summing up the geometric series

$$P_d(q,\omega) \simeq \frac{1}{Dq^2 - i\omega}$$ – the Diffusion inverse kernel of the diffusion operator

$\Rightarrow$ P_d is a solution to the diffusion equation

$$\boxed{\left[\frac{\partial}{\partial t} - D\Delta_{\vec{r}}\right] P_d(\vec{r},\vec{r}\,';t) = \delta(\vec{r}-\vec{r}\,')\delta(t)}$$

Usefull relation (check yourselves)

$$\Gamma_\omega(r,r') = \frac{1}{2\pi\rho_0\tau_e^2} P_d(r,r';\omega)$$

Normalization

$$P \simeq P_0 + P_d|_{diff/appr.} \simeq P_d|_{\substack{q=0 \\ \text{i.e. } \int d\vec{r}\,'}} = \frac{1}{-i\omega} = \frac{i}{\omega} \Big\} \text{ correct answer!}$$

To study Q-corrections let's change to the conductivity (technically simpler) discuss later generic problem