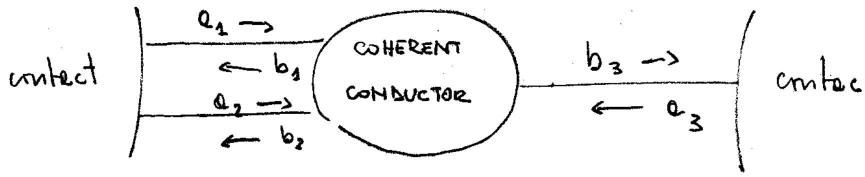
The S-matrix and its relations to the transmission function and the Green's function

The scattering matrix (in short S-matrix) is the matrix that relates the amplitudes of the incoming electrons to the one of the outgoing. Let's consider for example



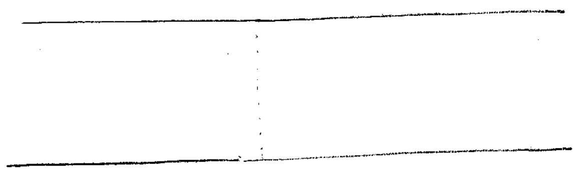
$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} \\ S_{21} & S_{22} & S_{23} \\ S_{31} & S_{32} & S_{33} \end{bmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

$$\underset{\text{out}}{\uparrow} \qquad\qquad\qquad\qquad\qquad \underset{\text{in}}{\uparrow}$$

S depends on the energy of the propagating modes and has dimension $M_T \times M_T$, where $M_T = \sum_p M_p(E)$ and p is labeling the leads and $M_p(E)$ is the number of subbands in p with minimum of energy $\varepsilon_m < E$.

In principle it is possible to calculate the S-matrix from the effective mass Schrödinger equation for the coherent conductor. In practice it can be usefull to split the conductor in parts and calculate the scattering matrixes of the different parts. In this way it is also possible to combine the different parts with different degree of coherence depending on the phase relaxation length.

Exercise: S-matrix for a single mode coherent conductor with δ like scatterer.



$$U(x,y) = U_0\,\delta(x)$$

Assume an energy $\varepsilon_{01} < E < \varepsilon_{02}$

The only relevant part of the Schrödinger equation is

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}\psi(x) + U_0\,\delta(x)\,\psi(x) = E\,\psi(x)$$

$$-\frac{d^2}{dx^2}\psi(x) + \frac{2m^* U_0}{\hbar^2}\delta(x)\,\psi(x) = \frac{2m^* E}{\hbar^2}\psi(x) \equiv k^2\psi(x)$$

$x<0$ $\quad \psi(x) = a_1 e^{+ikx} + b_1 e^{-ikx}$ $\qquad k = \sqrt{\dfrac{2m^*E}{\hbar^2}}$ $\qquad E \equiv \varepsilon - \varepsilon_{01}$.

$x>0$ $\quad \psi(x) = a_2 e^{-ikx} + b_2 e^{+ikx}$

In order to obtain the relations between a_1, a_2 and b_1, b_2 we impose the conditions on the wave function:

i) continuity: $\quad \psi(0^+) = \psi(0^-) \iff a_1 + b_1 = a_2 + b_2$

ii) discontinuity of the first derivative of ψ given by the δ-like potential.

$$\lim_{\varepsilon\to 0^+}\int_{-\varepsilon}^{\varepsilon} -\frac{d^2}{dx^2}\psi(x) + \frac{2m^*U_0}{\hbar^2}\delta(x)\,\psi(x)\,dx = \lim_{\varepsilon\to 0^+}\int_{-\varepsilon}^{\varepsilon} dx\, k^2\psi(x) = 0$$

$$[U_0] = [E]\cdot[L] \quad \Rightarrow \quad \frac{2m^*U_0}{\hbar^2} \equiv \bar{k}$$

$$\lim_{\varepsilon\to 0^+}\left[-\psi'(\varepsilon) + \psi'(-\varepsilon) + \bar{k}\,\psi(0)\right] = 0$$

$$-\left(ik a_2 + ik b_2\right) + \left(+ik a_1 - ik b_1\right) + \bar{k}\left(a_1 + b_1\right) = 0$$

The 2 equations read (after moving al b's to the left)

$$\begin{cases} b_1 - b_2 = a_2 - a_1 \\ -ik(b_1+b_2) + \bar{k}\, b_1 = -ik(a_1+a_2) - \bar{k} a_1 \end{cases}$$

In matrix form:

$$\begin{pmatrix} 1 & -1 \\ -ik+\bar{k} & -ik \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ -ik-\bar{k} & -ik \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \frac{1}{\bar{k} - 2ik} \begin{pmatrix} -ik & 1 \\ +ik-\bar{k} & 1 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ -ik-\bar{k} & -ik \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

$$S = \frac{1}{-\bar{k}+2ik} \begin{pmatrix} +\bar{k} & +2ik \\ +2ik & +\bar{k} \end{pmatrix}$$

$$SS^+ = \frac{1}{\bar{k}^2 + 4k^2} \begin{pmatrix} +\bar{k} & -2ik \\ -2ik & +\bar{k} \end{pmatrix} \begin{pmatrix} +\bar{k} & +2ik \\ +2ik & +\bar{k} \end{pmatrix} = \frac{1}{\bar{k}^2 + 4k^2} \begin{pmatrix} \bar{k}^2+4k^2 & 0 \\ 0 & \bar{k}^2+4k^2 \end{pmatrix} = \mathbb{1}$$

Analogously for S^+S $\Rightarrow$ S is unitary.

