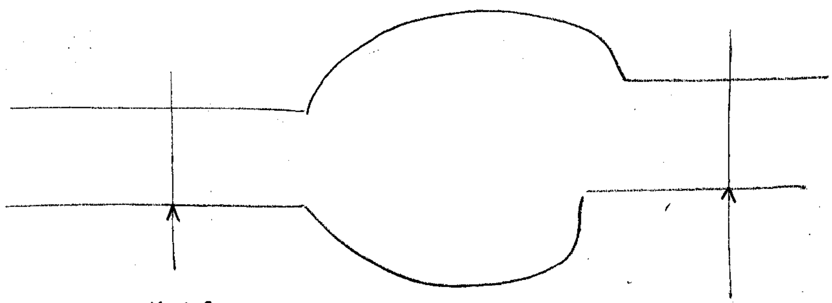
Notice that if we write the Green's function as a function of the energy we obtain

$$G^{R,A}(x, x'; \varepsilon) = -\frac{i}{\hbar v_\varepsilon} e^{i k_\varepsilon |x - x'|}$$

Fisher - Lee relation : it represents a connection between the Green's function and the S - matrix. Let's consider a different coordinate system in each lead.



$x_p = 0$ $x_q = 0$

G^R_{qp} is the Green's function calculated between a point on the $x_p = 0$ and a point on the $x_q = 0$ surface. G^R_{qp} is the solution of the Schrödinger equation in $x_q = 0$ with initial condition given by a delta function centered in $x_p = 0$. thus we can write:

$$G^R_{qp}(\varepsilon) = \delta_{qp} A^-_p(\varepsilon) + s'_{qp}(\varepsilon) A^+_p(\varepsilon)$$

- If $q = p$ => the wave function in q consists of 2 parts,

  1 - the component emerging from the δ-function and going towards the left. $A^-_p(\varepsilon)$ and the

  2 - component reflected by the scatterer: $A^+_p(\varepsilon)\, s'_{pp}(\varepsilon)$.

- If $q \neq p$ => only the transmitted component $A^+_p(\varepsilon)\, s'_{qp}(\varepsilon)$ is there.

N.B. No exponential factor are appearing by construction since we are considering the Green's function at the points connected by the S' matrix.

$$A_p^- = A_p^+ = -\frac{i}{\hbar v_p} \qquad v_p = \frac{\hbar k_p}{m} \qquad k_p = \frac{\sqrt{(E-\varepsilon_{01}^{(p)})2m}}{\hbar} \qquad S'_{qp} = S_{qp}\sqrt{v_p/v_q}$$

In other terms:

$$G^R_{qp}(\varepsilon) = -\frac{i}{\hbar v_p}\delta_{qp} - S_{qp}\sqrt{\frac{v_p}{v_q}}\frac{i}{\hbar v_p} = -\delta_{qp}\frac{i}{\hbar v_p} - S_{qp}\frac{i}{\sqrt{v_q v_p}}\frac{1}{\hbar}$$

$$\Rightarrow \quad S_{qp} = -\frac{\cancel{\sqrt{v_q v_p}}}{\cancel{v_p}}\delta_{qp} - \frac{\hbar\sqrt{v_q v_p}}{i}G^R_{qp}(\varepsilon)$$

$$\boxed{S_{qp} = -\delta_{qp} + i\hbar\sqrt{v_q v_p}\,G^R_{qp}(\varepsilon)}$$

N.B. a simplified version could be written for different leads with the same velocity in frequency. $S_{qp} = i v\, G^R_{qp}(\varepsilon) \qquad q \neq p.$

Multi-moded leads generalization

Never forget: $$G^R(\vec r, \vec r\,'; \varepsilon) = \sum_n \frac{\varphi_n(\vec r)\varphi_n^*(\vec r\,')}{\varepsilon - \varepsilon_n + i\eta} \leftarrow$$ general expression for the Green's function.

now: $\vec r \equiv x, y$

$n \equiv m, k$ where k is the longitudinal momentum

The Green's function for a multimoded lead reads:

$$G^R(x,y,x',y';\varepsilon) = \sum_{m,k}\frac{1}{L}\frac{\chi_m(y)e^{ikx}\chi_m^*(y')e^{-ikx'}}{\varepsilon - \varepsilon_{0m} - \frac{\hbar^2 k^2}{2m^*} + i\eta} = \sum_m \cancel{L}\int\frac{dk}{2\pi}\frac{1}{\cancel{L}}\cdots$$

