Scattering Theory on Graphs

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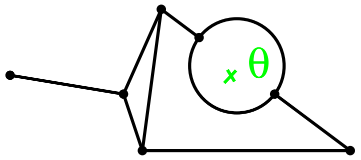
0. Foreword : definitions



Graph $\mathcal{G}$: network of 1d wires.

θ : magnetic flux

V : number of vertices α, β,... B : number of bonds $(\alpha\beta)$, $(\mu\nu)$,...

$2B$: number of arcs (oriented bond) $\alpha\beta$, $\mu\nu$,... (or i, j,...)

$a_{\alpha\beta}$: adjacency matrix $a_{\alpha\beta} = \begin{cases} 1 & \text{if } (\alpha\beta) \text{ is a bond} \\ 0 & \text{otherwise} \end{cases}$

$m_\alpha = \sum_\beta a_{\alpha\beta}$: coordinence of vertex α.

The bond $(\alpha\beta)$ is identified with $[0, l_{\alpha\beta}] \subset \mathbb{R}$.

A scalar function $\psi(x)$ on $\mathcal{G}$ has B components $\psi_{(\alpha\beta)}(x_{\alpha\beta})$.

We consider the Schrödinger operator $-\Delta + V(x)$ on $\mathcal{G}$

$$\boxed{\text{On a bond : } (\Delta\psi)_{(\alpha\beta)} = \mathrm{d}_x^2\psi_{(\alpha\beta)}(x) \quad + \quad \text{boundary conditions at vertices.}}$$

Outline

1. Introduction / Overview
2. Construction of the scattering matrix Σ
3. Spectrum of open graphs and Friedel sum rule
4. Local quantities :
   Local FSR, charge and current distributions
5. Summary

1. Introduction / Overview

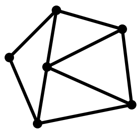
Interest of graphs in physics

⋆ Organic molecules Rudenberg, '53
⋆ Superconducting network Alexander, '83
Abilio *et al.*, '99

⋆ Quantum chaos Kottos & Smilansky, '97

⋆ Weak localisation in mesoscopic diffusive wires networks
Douçot & Rammal, '85
Pascaud & Montambaux, '99

Spectral properties of closed graphs



Spectral determinant :

$$S(\gamma) = \det(-\Delta + V(x) + \gamma) = \prod_n (\gamma + E_n)$$

Pascaud & Montambaux, PRL (1999)

Akkermans, Comtet, Desbois, Montambaux, Texier, Ann.Phys. (2000)

Desbois, J.Phys.A (2000), EPJB (2000), EPJB (2001)

- The Laplace operator ($V(x)=0$)

Continuity at vertices :

$\psi_{(\alpha\beta)}(0)=\psi_\alpha$ for β neighbour of α

$\sum_\beta a_{\alpha\beta}\mathrm{d}_x\psi_{(\alpha\beta)}(0)=0$

$\star$ A path integral derivation

$$S(\gamma)^{-1} = \frac{1}{\det(-\Delta+\gamma)} = \int_{\phi\text{ on Graph}}\mathcal{D}\phi\mathcal{D}\bar\phi\,\mathrm{e}^{-\frac{1}{2}\int_{\text{Graph}}\bar\phi(-\Delta+\gamma)\phi}$$
$$= \int\prod_{\text{vertices }\alpha}\mathrm{d}\phi_\alpha\mathrm{d}\bar\phi_\alpha\prod_{\substack{\text{bonds}\\(\alpha\beta)}}\int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta}\mathcal{D}\phi\mathcal{D}\bar\phi\,\mathrm{e}^{-\frac{1}{2}\int_0^{l_{\alpha\beta}}\mathrm{d}x\,\bar\phi(x)(-\mathrm{d}_x^2+\gamma)\phi(x)}$$

Contribution of a bond :

$$\int_{\phi(0)=\phi_\alpha}^{\phi(l_{\alpha\beta})=\phi_\beta}\mathcal{D}\phi\mathcal{D}\bar\phi\,\mathrm{e}^{-\frac{1}{2}\int_0^{l_{\alpha\beta}}\mathrm{d}x\,(|\mathrm{d}_x\phi|^2+\gamma|\phi|^2)}$$
$$= G_{l_{\alpha\beta}}^{\omega=\sqrt{\gamma}}(\vec\phi_\beta,\vec\phi_\alpha) = \langle\,\vec\phi_\beta\,|\mathrm{e}^{-\frac{l_{\alpha\beta}}{2}(-\vec\nabla_\phi^2+\gamma\vec\phi^{\,2})}|\,\vec\phi_\alpha\,\rangle$$

where

$$G_x^\omega(\vec\phi,\vec\phi\,') = \frac{\omega}{2\pi\,\mathrm{sh}(\omega x)}\mathrm{e}^{-\frac{\omega}{2\,\mathrm{sh}(\omega x)}(\mathrm{ch}(\omega x)(\vec\phi^{\,2}+\vec\phi\,'^2)-2\vec\phi\cdot\vec\phi\,')}$$

is the propagator of the 2d harmonic oscillator.

$$S(\gamma)^{-1} = \gamma^{\frac{B-V}{2}}\int\prod_{\alpha=1}^{V}\mathrm{d}\phi_\alpha\mathrm{d}\bar\phi_\alpha\prod_{(\alpha\beta)}G_{\sqrt{\gamma}l_{\alpha\beta}}^{\omega=1}(\vec\phi_\beta,\vec\phi_\alpha)$$

Then

$$S(\gamma) = \gamma^{\frac{V-B}{2}}\prod_{(\alpha\beta)}\mathrm{sh}\sqrt{\gamma}l_{\alpha\beta}\ \det M(\gamma)$$

where $M_{\alpha\beta} = \delta_{\alpha\beta}\sum_\mu a_{\alpha\mu}\coth\sqrt{\gamma}l_{\alpha\mu} - a_{\alpha\beta}\frac{1}{\mathrm{sh}\sqrt{\gamma}l_{\alpha\beta}}$

⋆ $\boxed{\text{An application : Weak localization}}$

→ correction due to disorder to thermodynamic and transport quantities in weakly disordered ($k_F\ell \gg 1$) and phase coherent ($L_\phi \gg \ell$) conductors.

ℓ : mean free path

L_ϕ : phase coherence length

→ Diffusive motion of electrons

Conductivity $\langle\sigma\rangle = \sigma_{\text{Drude}} + \langle\Delta\sigma\rangle$

weak localisation correction $\langle\Delta\sigma\rangle = -\frac{2e^2}{\pi\hbar}\frac{D}{\text{Vol}}\int_0^\infty \mathrm{d}t\, Z(t)\,\mathrm{e}^{-\gamma t}$.