It is easy to convince yourself that

$$T_{m\leftarrow n} = |S_{m\leftarrow n}|^2$$

where $T_{m\leftarrow n}$ is the transmission probability from the mode n into the mode m (n ingoing and m outgoing). In fact $S_{m\leftarrow n}$ gives the ratio between the (scattering) amplitudes $\Rightarrow$ $|S_{m\leftarrow n}|^2$ the ratio of the populations of the scattering states. In other terms the transmission probability.

Unitarity and flux normalization

In the simple example that we have presented the scattering matrix was relating the amplitudes of the scattering states and was unitary. With our definition of the scattering states this was simply the result of the fact that the group velocity of the first mode with energy E was equal in the 2 leads. Normally it is not the case. For this reason it is common to define

$$s_{nm} = \sqrt{\frac{v_n}{v_m}}\, s'_{nm}$$

where s'_{nm} connect the amplitudes of the incoming and outgoing waves. Current conservation imposes:

$$\sum_m v_m |a_m|^2 = \sum_m v_m |b_m|^2 .$$

$$\Rightarrow \sum_m \sqrt{v_m}\, a_m^* \sqrt{v_m}\, a_m = \sum_m \sqrt{v_m}\, b_m^* \sqrt{v_m}\, b_m$$

$$= \sum_m \sum_{nn'} \sqrt{v_m}\, s'^*_{mn} a_n^* \sqrt{v_m}\, s'_{mn'} a_{n'}$$

$$= \sum_{mnn'} \sqrt{v_n}\, s'^*_{nm} a_m^* \sqrt{v_n}\, s'_{nn'} a_{n'}$$

$$= \sum_{mnn'} \sqrt{\frac{v_n}{v_m}}\, (s'^{+})_{mn} \sqrt{\frac{v_n}{v_{n'}}}\, s'_{nn'} \sqrt{v_m}\, a_m^* \sqrt{v_{n'}}\, a_{n'}$$

Since $\{a\}$ is generic the relation is valid only if

$$\sum_n \sqrt{\frac{v_n}{v_m}} (s'^{+})_{mn} \sqrt{\frac{v_n}{v_{n'}}}\, s'_{nn'} = \delta_{mn'}$$ that is, the unitarity of s.

In terms of the elements of the S-matrix

$$\sum_{m=1}^{M_T} |S_{mn}|^2 = 1 = \sum_{m=1}^{M_T} |S_{nm}|^2$$

Physical interpretation:

$$\sum_{m=1}^{M_T} T_{m\leftarrow n} = 1$$ the electron must end up somewhere independently of where it comes from.

$$\sum_{m=1}^{M_T} T_{n\leftarrow m} = 1$$ the electron that outgoes in n must come from somewhere in the device.

Now we are ready for the microscopic derivations of the sum rules for the transmission function.

$$\sum_q \bar{T}_{qp} \equiv \sum_q \sum_{n\in q} \sum_{m\in p} T_{nm} = \sum_{m\in p} \underbrace{\sum_{n=1}^{M_T} |S_{nm}|^2}_{1} = M_p$$

$$\sum_q \bar{T}_{pq} \equiv \sum_q \sum_{n\in p} \sum_{m\in q} T_{nm} = \sum_{n\in p} \sum_{m=1}^{M_T} |S_{nm}|^2 = M_p$$

$\bar{T}_{pq}(E)$

xx	xx	xx	sum = M_1
xx	xx	xx	sum = M_2
xx	xx	xx	sum = M_3
sum = M_1	sum = M_2	sum = M_3	

$\Rightarrow$ for a 2-terminal device, independent of the presence of the magnetic field $\cancel{\bar{T}_{11}} + \bar{T}_{12} = \cancel{\bar{T}_{21}} + \bar{T}_{21}$.

For the conductance:

$$\sum_q G_{pq} = \sum_q G_{qp} = \frac{2e^2}{h}\int M_p(E)\left|-\frac{\partial f_0}{\partial E}\right| dE = \frac{2e^2}{h} M_p(\epsilon_f) \quad \text{at low temperatures.}$$

For coherent transport the unitarity of the S-matrix ensures the validity of the sum rule for the conductance.