The calculation for fixed m is the same of the one performed for the single subband case.

$$G^R(x,y,x',y';\varepsilon) = \sum_m -\frac{i}{\hbar v_m} \chi_m(y)\, \chi_m^*(y')\, e^{ik_m|x-x'|}$$

$$v_m = \frac{\hbar k_m}{m^*} \qquad k_m = \frac{\sqrt{2m^*(\varepsilon-\varepsilon_{om})}}{\hbar}$$

The physical meaning of $G^R(x,y,x',y';\varepsilon)$ is the wave function in x,y corresponding to an initial condition $\delta(x-x')\,\delta(y-y')$. Now, in analogy with the single mode case we restrict to $G^R(x_q,y_q;x_p,y_p;\varepsilon)$ and with $x_q=0$ and $x_p=0$. We define this particular G : $G^R_{qp}(y_q,y_p;\varepsilon)$

Certainly: $G^R_{qp}(y_q,y_p;\varepsilon) = \sum_{n\in q} c_n\, \chi_n(y_q)$ since it is a function of y_q and $\chi_n(y_q)$ is a complete basis. Since all modes in p can contribute to the wave function in q, the coefficient c_n reads:

$$c_n = \sum_m -\frac{i}{v_m\hbar}\, \delta_{nm}\, \chi_m^*(y_p) - \frac{i}{\hbar v_m}\, s'_{nm}\, \chi_m^*(y_p)$$

$$G^R_{qp}(y_q,y_p;\varepsilon) = \sum_{n\in q}\sum_{m\in p} -\frac{i}{v_m\hbar}\, \chi_n(y_q)\left[\delta_{nm} + \sqrt{\frac{v_m}{v_n}}\, s_{nm}\right]\chi_m^*(y_p)$$

We multiply by $\chi_{\bar n}^*(y_q)$ and $\chi_{\bar m}(y_p)$ and integrate over y_q and y_p.

$$\int dy_p\, dy_q\, G^R_{qp}(y_q,y_p;\varepsilon)\, \chi_{\bar n}^*(y_q)\, \chi_{\bar m}(y_p) = -\frac{i}{\sqrt{v_{\bar n} v_{\bar m}}\,\hbar}\left[\delta_{\bar n\bar m} + s_{\bar n\bar m}\right]$$

$\bar n \to n \quad \bar m \to m$

$$\Rightarrow \qquad s_{nm} = -\delta_{nm} + i\hbar\sqrt{v_n v_m}\int dy_q\, dy_p\, \chi_n^*(y_q)\left[G^R_{qp}(y_q,y_p)\right]\chi_m(y_p)$$

Suppose now $n \neq m$ and calculate $\bar{T}_{qp} = \sum_{n\in q}\sum_{m\in p} |s_{nm}|^2$

$$\bar{T}_{qp} = \sum_{n\in q}\sum_{m\in p} s_{nm} \cdot s_{nm}^* =$$

$$= \sum_{n\in q}\sum_{m\in p} \Big\{ i\hbar\sqrt{v_m v_n} \int dy_q\, dy_p\, \chi_n^*(y_q)\left[G^R_{qp}(y_q, y_p)\right]\chi_m(y_p) \cdot$$

$$(-i\hbar)\sqrt{v_n v_m}\int dy'_q\, dy'_p\, \chi_n(y'_q)\left[G^R_{qp}(y'_q, y'_p)\right]^* \chi_m^*(y'_p)\Big\} =$$

$$= \sum_{n\in q}\sum_{m\in p} \hbar^2 v_n v_m \int dy_q\, dy'_q\, dy_p\, dy'_p\, \chi_n(y'_q)\chi_n^*(y_q)\,\chi_m(y_p)\chi_m^*(y'_p)$$

$$\cdot\, G^R_{qp}(y_q, y_p) \cdot G^A_{pq}(y'_p, y'_q)$$

$$\Gamma_p(y_p, y'_p) = \sum_{m\in p} \chi_m(y_p)\chi_m^*(y'_p)\,\hbar v_m$$

$$= \int dy_q\, dy'_q\, dy_p\, dy'_p\; \Gamma_q(y'_q, y_q)\, G^R_{qp}(y_q, y_p)\, \Gamma_p(y_p, y'_p)\, G^A_{pq}(y'_p, y'_q)$$