Physical origin : increase of the coherent backscattering (due to interferences of time-reversed trajectories)

$Z(t) = \int \mathrm{d}\vec{r}\, P(\vec{r},\vec{r};t)$ is the heat kernel of

$$\left[\partial_t - D\left(\vec{\nabla} - \mathrm{i}\,2e\,\vec{A}\right)^2\right] P(\vec{r},\vec{r}\,';t) = \delta(\vec{r}-\vec{r}\,')$$

$\gamma^{-1} = \tau_\phi = L_\phi^2/D$: phase coherence time

$$\int_0^\infty \mathrm{d}t\, Z(t)\,\mathrm{e}^{-\gamma t} = \int_0^\infty \mathrm{d}t\,\mathrm{e}^{-\gamma t}\sum_n \mathrm{e}^{-E_n t} = \sum_n \frac{1}{\gamma+E_n}$$

$$\boxed{\langle\Delta\sigma\rangle = -\frac{2e^2}{\pi\hbar}\frac{D}{\text{Vol}}\frac{\partial}{\partial\gamma}\ln S(\gamma)} \qquad (\langle\Delta\sigma\rangle = 0 \text{ if no TRS})$$

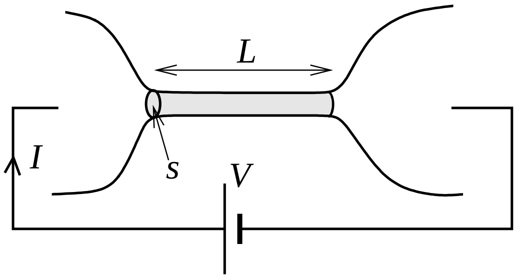
Fluctuations of conductivity :

$$\boxed{\left\langle\delta\sigma^2\right\rangle = -\frac{12e^4}{\beta\pi^2\hbar^2}\frac{D^2}{\text{Vol}^2}\frac{\partial^2}{\partial\gamma^2}\ln S(\gamma)}$$

$\beta = 1$: TRS

$\beta = 2$: no TRS

→ Diffusive wire connected to reservoirs



$L \gg \ell$: diffusive

$s \ll L^{d-1}$: quasi 1d

$L \ll L_\phi$: phase coherent

conductance : $G = \frac{I}{V} = \frac{e^2}{h} g = \frac{s}{L}\sigma$

wire perfectly connected $\Rightarrow$ Dirichlet ($\lambda = \infty$)

$$S(\gamma) = \frac{\mathrm{sh}(\sqrt{\gamma/D}\,L)}{\sqrt{\gamma}}$$

$$\frac{\partial}{\partial\gamma} \ln S(\gamma) = \frac{1}{2\gamma}\left(-1 + \sqrt{\tfrac{\gamma}{D}}\,L \coth(\sqrt{\tfrac{\gamma}{D}}\,L)\right) = \frac{L^2}{6D} - \frac{\gamma L^4}{90 D^2} + \cdots$$

$$\langle \Delta\sigma \rangle \simeq -\frac{2e^2}{\pi\hbar}\frac{D}{Ls}\frac{L^2}{6D} = -\frac{2}{3}\frac{e^2}{h}\frac{L}{s}$$

$$\boxed{\langle \Delta g \rangle = -\tfrac{2}{3}} \qquad \text{(with spin factor 2)}$$

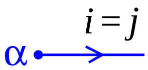
<u>UCF :</u>

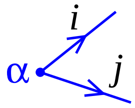
$$\left\langle \delta\sigma^2 \right\rangle \simeq \frac{12e^4}{\beta\pi^2\hbar^2}\frac{D^2}{(Ls)^2}\frac{L^4}{90D^2} = \frac{8}{15\beta}\left(\frac{e^2}{h}\right)^2\left(\frac{L}{s}\right)^2$$

$$\boxed{\left\langle \delta g^2 \right\rangle = \tfrac{8}{15\beta}} \qquad \text{(with spin factor 2)}$$

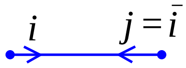
$\star$ $S(\gamma)$ in terms of arc variables :

$$S(\gamma) = \gamma^{\frac{V-B}{2}} \mathrm{e}^{\sqrt{\gamma}\,\mathcal{L}} \det(1 - QR)$$

$$Q_{ij} = \epsilon_{i\bar{j}} = \frac{2}{m_\alpha} - 1 \quad \text{if}$$ 

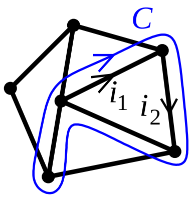
$$= \frac{2}{m_\alpha} \quad \text{if}$$ 

$$= 0 \quad \text{otherwise}$$

$$R_{ij} = \mathrm{e}^{-\sqrt{\gamma} l_i} \quad \text{if}$$ 

$$= 0 \quad \text{otherwise}$$

$\star$ Trace Formula for $Z(t) = \mathrm{Tr}\left\{\mathrm{e}^{t\Delta}\right\} = \sum_n \mathrm{e}^{-E_n t}$



$$S(\gamma) = \gamma^{\frac{V-B}{2}} \mathrm{e}^{\sqrt{\gamma}\,\mathcal{L}} \underbrace{\prod_{\tilde{C}}}_{\text{product over primitive orbits}} \left(1 - \alpha(\tilde{C})\mathrm{e}^{-\sqrt{\gamma}\, l(\tilde{C})}\right)$$

$\alpha(C) = \epsilon_{i_1 i_2}\epsilon_{i_2 i_3} \cdots \epsilon_{i_n i_1}$: weight of orbit $C = (i_1, i_2, \cdots, i_n)$.

Partition function : $\partial_\gamma \ln S(\gamma) = \sum_n \frac{1}{\gamma + E_n} = \int_0^\infty \mathrm{d}t\, Z(t)\, \mathrm{e}^{-\gamma t}$

$$Z(t) = \frac{\mathcal{L}}{2\sqrt{\pi t}} + \frac{V-B}{2} + \frac{1}{2\sqrt{\pi t}} \sum_C l(\tilde{C})\, \alpha(C)\, \mathrm{e}^{-\frac{l(C)^2}{4t}}$$

J.-P. Roth, C.R.A.S.P. (1983)

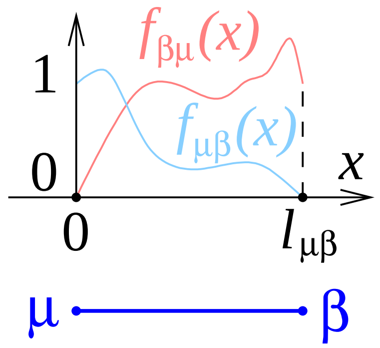
• The Schrödinger operator $-\Delta + V(x)$

Desbois, J.Phys.A (2000), EPJB (2000)

Introduce $f_{\mu\beta}(x)$ and $f_{\beta\mu}(x)$, solutions of

$$[\gamma - \mathrm{d}_x^2 + V_{(\mu\beta)}(x)]f(x) = 0$$

satisfying $\begin{cases} f_{\mu\beta}(\mu) = 1 \\ f_{\mu\beta}(\beta) = 0 \end{cases}$ and $\begin{cases} f_{\beta\mu}(\mu) = 0 \\ f_{\beta\mu}(\beta) = 1 \end{cases}$