Also the reciprocity can be microscopically deduced for coherent transport from the properties of the S-matrix:

$$[S]_{+B} = [S^T]_{-B} \quad \text{that is} \quad [s_{mn}]_{+B} = [s_{nm}]_{-B}$$

In fact S comes from the solution of

$$\left[E_s + \frac{(i\hbar\nabla + eA)^2}{2m^*} + U(x,y)\right]\psi(x,y) = E\,\psi(x,y) \quad . \quad (*)$$

The complex conjugate of (*) gives

$$\left[E_s + \frac{(-i\hbar\nabla + eA)^2}{2m^*} + U(x,y)\right]\psi^*(x,y) = E\,\psi^*(x,y)$$

At the same time let's reverse A and => B

$$\left[E_s + \frac{(i\hbar\nabla + eA)^2}{2m^*} + U(x,y)\right]\psi^*(x,y) = E\,\psi^*(x,y)$$

=> $\psi^*(x,y)$ solves the same equation (*) if we invert B

$$[\psi^*(x,y)]_{-B} = [\psi(x,y)]_B$$

But the complex conjugation brings $\{b\} \to \{e\}$ and viceversa.

Inserting the velocities in the amplitudes:

$$\{b\} = [S]_{+B}\{a\} \quad \Rightarrow \quad \{b^*\} = [S^*]_B\{a^*\}$$

But

$$\{a^*\} = [S]_{-B}\{b^*\} \quad \Rightarrow \quad \{b^*\} = [S^{-1}]_B\{a^*\}$$

$$\Downarrow$$

$$[S^*]_{+B} = [S^{-1}]_B \overset{\text{unitarity}}{=} [S^+]_B = [S^*]^T_{-B}$$

$$\Rightarrow \quad [S]_{-B} = [S^T]_B .$$

It follows thus immediately:

$$[\overline{T}_{pq}]_B = \sum_{n\in p}\sum_{m\in q}\left[|S_{nm}|^2\right]_B =$$

$$= \sum_{n\in p}\sum_{m\in q}[|S_{mn}|^2]_{-B} = [\overline{T}_{qp}]_{-B} .$$

The relation for the conductance follows trivially: $[G_{pq}]_B = [G_{qp}]_{-B}$.

Notice that the reciprocity relations holds only at small biases since we are neglecting in their derivation the possible change of $V(x,y)$. In fact the Hall potential changes sign when the magnetic field reverses. This effect can nevertheless be neglected in conductance calculations.

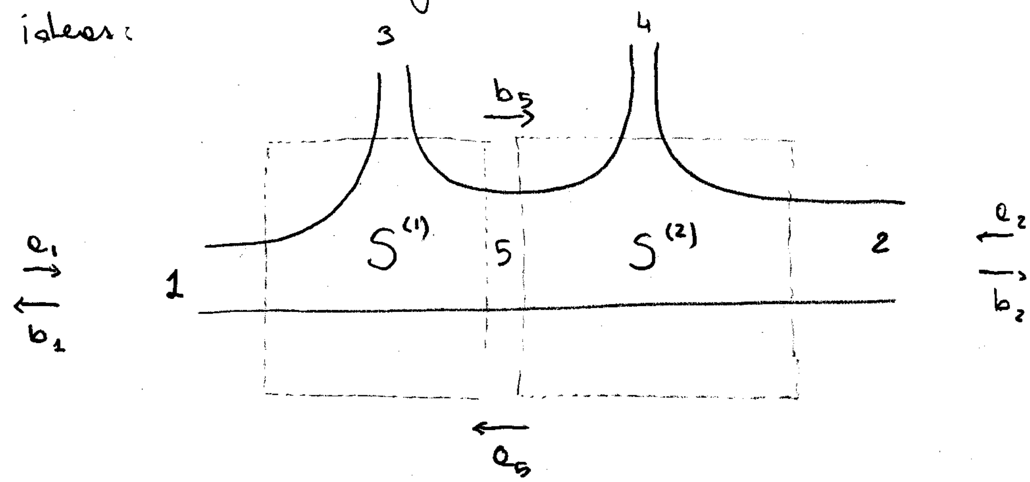
As clear from the beginning that the conductance that we are calculating is in the leads and NOT in the contacts. This is though harmless for reflectionless contacts.

Coherent combination of S-matrices

A coherent conductor can be splitted into parts (ex 1 and 2). The scattering matrices for part 1 and 2 are calculated $S^{(1)}$ and $S^{(2)}$. Eventually the total scattering matrix S can be obtained from $S^{(1)}$ and $S^{(2)}$:

$$S = S^{(1)} \otimes S^{(2)}$$

What is the meaning of $\otimes$? Let's consider an example to fix the ideas:



$$\begin{pmatrix} b_{13} \\ b_5 \end{pmatrix} = \begin{bmatrix} r^{(1)} & t'^{(1)} \\ t^{(1)} & r'^{(1)} \end{bmatrix} \begin{pmatrix} a_{13} \\ a_5 \end{pmatrix}$$

$$\begin{pmatrix} a_5 \\ b_{24} \end{pmatrix} = \begin{bmatrix} r^{(2)} & t'^{(2)} \\ t^{(2)} & r'^{(2)} \end{bmatrix} \begin{pmatrix} b_5 \\ a_{24} \end{pmatrix}$$

- b_{13} is an expression to include all coefficients of outgoing waves in leads 1 and 3. Analogously for a_{13}, b_{24} and a_{24}.