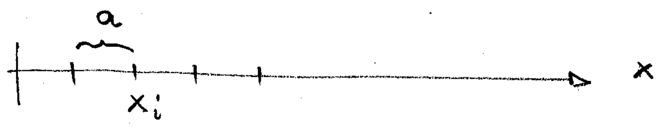
$$= \mathrm{Tr}\left\{ \Gamma_q\, G^R_{qp}\, \Gamma_p\, G^A_{pq} \right\}$$

Method of finite differences

How to calculate the Green's function and ⇒ the S-matrix for a conductor with arbitrary shape.

1D $$\left[E - H_{op}(x) + i\eta\right] G^R(x;x') = \delta(x-x')$$

Numerically I can discretize the space



$$\left[(E+i\eta)\mathbb{1} - H\right] G^R = \frac{1}{a}\mathbb{1}$$

All functions of x are transformed into vectors by the relation:

$$x \to x_i$$
$$f(x) \to f_i \equiv f(x_i)$$

Consequently the H_{op} that transforms $\psi(x)$ into $(H\psi)(x)$ and is a linear operator, is transformed into a matrix:

$$H_{ij} = \delta_{ij} U_i - t\left(\delta_{ij+1} + \delta_{ij-1}\right) + 2t\,\delta_{ij} \qquad t = \frac{\hbar^2}{2m^* a^2}$$

The first question concerns the consequences of the discretization on the spectrum. Let's assume $U_i = U_0 \ \forall i$. In the continuum we would have:

$$\psi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} \qquad E = U_0 + \frac{\hbar^2 k^2}{2m^*}$$ (periodic boundary conditions ...)

In the discrete:

$$E\psi_j = (U_0 + 2t)\psi_j - t\psi_{j-1} - t\psi_{j+1}$$

This equation is solved by

$$\psi_k(j) = \frac{1}{\sqrt{Na}} \exp(ikja)$$

$$E = U_0 + 2t - te^{-ika} - te^{ika} = U_0 + 2t(1 - \cos(ka))$$

In the limit $N \to \infty$ all k are allowed between $-\pi/a$ and π/a.

$$a \to 0 \qquad U_0 + 2t(1 - \cos(ka)) \to U_0 + \cancel{2}t\frac{k^2a^2}{\cancel{2}} = U_0 + \frac{\hbar^2}{2m^*\cancel{a^2}} \cdot k^2\cancel{a^2}.$$

$$v = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{2at}{\hbar}\sin(ka)$$

Summarizing: the discretization imposes limits to the available k. The spectrum is also distorted and the dispersion relation recovers the continuum only for low k's.

The matrix representation in 2D and in presence of a vector potential reads:

$$\begin{aligned} H_{ij} &= U(\vec{r}_i) + zt & & i=j \\ &= -\tilde{t}_{ij} & & i \text{ and } j \text{ nearest neighbours} \\ &= 0 & & \text{otherwise} \end{aligned}$$

z is the # of nearest neighbours. $\tilde{t}$ contains a factor that accounts for the vector potential:

$$\tilde{t}_{ij} = t \exp\left[\frac{ie\vec{A}\cdot(\vec{r}_i - \vec{r}_j)}{\hbar}\right]$$

$\vec{A}$ is calculated at $\frac{\vec{r}_i + \vec{r}_j}{2}$.

With these prescriptions we are now able to write a discretized version of the Hamiltonian. The Green's function can be obtained by matrix inversion.

A problem is nevertheless still open: the Green's function in the conductor contains information about the lead. Since the lead is infinite the problem still appears as numerically intractable.