Ex. : $V(x) = 0 \Rightarrow f_{\mu\beta}(x) = \frac{\mathrm{sh}\sqrt{\gamma}(l_{\mu\beta}-x)}{\mathrm{sh}\sqrt{\gamma}l_{\mu\beta}}$

$$S(\gamma) = \gamma^{V/2} \prod_{(\alpha\beta)} \left(\frac{\mathrm{d}f_{\beta\alpha}}{\mathrm{d}x_{\alpha\beta}}(\alpha) \right)^{-1} \det M$$

where

$$M_{\mu\beta} = \frac{1}{\sqrt{\gamma}} \left(-\delta_{\mu\beta} \sum_{\nu} a_{\mu\nu} \frac{\mathrm{d}f_{\mu\nu}}{\mathrm{d}x_{\mu\nu}}(\mu) + a_{\mu\beta} \frac{\mathrm{d}f_{\mu\beta}}{\mathrm{d}x_{\mu\beta}}(\beta) \right)$$

• Generalized boundary conditions at vertices

Desbois, EPJB (2001)

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \vdots \\ \psi_{2B}(x) \end{pmatrix} \quad \Rightarrow \quad C\psi(0) + D\psi'(0) = 0$$

$CD^\dagger$ is self-adjoint and (C, D) is of maximal rank $2B$

$$S(\gamma) = \gamma^{-B/2} \ \det(C - \sqrt{\gamma} D) \prod_{(\alpha\beta)} (R_{\alpha\beta})^{-1} \ \det(1 - QR)$$

where $R = (1 - \Omega)(1 + \Omega)^{-1}$

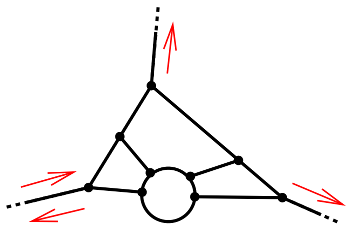
and $Q = (\sqrt{\gamma} D - C)^{-1}(\sqrt{\gamma} D + C)$

$\Omega_{\alpha\beta,\alpha\beta} = -\frac{1}{\sqrt{\gamma}} \frac{\mathrm{d} f_{\alpha\beta}}{\mathrm{d} x_{\alpha\beta}}(\alpha)$ and $\Omega_{\alpha\beta,\beta\alpha} = \frac{1}{\sqrt{\gamma}} \frac{\mathrm{d} f_{\alpha\beta}}{\mathrm{d} x_{\alpha\beta}}(\beta)$

An application (Desbois, 2001) :

the generating function of the number of closed paths in a graph with a given length and a given number of backtrackings.

Scattering on open graphs



→ Importance of scattering approach
in mesoscopic physics

⋆ Transport in phase coherent networks

Aharonov-Bohm oscillations

Büttiker, Imry & Azbel '84

Gefen, Imry & Azbel '84

Webb & Washburn, '85

...

⋆ Quantum chaos

Kottos & Smilansky, '00

⋆ Aharonov-Bohm cage effect

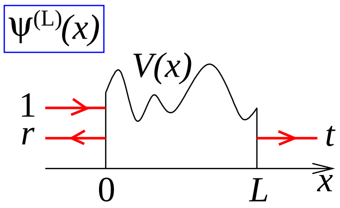
Vidal, Montambaux & Douçot '00

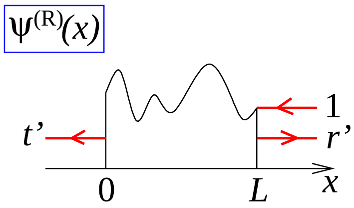
Naud *et al.* '01

Description of scattering in 1d

The 2 stationary scattering states :

solutions of $[-\mathrm{d}_x^2 + V(x)]\psi(x) = k^2\psi(x)$

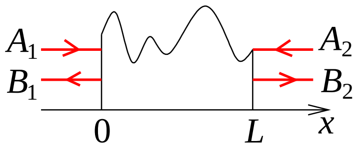




$$\psi^{(L)} = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + r\,\mathrm{e}^{-\mathrm{i}kx} & ;\ x < 0 \\ t\,\mathrm{e}^{\mathrm{i}k(x-L)} & ;\ x > L \end{cases} \qquad \psi^{(R)} = \begin{cases} t'\,\mathrm{e}^{-\mathrm{i}kx} \\ \mathrm{e}^{-\mathrm{i}k(x-L)} + r'\,\mathrm{e}^{\mathrm{i}k(x-L)} \end{cases}$$

The on-shell scattering matrix :

$$\varphi(x) = A_1\,\psi^{(L)}(x) + A_2\,\psi^{(R)}(x)$$



$$A = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} : \text{ incoming amplitudes} \qquad B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} : \text{ outgoing amplitudes}$$

$$\boxed{B = \Sigma A}$$

in one dimension : $\Sigma = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix}$.

Our purpose : Construct Σ with matrices encoding characteristics (topology, potential, fluxes) of the graph.

2. Construction of Σ

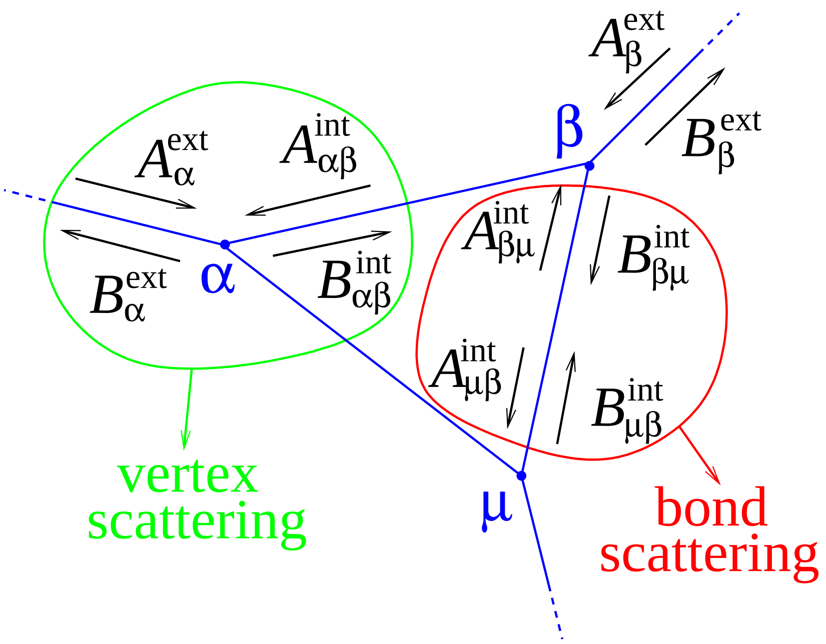
$$\left[-(\mathrm{d}_x - \mathrm{i}A(x))^2 + V(x)\right]\psi(x) = k^2\psi(x) \text{ with } x \in \mathcal{G}$$