- Notice the apparently inverted roles of a_5 and b_5 coeficients in the equations for $S^{(2)}$.

- r stands for reflected, t for transmitted.

Keep in mind that each lead contains in principle many modes. $\Rightarrow$ $r^{(i)}$ $t^{(i)}$ $r'^{(i)}$ $t'^{(i)}$ are matrices.

We want to obtain the equation

$$\begin{pmatrix} b_{13} \\ b_{24} \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_{13} \\ a_{24} \end{pmatrix}$$

For these purpose we have to eliminate a_5 and b_5 from the equations

$$b_5 = t^{(1)} a_{13} + r'^{(1)} a_5$$
$$a_5 = r^{(2)} b_5 + t'^{(2)} a_{24}$$

If I multiply the first eq. by $r^{(2)}$ and sum to the second and multiply the second by $r'^{(1)}$ and sum to the first

$$\cancel{r^{(2)} b_5} + a_5 = r^{(2)} t^{(1)} a_{13} + r^{(2)} r'^{(1)} a_5 + \cancel{r^{(2)} b_5} + t'^{(2)} a_{24}$$
$$\cancel{r'^{(1)} a_5} + b_5 = r'^{(1)} r^{(2)} b_5 + r'^{(1)} t'^{(2)} a_{24} + t^{(1)} a_{13} + \cancel{r'^{(1)} a_5}$$

$$\left(\mathbb{1} - r^{(2)} r'^{(1)}\right) a_5 = r^{(2)} t^{(1)} a_{13} + t'^{(2)} a_{24}$$
$$\left(\mathbb{1} - r'^{(1)} r^{(2)}\right) b_5 = r'^{(1)} t'^{(2)} a_{24} + t^{(1)} a_{13}$$

$$a_5 = \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} r^{(2)} t^{(1)} a_{13} + \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} t'^{(2)} a_{24}$$
$$b_5 = \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} t^{(1)} a_{13} + \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} r'^{(1)} t'^{(2)} a_{24}$$

$$b_{13} = r^{(1)} a_{13} + t'^{(1)} \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} r^{(2)} t^{(1)} a_{13} + t'^{(1)} \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} t'^{(2)} a_{24}$$

$$b_{24} = t^{(2)} \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} t^{(1)} a_{13} + t^{(2)} \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} r'^{(1)} t'^{(2)} a_{24} + r'^{(2)} a_{24}$$

We can thus identify all the different components of the S-matrix.

$$r = r^{(1)} + t'^{(1)} \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} r^{(2)} t^{(1)}$$

$$t = t^{(2)} \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} t^{(1)}$$

$$t' = t'^{(1)} \left(\mathbb{1} - r^{(2)} r'^{(1)}\right)^{-1} t'^{(2)}$$

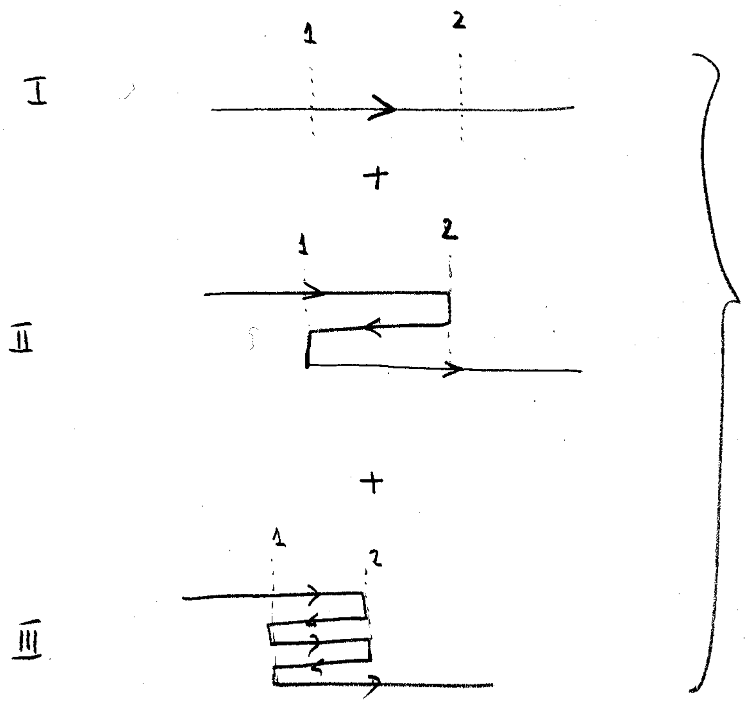
$$r' = r'^{(2)} + t^{(2)} \left(\mathbb{1} - r'^{(1)} r^{(2)}\right)^{-1} r'^{(1)} t'^{(2)}$$