Let's formulate better the problem:

$$G^R = \frac{1}{a^2}\left[(E+i\eta) - H\right]^{-1}$$

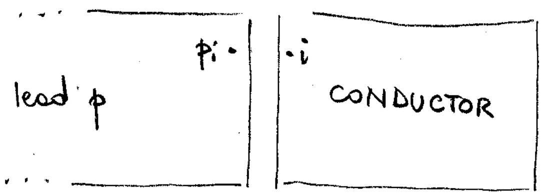
$$\begin{bmatrix} G_p & G_{pC} \\ G_{Cp} & G_C \end{bmatrix} \equiv \frac{1}{a^2}\begin{bmatrix} (E+i\eta) - H_p & \tilde{\tau}_p \\ \tau_p^{+} & E - H_c \end{bmatrix}^{-1}$$

G_p is the Green's function calculated in points belonging to the lead p

G_C ″ ″ conductor

G_{pC} and G_{Cp} are mixed.

For the calculation of the transmission we need G_c.



The dimension of H_c is $N \times N$

H_p is $\infty \times \infty$

τ_p is $\infty \times N$

G_c contains H_c, H_p, τ_p.

The crucial observation is that $\tau_p = t$ only for the points on the border $\tau_p(p_i, i) = t$ and zero otherwise.

$$\left[(E+i\eta)-H_p\right]G_{pc}+\left[\tau_p\right]G_c=0 \quad \Rightarrow \quad G_{pc}=-g_p^R\,\tau_p\,G_c\,a^2$$

$$\left[E-H_c\right]G_c+\left[\tau_p^{\dagger}\right]G_{pc}=\frac{1}{a^2} \qquad \text{where} \quad g_p^R=\frac{1}{a^2}\left[E+i\eta-H_p\right]^{-1}$$

$$G_c=\frac{1}{a^2}\left[E-H_c-\tau_p^{\dagger}g_p^R\tau_p a^2\right]^{-1}$$

Due to the particular form of τ_p we need only a finite number of elements of g_p^R. Namely: $\left[\tau_p^{\dagger}g_p^R\tau_p\right]_{ij}=t^2 g_p^R(p_i,p_j)$ where p_i and p_j are on the frontier of the lead p. It is interesting to note before proceeding with the calculation of g_p^R that the coupling to the leads is (clearly) additive:

$$G_c=\frac{1}{a^2}\left[E-H_c-\sum_p\Sigma_p^R\right]^{-1}$$

where the symbol Σ_p^R = "retarded self energy relative to lead p" has been introduced:

$$\Sigma_p^R=\tau_p^{\dagger}g_p^R\tau_p a^2.$$

<u>Self energy for a semi-infinite lead</u>

We will now prove that for a multi-moded semiinfinite lead

$$g_p^R(p_i,p_j)=-\frac{1}{at}\sum_m \chi_m(p_i)\,e^{ik_m a}\,\chi_m^*(p_j)$$

$$\Rightarrow \Sigma_p^R(i,j)=-at\sum_{m\in p}\chi_m(p_i)\,e^{ik_m a}\,\chi_m^*(p_j)$$

Continuous semi-infinite lead

eigenfunctions $\quad \psi_{m,\beta}(x) = \sqrt{\frac{2}{L}}\, \chi_m(y) \sin(\beta x) \qquad \varepsilon_{m,\beta} = \varepsilon_{m,0} + \frac{\hbar^2\beta^2}{2m^*}$

$$\Rightarrow \quad G^R(x,y;x,y') = \frac{2}{L} \sum_m \sum_{\beta=0}^{\infty} \frac{\chi_m(y)\chi_m^*(y') \sin^2(\beta x)}{\varepsilon - \varepsilon_{m,0} - \frac{\hbar^2\beta^2}{2m^*} + i\eta}$$

$\sum_\beta \to \frac{L}{\pi}\int d\beta$ different from the periodic boundary conditions since the number of states is more.

$$G^R(x,y;x,y') = \frac{2}{\pi} \sum_m \chi_m(y)\chi_m^*(y') \int_0^\infty \frac{\sin^2 \beta x}{E - \varepsilon_{m,0} - \frac{\hbar^2\beta^2}{2m^*} + i\eta}\, d\beta$$

$$\sin^2(\beta x) = \frac{2 - \exp(2i\beta x) - \exp(-2i\beta x)}{4}$$

$$G^R(x,y;x,y') = \frac{1}{2\pi} \sum_m \chi_m(y)\chi_m^*(y') \int_{-\infty}^{+\infty} \frac{[1 - \exp(i2\beta x)]}{E - \varepsilon_{m0} - \frac{\hbar^2\beta^2}{2m^*} + i\eta}\, d\beta$$