+ boundary conditions at vertices

A. Arc Formulation

Arc $\equiv$ oriented bond

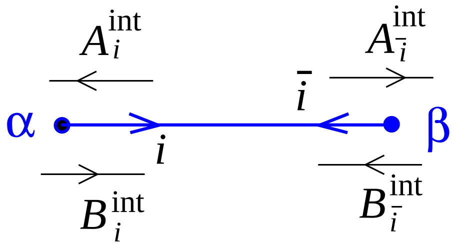
$$\boxed{B^{\mathrm{ext}} = \Sigma\, A^{\mathrm{ext}}}$$



L couples of external amplitudes : A_j^{ext}, B_j^{ext}

$2B$ couples of internal amplitudes : A_j^{int}, B_j^{int}

Scattering by bonds :

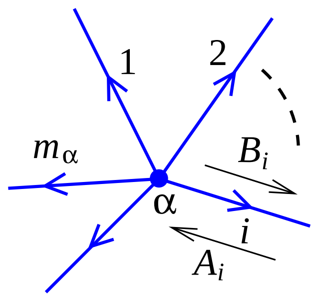


$$\begin{pmatrix} A_i^{\mathrm{int}} \\ A_{\bar{i}}^{\mathrm{int}} \end{pmatrix} = \begin{pmatrix} r_i & t_{\bar{i}} \\ t_i & r_{\bar{i}} \end{pmatrix} \begin{pmatrix} B_i^{\mathrm{int}} \\ B_{\bar{i}}^{\mathrm{int}} \end{pmatrix}$$

$$\boxed{A^{\mathrm{int}} = R\,B^{\mathrm{int}}} \qquad \text{with } R_{ij} = r_i \delta_{i,j} + t_{\bar{i}} \delta_{\bar{i},j}$$

Ex. : $V(x) = 0 \Rightarrow R_{ij} = \mathrm{e}^{ikl_j} \delta_{\bar{i},j}$

Scattering by vertices :



$$\begin{pmatrix} B_1 \\ \vdots \\ B_{m_\alpha} \end{pmatrix} = Q_\alpha \begin{pmatrix} A_1 \\ \vdots \\ A_{m_\alpha} \end{pmatrix}$$

$$B = \begin{pmatrix} B^{\mathrm{int}} \\ B^{\mathrm{ext}} \end{pmatrix} \text{ and } A = \begin{pmatrix} A^{\mathrm{int}} \\ A^{\mathrm{ext}} \end{pmatrix}$$

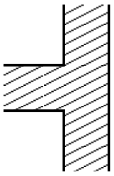
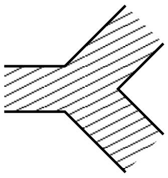
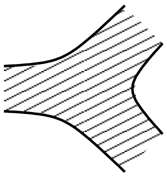
$$\boxed{B = Q\,A}$$

$$Q = \underbrace{\left(\begin{array}{c|c|c|c} Q_1 & 0 & \cdots & 0 \\ \hline 0 & Q_2 & \cdots & 0 \\ \hline \vdots & \vdots & \ddots & \vdots \\ \hline 0 & 0 & \cdots & Q_V \end{array}\right)}_{2B+L \text{ arcs}}$$

More on the scattering by vertices...

$\rightarrow$ how to choose Q_α ?

In a real network :

 ,  or 

are described by different Q_α

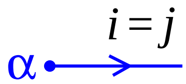
$\rightarrow$ If we choose to impose continuity of $\psi(x)$ at the vertices

- $\psi_{(\alpha\beta_i)}(x_{\alpha\beta_i} = 0) = \psi_\alpha \qquad$ for $\quad i = 1, \cdots, m_\alpha$
- $\displaystyle\sum_\beta a_{\alpha\beta}\, \mathrm{D}_x \psi_{(\alpha\beta)}(x = 0) = \lambda_\alpha \psi_\alpha$,

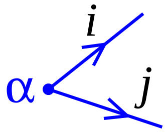
$$\lambda_\alpha = 0 : \text{Neumann}$$
$$\lambda_\alpha = \infty : \text{Dirichlet}$$

Then

$$Q_{ij} = \frac{2}{m_\alpha + \mathrm{i}\lambda_\alpha/k} - 1 \quad \text{if}$$



$$= \frac{2}{m_\alpha + \mathrm{i}\lambda_\alpha/k} \quad \text{if}$$



$$= 0 \quad \text{otherwise .}$$

$\rightarrow$ more general boundary conditions : Any unitary matrix Q.

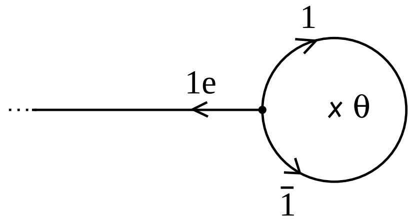
Scattering by the whole graph :

- $A^{\text{int}} = R\, B^{\text{int}}$
- $\begin{pmatrix} B^{\text{int}} \\ B^{\text{ext}} \end{pmatrix} = \left(\begin{array}{c|c} Q^{\text{int}} & \tilde{Q}^{\mathrm{T}} \\ \hline \tilde{Q} & Q^{\text{ext}} \end{array}\right) \begin{pmatrix} A^{\text{int}} \\ A^{\text{ext}} \end{pmatrix}$

Then

$$\boxed{\Sigma = Q^{\text{ext}} + \tilde{Q}\,(R^{\dagger} - Q^{\text{int}})^{-1}\,\tilde{Q}^{\mathrm{T}}}$$

Example : ring with $V(x) = 0$



Bond scattering :

$$R = \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}kl-\mathrm{i}\theta} \\ \mathrm{e}^{\mathrm{i}kl+\mathrm{i}\theta} & 0 \end{pmatrix}$$

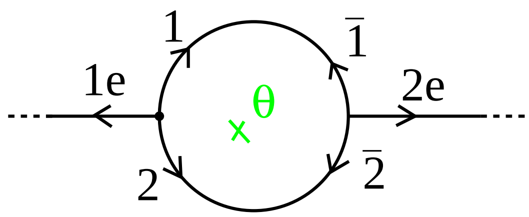
Vertex scattering :

$$Q = \left(\begin{array}{cc|c} -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \\ \hline 2/3 & 2/3 & -1/3 \end{array}\right)$$

$$\Sigma = -\tfrac{1}{3} + \begin{pmatrix} 2/3 & 2/3 \end{pmatrix} \begin{pmatrix} 1/3 & \mathrm{e}^{-\mathrm{i}kl-\mathrm{i}\theta} - 2/3 \\ \mathrm{e}^{-\mathrm{i}kl+\mathrm{i}\theta} - 2/3 & 1/3 \end{pmatrix}^{-1} \begin{pmatrix} 2/3 \\ 2/3 \end{pmatrix}$$

$$\Sigma(E) = \mathrm{e}^{\mathrm{i}\delta(E)} = -\frac{2(\cos kl - \cos\theta) + \mathrm{i}\sin kl}{2(\cos kl - \cos\theta) - \mathrm{i}\sin kl}$$