An interesting interpretation of these formulas can be given in terms of Feynman paths. Let's consider t in order to fix the ideas. We expand in the geometric series

$$t = t^{(2)} \sum_{n=0}^{\infty} \left[r'^{(1)} r^{(2)}\right]^n t^{(1)}$$

[notice that convergence is ensured by the fact that if $\{\lambda\}$ is the spectrum of $r'^{(1)} r^{(2)} \Rightarrow |\{\lambda\}| < 1$]

$$= t^{(2)} t^{(1)} + t^{(2)} r'^{(1)} r^{(2)} t^{(1)} + t^{(2)} r'^{(1)} r^{(2)} r'^{(1)} r^{(2)} t^{(1)} + \dots$$



Feynman paths

More specifically

$$t_{mn} = \sum_{P} A^{(P)}_{mn}$$ where A_P is the amplitude of transmission corresponding to a specific path P.

For example $A^{(II)}_{mn}$

$$A^{(II)}_{mn} = \left(t^{(2)} r'^{(1)} r^{(2)} t^{(1)} \right)_{mn} = \sum_{m_1} \sum_{m_2} \sum_{m_3} \left(t^{(2)} \right)_{m m_3} \left(r'^{(1)} \right)_{m_3 m_2} \left(r^{(2)} \right)_{m_2 m_1} \left(t^{(1)} \right)_{m_1 n}$$

The transmission probability is the square of the transmission amplitude

$$T_{mn} = t_{mn} \cdot t_{mn}^{*} = \sum_{P} A^{(P)} \cdot A^{(P)*} + \sum_{P} \sum_{P' \neq P} A^{(P)} \cdot A^{(P')*}$$

INCOHERENT vs. COHERENT combination of successive sections

$$T^{I}_{mn} = \sum_{P} |A^{P}|^2$$

In order to fix the ideas let's consider a single mode structure

$$S^{(1)} = \begin{pmatrix} r_1 & t'_1 \\ t_1 & r'_1 \end{pmatrix} \qquad S^{(2)} = \begin{pmatrix} r_2 & t'_2 \\ t_2 & r'_2 \end{pmatrix}$$

$$\mathcal{S}^{(1)} = \begin{pmatrix} R_1 & T_1 \\ T_1 & R_1 \end{pmatrix} \qquad \mathcal{S}^{(2)} = \begin{pmatrix} R_2 & T_2 \\ T_2 & R_2 \end{pmatrix}$$

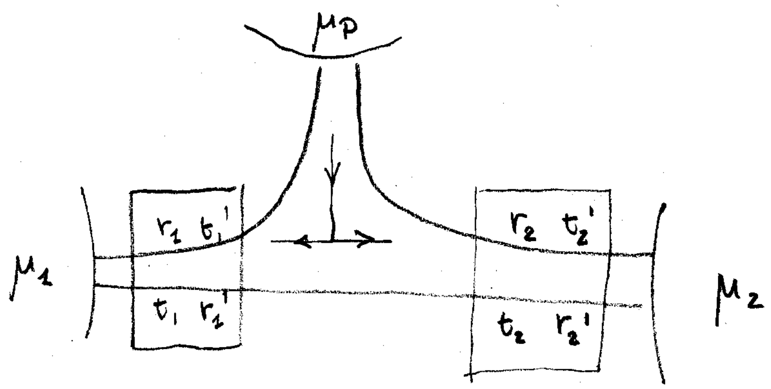
$$t = \frac{t_1 t_2}{1 - r'_1 r_2} \Rightarrow T^{C} = |t|^2 = \frac{T_1 T_2}{1 - 2\sqrt{R_1 R_2}\cos\theta + R_1 R_2}$$

$$\theta = \varphi_1 + \varphi_2 \qquad \varphi_1 = \arg r'_1 \qquad \varphi_2 = \arg r_2$$

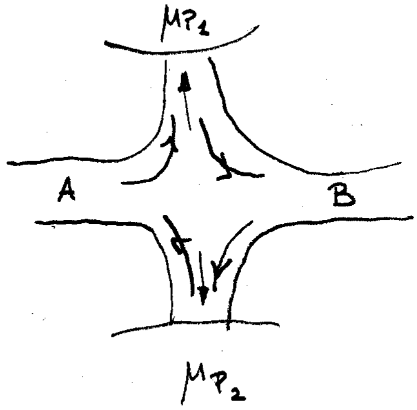
$$T^{I} = \frac{T_1 T_2}{1 - R_1 R_2}.$$ This result if phase independent as expected!

Combining successive sections with PARTIAL COHERENCE

We have already mentioned that voltage probes can be considered as sources of dephasing. The only problem is that they are also introducing, typically, momentum relaxation and thus Resistance.



The voltage probe is at potential μ_P and accept electrons from 2 and 1 but it also gives back them in both direction. If we just want to model dephasing without momentum relaxation we can introduce a system of twin probes like



The corresponding S-matrix can be written as a function of a single parameter α. $\alpha \in [0,1]$.