contour integration

$$G^R(x,y;x,y') = -\frac{1}{\cancel{2\pi}}\, \cancel{2\pi} i \sum_m \chi_m(y)\chi_m^*(y') \frac{1}{\hbar v_m}\left(1 - \exp(i2k_m|x|)\right)$$

$$k_m = \frac{\sqrt{2m^*(\varepsilon - \varepsilon_{m,0})}}{\hbar} \qquad v_m = \frac{\hbar k_m}{m^*}$$

$$1 - e^{2i\alpha} = e^{i\alpha}\left(\frac{e^{-i\alpha} - e^{i\alpha}}{2i}\right) 2i = -2i\, e^{i\alpha} \sin\alpha$$

$$G^R(x,y;x,y') = -\sum_m \chi_m(y)\chi_m^*(y') \frac{2\sin k_m|x|}{\hbar v_m} e^{ik_m|x|}$$

Now, in the discrete limit we set $x=-a$ (the first point in the lead!)

$$g^R(p_i,p_j) = \left[G^R(x,y;x,y') \right]_{x=-a,\ y=p_i,\ y'=p_j}$$

$$= -\sum_m \frac{2\sin(k_m a)}{\hbar v_m} \chi_m(p_i)\chi^*_m(p_j)\, e^{ik_m a} \ominus$$

$$\hbar v_m = \left.\frac{\partial E_m}{\partial \beta}\right|_{\beta=k_m} = 2at\sin(k_m a)$$

$$\ominus -\frac{1}{at}\sum_m \chi_m(p_i)\chi^*_m(p_j)\, e^{ik_m a}$$

QED.

We have already proven in the continuum limit the relation

$$T_{pq} = \mathrm{Tr}\left[\Gamma_p G^R \Gamma_q G^A\right]$$ see page 159

where $\Gamma_p = \sum_m \chi_m(y_p)\,\hbar v_m\, \chi^*_m(y'_p)$.

The discrete version reads.

$$T_{pq} = a^4 \sum_{ijrs} \Gamma_q(i,j)\, G^R_{qp}(j,r)\, \Gamma_p(r,s)\, G^A_{pq}(s,i) .$$

From the definition of the self energy we can readily see that

$$i\left(\Sigma^R_p(r,s) - \Sigma^A_p(r,s)\right) = ia\Big[(-t)\sum_{m\in p} \chi_m(p_r)\, e^{ik_m a}\chi^*_m(p_s) + t\sum_{m\in p} \chi^*_m(p_s)\, e^{-ik_m a}\chi_m(p_r)\Big]$$

$$= 2a\sum_{m\in p} \chi_m(p_r)\sin(k_m a)\,\chi^*_m(p_s) = \Gamma_p(r,s)$$

N.B. a redefinition of the Green's function as $1/E$ would compensate the factor a^4 of the transmission. Some authors adopt this convention.

Again the sum rule

$$\sum_q T_{pq} = \mathrm{Tr}\left[\Gamma_p G^R \Gamma G^A\right] \qquad \text{where} \quad \Gamma \equiv \sum_p \Gamma_p = \sum_p i\left[\Sigma_p^R - \Sigma_p^A\right]$$

The sum rule on the transmission requires

$$\mathrm{Tr}\left[\Gamma_p G^R \Gamma G^A\right] = \mathrm{Tr}\left[\Gamma G^R \Gamma_p G^A\right]$$

Using the cyclic property of the trace one obtains

$$\mathrm{Tr}\left[\Gamma_p G^R \Gamma G^A\right] = \mathrm{Tr}\left[\Gamma_p G^A \Gamma G^R\right]$$

The point is that $G^R \Gamma G^A = G^A \Gamma G^R = A \equiv i\left[G^R - G^A\right]$

proof:

$$[G^R]^{-1} - [G^A]^{-1} = \Sigma^A - \Sigma^R = i\Gamma$$

if now we multiply by G^R on the left and G^A on the right

$$G^A - G^R = i G^R \Gamma G^A$$

$$i\left(G^R - G^A\right) = G^R \Gamma G^A$$

We can repeat the operation multiplying G^R on the right and G^A on the left

QED