Example 2 :



in the basis $\{1,2,\bar{1},\bar{2}\}$

$$R=\begin{pmatrix} 0 & 0 & \mathrm{e}^{\mathrm{i}kl_1-\mathrm{i}\theta_1} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}kl_2-\mathrm{i}\theta_2} \\ \mathrm{e}^{\mathrm{i}kl_1+\mathrm{i}\theta_1} & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}kl_2+\mathrm{i}\theta_2} & 0 & 0 \end{pmatrix}$$

$$Q=\left(\begin{array}{cccc|cc} -1/3 & 2/3 & 0 & 0 & 2/3 & 0 \\ 2/3 & -1/3 & 0 & 0 & 2/3 & 0 \\ 0 & 0 & -1/3 & 2/3 & 0 & 2/3 \\ 0 & 0 & 2/3 & -1/3 & 0 & 2/3 \\ \hline 2/3 & 2/3 & 0 & 0 & -1/3 & 0 \\ 0 & 0 & 2/3 & 2/3 & 0 & -1/3 \end{array}\right)=\left(\begin{array}{c|c} Q^{\mathrm{int}} & \tilde{Q}^{\mathrm{T}} \\ \hline \tilde{Q} & Q^{\mathrm{ext}} \end{array}\right)$$

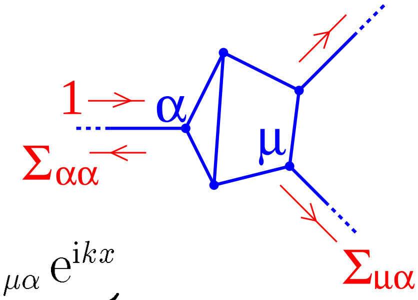
...

B. Vertex Formulation

If the wave function is continuous at the vertices

Starting point :

Consider the stationary scattering state $\psi^{(\alpha)}(x)$:



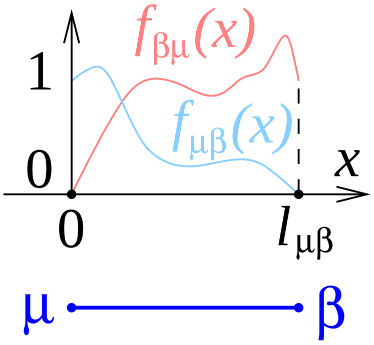
On the lead μ : $$\psi^{(\alpha)}_{\mathrm{lead}\ \mu}(x) = \underbrace{\delta_{\mu\alpha}\,\mathrm{e}^{-\mathrm{i}kx}}_{\text{incoming}} + \underbrace{\Sigma_{\mu\alpha}\,\mathrm{e}^{\mathrm{i}kx}}_{\text{outgoing}}$$

On the bond $(\mu\beta)$: $$\psi^{(\alpha)}_{(\mu\beta)}(x) = \psi^{(\alpha)}_{\mu}\, f_{\mu\beta}(x) + \psi^{(\alpha)}_{\beta}\, f_{\beta\mu}(x)$$

$f_{\mu\beta}(x)$ and $f_{\beta\mu}(x)$ are solutions of

$$[-\mathrm{d}_x^2 + V_{(\mu\beta)}(x)]f(x) = k^2 f(x)$$

satisfying $\begin{cases} f_{\mu\beta}(\mu) = 1 \\ f_{\mu\beta}(\beta) = 0 \end{cases}$ and $\begin{cases} f_{\beta\mu}(\mu) = 0 \\ f_{\beta\mu}(\beta) = 1 \end{cases}$



Coupling of the graph to the leads :

In the basis {connected vertices, internal vertices} :

$$W = \left(\begin{array}{cccc|ccc} 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 & \cdots & 0 \end{array}\right)$$

(1) Continuity

$$\psi^{(\alpha)}_{\mathrm{lead}\,\mu}(0) = \psi^{(\alpha)}_{\mu} = \delta_{\mu\alpha} + \Sigma_{\mu\alpha} \quad \text{for } \mu = 1, \cdots, L$$

(2) Current conservation

$$\textstyle\sum_\beta a_{\mu\beta} \frac{\mathrm{d}\psi^{(\alpha)}_{(\mu\beta)}}{\mathrm{d}x_{\mu\beta}}(\mu) + (W^{\mathrm{T}}W)_{\mu\mu} \frac{\mathrm{d}\psi^{(\alpha)}_{\mathrm{lead}\,\mu}}{\mathrm{d}x}(\mu) = \lambda_\mu \psi^{(\alpha)}_\mu \quad \text{for } \mu = 1, \cdots, V$$

(2') $\quad (W^{\mathrm{T}}W)_{\mu\mu}\, (\delta_{\mu\alpha} - \Sigma_{\mu\alpha}) = \sum_\beta M_{\mu\beta} \psi^{(\alpha)}_\beta \quad \text{for } \mu = 1, \cdots, V$

where

$$M_{\mu\beta} = \frac{\mathrm{i}}{k} \left(\delta_{\mu\beta} \left[\lambda_\mu - \sum_\nu a_{\mu\nu} \frac{\mathrm{d} f_{\mu\nu}}{\mathrm{d}x_{\mu\nu}}(\mu) \right] + a_{\mu\beta} \frac{\mathrm{d} f_{\mu\beta}}{\mathrm{d}x_{\mu\beta}}(\beta) \right)$$

$\psi^{(\alpha)}_\mu \longrightarrow$ the $V \times L$ matrix Ψ

$$(1)+(2') \quad \Rightarrow \quad \begin{cases} 1 + \Sigma & = W\Psi \\ W^{\mathrm{T}}(1 - \Sigma) & = M\Psi \end{cases}$$

Then

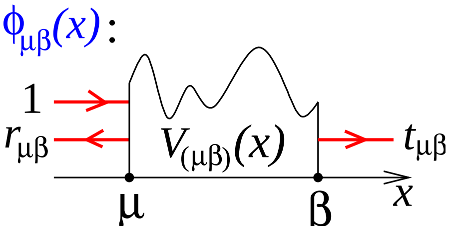
$$\boxed{\Sigma = -1 + 2\, W \left(M + W^{\mathrm{T}}W \right)^{-1} W^{\mathrm{T}}}$$

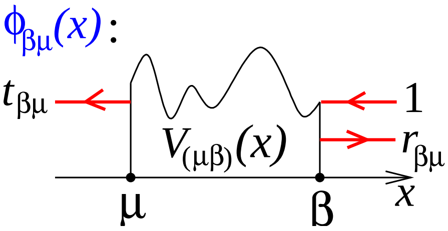
- $a_{\mu\nu}$: structure of the graph
- $f_{\mu\nu}(x)$, $f_{\nu\mu}(x)$: potential
- W : connection to the wires

Relation with reflexion/transmission coefficients of each bond ?