The "connecting" scattering matrix reads

	A	B	P_1	P_2
A	0	$\sqrt{1-\alpha}$	0	$-\sqrt{\alpha}$
B	$\sqrt{1-\alpha}$	0	$-\sqrt{\alpha}$	0
P_1	$\sqrt{\alpha}$	0	$\sqrt{1-\alpha}$	0
P_2	0	$\sqrt{\alpha}$	0	$\sqrt{1-\alpha}$

$\alpha = 1$ incoherent

$\alpha = 0$ coherent

Single electron Green's function: generalization of S-matrix theory.

The starting point is again the Schrödinger equation

$$i\hbar \partial_t \psi = H\psi \qquad \psi = \psi(\vec{r},t)$$

Let's consider the initial condition $\psi(\vec{r}, t=0) = \delta(\vec{r}-\vec{r}\,')$. We can find a solution of the Schrödinger equation for this particular case

$$\psi(\vec{r},t) = \sum_n e^{-i\omega_n t} c_n \varphi_n(\vec{r}) \qquad H\varphi_n(\vec{r}) = \hbar\omega_n \varphi_n(\vec{r})$$

From the initial condition I should be able to calculate c_n.

$$\psi(\vec{r},0) = \delta(\vec{r}-\vec{r}\,') = \sum_n c_n \varphi_n(\vec{r})$$

If I multiply by $\varphi^*_m(\vec{r})$ and integrate over $\vec{r}$

$$\varphi^*_m(\vec{r}\,') = \sum_n \int d\vec{r}\, c_n \varphi^*_m(\vec{r})\varphi_n(\vec{r}) = c_m .$$

$$\Rightarrow \quad \psi(\vec{r},t) = \sum_n e^{-i\omega_n t} \varphi^*_n(\vec{r}\,')\varphi_n(\vec{r}).$$

This special "wave function" with δ initial condition is called Green's function: (RETARDED)

$$iG^R(\vec{r},\vec{r}',t) = \sum_n e^{-i\varepsilon_n t/\hbar}\varphi_n^*(\vec{r}')\varphi_n(\vec{r})\,\theta(t)$$

Similarly one can define an advanced Green's function:

$$-iG^A(\vec{r},\vec{r}',t) = \sum_n e^{-i\varepsilon_n t/\hbar}\varphi_n^*(\vec{r}')\varphi_n(\vec{r})\,\theta(-t)$$

note that $\lim_{t\to 0^+} iG^R(\vec{r},\vec{r}';t) = \lim_{t\to 0^-} -iG^A(\vec{r},\vec{r}',t) = \delta(\vec{r}-\vec{r}')$. Now we can ask ourselves which is the equation of motion for the Green's functions

$$i\hbar\frac{\partial}{\partial t}(iG^R) = \sum_n \varepsilon_n e^{-i\varepsilon_n t/\hbar}\varphi_n^*(\vec{r}')\varphi_n(\vec{r})\,\theta(t) +$$

$$\sum_n i\hbar e^{-i\varepsilon_n t/\hbar}\varphi_n^*(\vec{r}')\varphi_n(\vec{r})\,\delta(t)$$

$$H(\vec{r})(iG^R) = \sum_n e^{-i\varepsilon_n t/\hbar}H(\vec{r})\varphi_n(\vec{r})\varphi_n^*(\vec{r}')\,\theta(t) = \sum_n \varepsilon_n e^{-i\varepsilon_n t/\hbar}\varphi_n^*(r')\varphi_n(r)\theta(t)$$

$$\left(i\hbar\frac{\partial}{\partial t} - H(\vec{r})\right)\cancel{i}G^R(\vec{r},\vec{r}';t) = \cancel{i}\hbar\,\delta(t)\,\delta(\vec{r}-\vec{r}')$$

$$\left(i\hbar\frac{\partial}{\partial t} - H(\vec{r})\right)G^A(\vec{r},\vec{r}';t) = \hbar\,\delta(t)\,\delta(\vec{r}-\vec{r}')$$

The general solution of the Schrödinger equation with a given initial condition $\psi(\vec{r},0)$ can be written in terms of the Green's function:

$$\psi(\vec{r},t) = \sum_n e^{-i\varepsilon_n t/\hbar}c_n\varphi_n(\vec{r})$$

$$c_n = \int d^3\vec{r}\;\psi(\vec{r},0)\,\varphi_n^*(\vec{r})$$

$$\psi(\vec{r},t>0) = \sum_n e^{-i\varepsilon_n t/\hbar}\int d\vec{r}'\,\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}')\,\psi(\vec{r}',0)\,\theta(t)$$

$$= \int d\vec{r}'\underbrace{\sum_n e^{-i\varepsilon_n t/\hbar}\varphi_n(\vec{r})\varphi_n^*(\vec{r}')\theta(t)}_{iG^R}\psi(\vec{r}',0)$$

$$\psi(\vec{r},t) = i\int d\vec{r}\,'\, G^R(\vec{r},\vec{r}\,';t)\,\psi(\vec{r}\,',0)$$

The final expression justifies also the name propagator for the Green's function.