Another expression of the matrix $M(-k^2)$

$\phi_{\mu\beta}(x)$ and $\phi_{\beta\mu}(x)$: left and right scattering states for $V_{(\mu\beta)}(x)$:





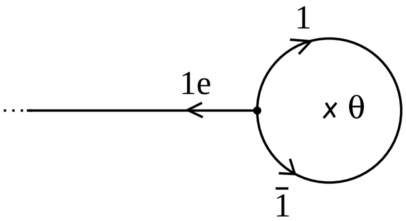
$$f_{\mu\beta}(x) = \frac{(1+r_{\beta\mu})\,\phi_{\mu\beta}(x) - t_{\mu\beta}\,\phi_{\beta\mu}(x)}{(1+r_{\mu\beta})(1+r_{\beta\mu}) - t_{\mu\beta}\,t_{\beta\mu}}$$

$$\boxed{M_{\alpha\beta} \;=\; \delta_{\alpha\beta}\left(\mathrm{i}\frac{\lambda_\alpha}{k} + \sum_\mu a_{\alpha\mu}\frac{(1-r_{\alpha\mu})(1+r_{\mu\alpha}) + t_{\alpha\mu}\,t_{\mu\alpha}}{(1+r_{\alpha\mu})(1+r_{\mu\alpha}) - t_{\alpha\mu}\,t_{\mu\alpha}}\right) - a_{\alpha\beta}\frac{2\,t_{\alpha\beta}}{(1+r_{\alpha\beta})(1+r_{\beta\alpha}) - t_{\alpha\beta}\,t_{\beta\alpha}}\,.}$$

if $V(x)=0$:

$$M_{\alpha\beta}(-k^2) = \mathrm{i}\,\delta_{\alpha\beta}\left(\frac{\lambda_\alpha}{k} + \sum_\mu a_{\alpha\mu}\,\mathrm{cotg}\,kl_{\alpha\mu}\right) - a_{\alpha\beta}\frac{\mathrm{i}\,\mathrm{e}^{\mathrm{i}\theta_{\alpha\beta}}}{\sin kl_{\alpha\beta}}$$

Example : ring with $V(x)=0$



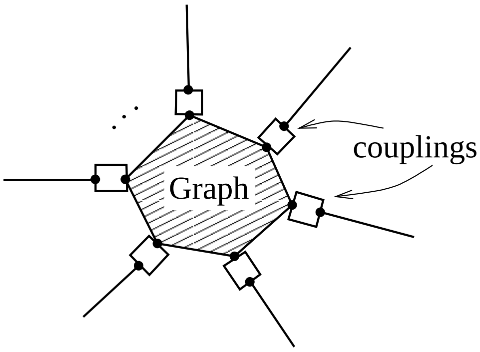
$$M = 2\mathrm{i}\left(\mathrm{cotg}\,kl - \frac{\cos\theta}{\sin kl}\right)$$

$$\Sigma = -1 + \frac{2}{M+1} = \frac{\mathrm{i}\sin kl + 2(\cos kl - \cos\theta)}{\mathrm{i}\sin kl - 2(\cos kl - \cos\theta)}$$

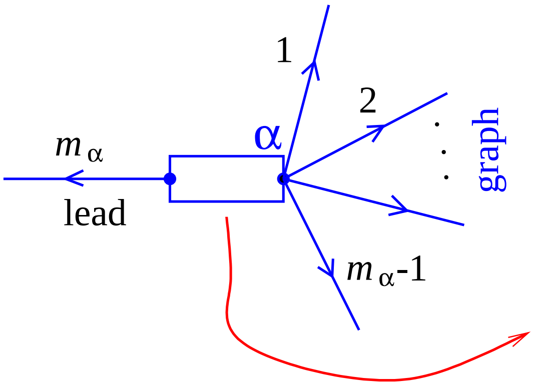
More efficient than the arc approach !

C. Tuning the coupling to the leads

$\rightarrow$ Go continuously from isolated graph to connected graph



Scattering at external vertices :



Bond scattering :

$$R = \begin{pmatrix} \cos\xi_\alpha & \sin\xi_\alpha \\ \sin\xi_\alpha & -\cos\xi_\alpha \end{pmatrix}$$

$\xi_\alpha = 0$: lead α disconnected

$\xi_\alpha = \frac{\pi}{2}$: lead α maximally coupled

$$Q_\alpha = \frac{2}{m^\star_\alpha} \left(\begin{array}{cccc|c} 1 & 1 & \cdots & 1 & w_\alpha \\ 1 & 1 & \cdots & 1 & w_\alpha \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & w_\alpha \\ \hline w_\alpha & w_\alpha & \cdots & w_\alpha & w_\alpha^2 \end{array} \right) - 1$$

$w_\alpha = \tan(\xi_\alpha/2)$

where

$m^\star_\alpha = m_\alpha - 1 + w_\alpha^2 + \mathrm{i}\lambda_\alpha/k.$

transmission amplitude between graph and lead : $t_\alpha = \frac{2w_\alpha}{1+w_\alpha^2}$

- $w_\alpha = 1$: we recover the previous Q_α.
- $w_\alpha = 0$: lead α disconnected.

The "continuity" at external vertices now reads :

$$\psi^{(\alpha)}_{\mathrm{lead}\,\mu}(0) = w_\mu \psi^{(\alpha)}_\mu$$

- "Continuity"

$$\delta_{\mu\alpha} + \Sigma_{\mu\alpha} = w_\mu \psi^{(\alpha)}_\mu \quad \text{for } \mu = 1, \cdots, L$$

- Current conservation

$$\psi^{(\alpha)^*}_\mu \sum_\beta a_{\mu\beta}\, \mathrm{d}_x \psi^{(\alpha)}_{(\mu\beta)}(\mu) + \psi^{(\alpha)*}_{\mathrm{lead}\,\mu}(\mu)\, \mathrm{d}_x \psi^{(\alpha)}_{\mathrm{lead}\,\mu}(\mu) = \lambda_\mu |\psi^{(\alpha)}_\mu|^2$$

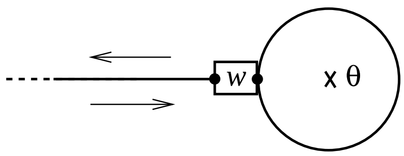
$\Rightarrow$

$$\sum_\beta a_{\mu\beta} \mathrm{d}_x \psi^{(\alpha)}_{(\mu\beta)}(\mu) + w_\mu \mathrm{d}_x \psi^{(\alpha)}_{\mathrm{lead}\,\mu}(\mu) = \lambda_\mu \psi^{(\alpha)}_\mu$$

$$\Sigma = -1 + 2\, W \left(M + W^{\mathrm{T}} W\right)^{-1} W^{\mathrm{T}} \quad \text{still holds with}$$

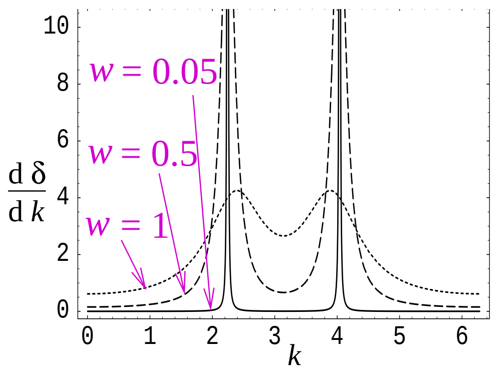
$$W = \left(\begin{array}{cccc|ccc} w_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_L & 0 & \cdots & 0 \end{array}\right)$$