The Green's function also admit a spectral representation:

$$i\,G^R(\vec{r},\vec{r}\,';\omega) = \int_{-\infty}^{+\infty} dt\; i\,G^R(\vec{r},\vec{r}\,';t)\,e^{i\omega t} =$$

$$\omega_n \equiv \frac{\varepsilon_n}{\hbar}$$

$$= \sum_n \varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,') \int_{-\infty}^{+\infty} dt\; e^{i\omega t}\, e^{-i\omega_n t}\,\theta(t) \;=$$

$$\int_{-\infty}^{+\infty} dt\; e^{i\omega t}\,\theta(t) = \lim_{\eta\to 0^+} \int_0^{\infty} dt\; e^{i\omega t - \eta t} = \lim_{\eta\to 0^+} \frac{-1}{i\omega - \eta}$$

$$= \lim_{\eta\to 0^+} \frac{i}{\omega + i\eta}$$

$$= i\sum_n \frac{\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')}{\omega - \omega_n + i\eta}$$

It follows that

$$\boxed{\begin{aligned} G^R(\vec{r},\vec{r}\,';\omega) &= \sum_n \frac{\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')}{\omega - \omega_n + i\eta} \\ G^A(\vec{r},\vec{r}\,';\omega) &= \sum_n \frac{\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')}{\omega - \omega_n - i\eta} \end{aligned}}$$

Formally it is thus possible to define a Green's function operator

$$\hat{G}^{R,A}(\omega) = \frac{1}{\omega - \frac{\hat{H}}{\hbar} \pm i\eta}$$ and, in the time domain $$i\,\hat{G}^{R,A}(t) = \pm e^{-i\hat{H}t/\hbar}\,\theta(\pm t)$$

In the final form is even clearer the rôle of propagator of the Green's function.

$$\Rightarrow \quad i\, G^{R,A}(\vec{r},\vec{r}\,';t) = \pm \langle \vec{r}\,| \, e^{-i\hat{H}t/\hbar} \,|\vec{r}\,'\rangle \, \theta(\pm t)$$

Physical interpretation: G is the "probability" that, if a particle is at time t=0 in r', I will find it at time t in $\vec{r}$.

The equation of motion for the formal Green's function read

$$\left(\hbar\omega - \hat{H} \pm i\eta\right) \hat{G}^{R,A}(\omega) = \mathbb{1}$$

From the spectral form of the Green's function it is natural to introduce the spectral function:

$$G^R(\vec{r},\vec{r}\,';\omega) = \sum_n \frac{\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')}{\omega - \omega_n + i\eta} =$$

$$= \int_{-\infty}^{+\infty} d\omega' \sum_n \frac{\varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')}{\omega - \omega' + i\eta}\, \delta(\omega' - \omega_n)$$

$$= \int_{-\infty}^{+\infty} d\omega' \,\frac{A(\vec{r},\vec{r}\,';\omega')}{\omega - \omega' + i\eta}$$

$$A(\vec{r},\vec{r}\,';\omega') = \sum_n \varphi_n(\vec{r})\varphi_n^*(\vec{r}\,')\,\delta(\omega' - \omega_n) \longleftarrow \text{spectral function.}$$

$A(\vec{r},\vec{r};\omega) = \sum_n |\varphi_n(\vec{r})|^2\, \delta(\omega - \omega_n)$ is the local density of states.

$$G^R(\vec{r},\vec{r}\,';\omega) - G^A(\vec{r},\vec{r}\,';\omega) = -\sum_n \varphi_n(\vec{r})\varphi_n^*(\vec{r}\,')\,\frac{2i\eta}{(\omega-\omega_n)^2+\eta^2}$$

$$= -\sum_n 2\pi i\, \varphi_n(\vec{r})\,\varphi_n^*(\vec{r}\,')\,\delta(\omega - \omega_n)$$

$$A(\vec{r},\vec{r}';\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^r(\vec{r},\vec{r}';\omega)$$

Starting from the spectral function we can also calculate the density of states:

$$g(\varepsilon) = \frac{1}{V}\sum_n \delta(\varepsilon-\varepsilon_n) = \frac{1}{V}\sum_n \delta(\varepsilon - \hbar\omega_n) = \frac{1}{\hbar V}\sum_n \delta\left(\frac{\varepsilon}{\hbar}-\omega_n\right) =$$

$$= \frac{1}{\hbar V}\sum_n \int dr\, |\varphi_n(r)|^2\, \delta\left(\frac{\varepsilon}{\hbar}-\omega_n\right) = \frac{1}{\hbar V}\int dr\, A\left(\vec{r},\vec{r};\frac{\varepsilon}{\hbar}\right)$$