Example :



$$\Sigma = \mathrm{e}^{\mathrm{i}\delta} = -1 + \frac{2w^2}{M + w^2}$$
$$= \frac{\mathrm{i}w^2 \sin kl + 2(\cos kl - \cos\theta)}{\mathrm{i}w^2 \sin kl - 2(\cos kl - \cos\theta)}$$

- resonance structure if $w \to 0$



3. Spectrum and Friedel sum rule

Existence of localized states in certain graphs

In the arc picture, the Schrödinger equation leads to :

$$\begin{cases} A^{\text{int}} = R\, B^{\text{int}} \\ B^{\text{int}} = Q^{\text{int}} A^{\text{int}} + \tilde{Q}^{\text{T}} A^{\text{ext}} \\ B^{\text{ext}} = \tilde{Q} A^{\text{int}} + Q^{\text{ext}} A^{\text{ext}} \end{cases} \quad \Rightarrow \quad \begin{cases} \tilde{Q}^{\text{T}}\, A^{\text{ext}} &= (R^\dagger - Q^{\text{int}})\, A^{\text{int}} \\ B^{\text{ext}} &= \tilde{Q}\, A^{\text{int}} + Q^{\text{ext}}\, A^{\text{ext}} \end{cases}$$

- In the general case $\det(R^\dagger - Q^{\text{int}}) \neq 0\ \forall\ E$.

  $\Rightarrow$ all solutions are the scattering states

- If $\det(R^\dagger - Q^{\text{int}}) = 0$ has a discrete set of solutions $E = E_1, E_2, \cdots$.

  $\Rightarrow$ solutions are the scattering states

  and at $E = E_n$: $A^{\text{ext}} = B^{\text{ext}} = 0$

  $$(R^\dagger - Q^{\text{int}})A^{\text{int}} = 0$$

  $$\tilde{Q} A^{\text{int}} = 0$$

  $\longrightarrow$ State localized in the graph

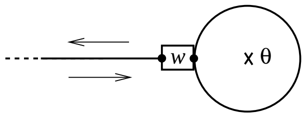
  $\longrightarrow$ These states are not probed by scattering

Coexistence of continuous and discrete parts in the spectrum :

The LDoS $\rho(x;E) = \langle\, x\, | \delta(E-H) |\, x\,\rangle$ reads :

$$\rho(x;E) = \underbrace{\sum_\alpha |\psi^{(\alpha)}(x)|^2}_{\text{continuous spectrum}} + \underbrace{\sum_n \sum_{j=1}^{g_n} \delta(E-E_n)\, |\varphi_{n,j}(x)|^2}_{\text{discrete spectrum}}$$

Example : ring threaded by a flux



$$R^\dagger - Q^{\rm int} = \begin{pmatrix} \frac{w^2}{2+w^2} & \mathrm{e}^{-\mathrm{i}kl-\mathrm{i}\theta} - \frac{2}{2+w^2} \\ \mathrm{e}^{-\mathrm{i}kl+\mathrm{i}\theta} - \frac{2}{2+w^2} & \frac{w^2}{2+w^2} \end{pmatrix}$$

$$\det(R^\dagger - Q^{\rm int}) = \tfrac{2}{2+w^2}\mathrm{e}^{-\mathrm{i}kl}\left[2(\cos\theta - \cos kl) + \mathrm{i}w^2\sin kl\right]$$

- Non degenerate spectrum $\boldsymbol{\theta \neq 0}$ and $\boldsymbol{\pi}$

$$\det(R^\dagger - Q^{\rm int}) \neq 0$$

$$\rho(x;E) = |\psi(x)|^2 = \left|\frac{w}{\sqrt{\pi k}}\frac{\sin k(l-x) + \mathrm{e}^{-\mathrm{i}\theta}\sin kx}{2(\cos\theta - \cos kl) + \mathrm{i}w^2\sin kl}\right|^2$$

- Degenerate spectrum $\boldsymbol{\theta = 0}$

$$\det(R^\dagger - Q^{\rm int}) = \tfrac{4}{2+w^2}\mathrm{e}^{-\mathrm{i}kl}\left[2\sin(kl/2) + \mathrm{i}w^2\cos(kl/2)\right]\sin(kl/2)$$

$$\det(R^\dagger - Q^{\rm int}) = 0 \text{ for } k_n = 2n\pi/l.$$

$\star$ At $\boxed{k \neq k_n}$ $\Rightarrow$ solution is the scattering state.

$\star$ At $\boxed{k = k_n}$ $\Rightarrow$ two solutions

- $A^{\rm int} = (1,1) \times A^{\rm ext}/w$ is the scattering state
- $A^{\rm int} = (1,-1)$ with $A^{\rm ext} = B^{\rm ext} = 0$
  is localized in the ring : $(R^\dagger - Q^{\rm int})A^{\rm int} = 0$ & $\tilde{Q}A^{\rm int} = 0$

$$\rho(x;E) = \left|\frac{w}{\sqrt{\pi k}}\frac{\cos k(x-l/2)}{2\sin(kl/2) + \mathrm{i}w^2\cos(kl/2)}\right|^2 + \sum_{n=1}^{\infty}\delta(E-k_n^2)\left|\sqrt{2/l}\,\sin k_n x\right|^2$$

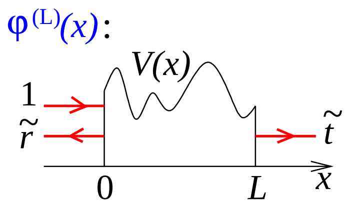
Friedel Sum Rule :

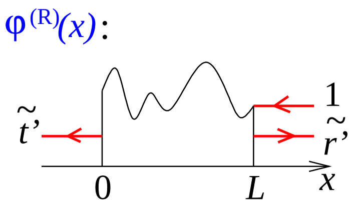
Relation between spectral and scattering properties

$\rightarrow$ Count the states with the scattering matrix

KREIN-FRIEDEL RELATION IN $d = 1$

Local DoS : $\rho(x;E) = \langle\, x\,|\delta(E-H)|\, x\,\rangle$.