Exercise: plane waves in 1D

$$\varphi_n(x) = \varphi_k(x) = \frac{1}{\sqrt{L}}e^{ikx} \qquad \omega_n = \omega_k = \frac{\hbar^2 k^2}{2m}$$

$$G^R(x,x';\omega) = \sum_n \frac{\varphi_n(x)\varphi_n^*(x')}{\omega-\omega_n+i\eta} = \sum_k \frac{\varphi_k(x)\varphi_k^*(x')}{\omega-\omega_k+i\eta}$$

$$= \cancel{\frac{L}{2\pi}}\int_{-\infty}^{+\infty} dk\, \frac{\frac{1}{\cancel{\sqrt{L}}}e^{ikx}\,\frac{1}{\cancel{\sqrt{L}}}e^{-ikx'}}{\omega - \frac{\hbar^2k^2}{2m}+i\eta} = \int \frac{dk}{2\pi}\, e^{ik(x-x')}\,\frac{1}{\omega-\omega_k+i\eta}$$

$$\Rightarrow \quad G(k,\omega) = \frac{1}{\omega-\omega_k+i\eta}$$

$$G^R(x,x';\omega) = \int_{-\infty}^{+\infty}\frac{dk}{2\pi}\,\frac{e^{ik(x-x')}}{\frac{\hbar}{2m}\left(k_\omega^2-k^2+i\eta\right)} \;\ominus$$

$$\frac{1}{k_\omega^2-k^2+i\eta} = -\frac{1}{2k_\omega}\left[\frac{1}{k-k_\omega-i\eta} - \frac{1}{k+k_\omega+i\eta}\right]$$

$$\ominus\; \frac{2m}{\hbar}\int\frac{dk}{2\pi}\left(-\frac{1}{2k_\omega}\right)\left[\frac{1}{k-k_\omega-i\eta}-\frac{1}{k+k_\omega+i\eta}\right]e^{ik(x-x')} =$$

$$= -\frac{1}{v_\omega}\left[\int \frac{dk}{2\pi}\,\frac{e^{ik(x-x')}}{k-k_\omega-i\eta} - \int \frac{dk}{2\pi}\,\frac{e^{ik(x-x')}}{k+k_\omega+i\eta}\right]$$

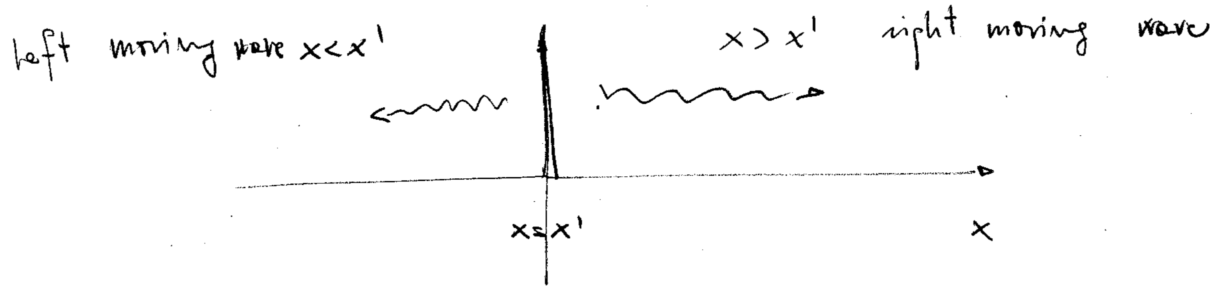
i) $x-x'>0$ $\Rightarrow$ the integration should be done with $\mathrm{Im}\,k>0$

$$G^R(x,x';\omega) = -\frac{1}{v_\omega}\frac{\cancel{2\pi} i}{\cancel{2\pi}}\, e^{ik_\omega(x-x')} = -\frac{i}{v_\omega}\, e^{ik_\omega(x-x')}$$

ii) $x-x'<0$ $\Rightarrow$ the integration should be done in the half plane $\mathrm{Im}\,k<0$

$$G^R(x,x';\omega) = -\frac{1}{v_\omega}(-1)(-2\cancel{\pi} i)\frac{1}{\cancel{2\pi}}\, e^{-ik_\omega(x-x')} = -\frac{i}{v_\omega}\, e^{-ik_\omega(x-x')}$$

$$\Rightarrow \quad G^R(x,x';\omega) = -\frac{i}{v_\omega}\, e^{ik_\omega|x-x'|}$$



$$g(\varepsilon) = -\frac{1}{L\pi\hbar}\int dx\; \mathrm{Im}\, G^R\!\left(x,x;\frac{\varepsilon}{\hbar}\right) = -\frac{1}{L\pi\hbar}\int\left(-\frac{1}{v_\varepsilon}\right)dx = \frac{1}{\pi\hbar\,\frac{\hbar k_\varepsilon}{m}}$$

$$= \frac{m}{\pi\hbar^2 k}$$

With spin: $\dfrac{2m}{\pi\hbar^2 k} = \dfrac{1}{\pi}\dfrac{k}{\varepsilon_k}$

The spectral function: $A(x,x';\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G^R(x,x';\omega) = \frac{1}{\pi v_\omega}\cos\left(k_\omega|x-x'|\right)$

the absolute value can be dropped.