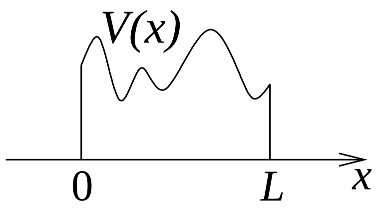
$$\varphi^{(L)} = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + \tilde{r}\,\mathrm{e}^{-\mathrm{i}kx} & ;\ x < 0 \\ \tilde{t}\,\mathrm{e}^{\mathrm{i}kx} & ;\ x > L \end{cases} \qquad \varphi^{(R)} = \begin{cases} \tilde{t}'\,\mathrm{e}^{-\mathrm{i}kx} \\ \mathrm{e}^{-\mathrm{i}kx} + \tilde{r}'\,\mathrm{e}^{\mathrm{i}kx} \end{cases}$$

$$\tilde{\Sigma} = \begin{pmatrix} \tilde{r} & \tilde{t}' \\ \tilde{t} & \tilde{r}' \end{pmatrix} = \mathcal{U} \begin{pmatrix} \mathrm{e}^{2\mathrm{i}\eta_1} & 0 \\ 0 & \mathrm{e}^{2\mathrm{i}\eta_2} \end{pmatrix} \mathcal{U}^\dagger$$

Variation of the total DoS due to the presence of $V(x)$:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\ [\rho(x;E) - \rho_0(x;E)] = \frac{1}{\pi}\sum_\sigma \frac{\mathrm{d}\eta_\sigma}{\mathrm{d}E} = \frac{1}{2\mathrm{i}\pi}\mathrm{Tr}\{\tilde{\Sigma}^\dagger \frac{\mathrm{d}\tilde{\Sigma}}{\mathrm{d}E}\}$$

$\boxed{\text{THE SMITH RELATION}}$



One-dimensional case :

LDoS integrated in the scattering region :

$$\int_0^L \mathrm{d}x\, \rho(x;E) = \sum_{\alpha=L,R} \int_0^L \mathrm{d}x\, |\psi^{(\alpha)}(x)|^2$$

$$= \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\mathrm{Tr}\left\{\Sigma - \Sigma^\dagger\right\}\right)$$

Case of graphs :

If ψ is solution of $(-\mathrm{D}_x^2 + V(x))\psi(x) = E\psi(x)$ then

$$\frac{\mathrm{d}}{\mathrm{d}x}\Omega(x) = |\psi(x)|^2$$

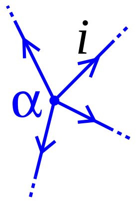
where $\Omega = (\mathrm{D}_x\psi)^* \frac{\mathrm{d}\psi}{\mathrm{d}E} - \psi^* \left(\mathrm{D}_x \frac{\mathrm{d}\psi}{\mathrm{d}E}\right)$

On the bond : $\psi_{(\mu\beta)}(x_{\mu\beta}) \longrightarrow \Omega_{\mu\beta}(x_{\mu\beta})$

$$\boxed{\int_0^{l_{\mu\beta}} \mathrm{d}x\, |\psi_{(\mu\beta)}(x)|^2 = -\Omega_{\mu\beta}(\mu) - \Omega_{\beta\mu}(\beta)}$$

At the vertex α :

$$\sum_i \mathrm{D}_x\psi_i(\alpha) = \lambda_\alpha\psi_\alpha \;\Rightarrow\; \sum_i \Omega_i(\alpha) = 0$$



$$\boxed{\sum_\beta a_{\mu\beta}\, \Omega_{\mu\beta}(\mu) + (W^{\mathrm{T}}W)_{\mu\mu}\, \Omega_{\mathrm{lead}\,\mu}(\mu) = 0}$$

Integration in the graph :

$$\int_{\text{Graph}} \mathrm{d}x \, |\psi^{(\alpha)}(x)|^2 = \sum_{(\mu\beta)} \int_0^{l_{\mu\beta}} \mathrm{d}x \, |\psi^{(\alpha)}_{(\mu\beta)}(x)|^2$$
$$= -\sum_{\text{arc }\mu\beta} \Omega^{(\alpha)}_{\mu\beta}(\mu) = \sum_{\mu} \Omega^{(\alpha)}_{\text{lead }\mu}(\mu)$$

In the lead :

$$\psi^{(\alpha)}_{\text{lead }\mu}(x) = \frac{1}{\sqrt{4\pi k}} \left(\delta_{\mu\alpha} \, \mathrm{e}^{-\mathrm{i}kx} + \Sigma_{\mu\alpha} \, \mathrm{e}^{\mathrm{i}kx}\right)$$

then

$$\Omega^{(\alpha)}_{\text{lead }\mu}(\mu) = -\frac{\mathrm{i}}{2\pi} \Sigma^*_{\mu\alpha} \frac{\mathrm{d}\Sigma_{\mu\alpha}}{\mathrm{d}E} - \frac{\mathrm{i}}{8\pi E} \left(\delta_{\mu\alpha} + \Sigma^*_{\mu\alpha}\right) \left(-\delta_{\mu\alpha} + \Sigma_{\mu\alpha}\right)$$

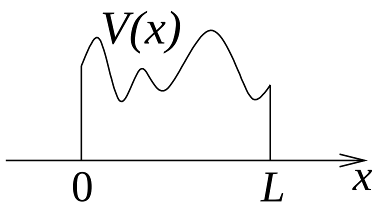
$$\int_{\text{Graph}} \mathrm{d}x \, |\psi^{(\alpha)}(x)|^2 = -\frac{\mathrm{i}}{2\pi} \left(\Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right)_{\alpha\alpha} - \frac{\mathrm{i}}{8\pi E} \left(\Sigma - \Sigma^\dagger\right)_{\alpha\alpha}$$

$$\boxed{\sum_{\alpha} \int_{\text{Graph}} \mathrm{d}x \, |\psi^{(\alpha)}(x)|^2 = \frac{1}{2\mathrm{i}\pi} \left(\mathrm{Tr}\left\{ \Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E} \right\} + \frac{1}{4E} \mathrm{Tr}\left\{ \Sigma - \Sigma^\dagger \right\} \right)}$$

$\longrightarrow$ This is not always related to the DoS of the graph

Relation between spectral and scattering properties

$\boxed{\text{THE SMITH RELATION}}$ (Another derivation)



• One-dimensional case :

Local DoS : $\rho(x;E) = \langle x|\delta(E-H)|x\rangle$.

LDoS integrated in the scattering region :

$$\int_0^L \mathrm{d}x\,\rho(x;E) = \sum_{\alpha=L,R}\int_0^L \mathrm{d}x\,|\psi^{(\alpha)}(x)|^2$$
$$= \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\mathrm{Tr}\left\{\Sigma-\Sigma^\dagger\right\}\right)$$

• Case of graphs :

On the bond $(\mu\beta)$: $\quad \psi^{(\alpha)}_{(\mu\nu)}(x) = \psi^{(\alpha)}_\mu\, f_{\mu\nu}(x) + \psi^{(\alpha)}_\nu\, f_{\nu\mu}(x)$

Wave function $\psi^{(\alpha)}(x)$ at the nodes μ, $\psi^{(\alpha)}_\mu \equiv \Psi_{\mu\alpha}$:

$$\Psi = \frac{1}{\sqrt{\pi k}}\frac{1}{M+W^\mathrm{T}W}W^\mathrm{T}$$

We define

$$\rho^{(\alpha,\beta)}(E) = \int_{\mathrm{Graph}}\mathrm{d}x\,\psi^{(\alpha)}_E(x)^*\,\psi^{(\beta)}_E(x) = \sum_{(\mu\nu)}\int_0^{l_{\mu\nu}}\mathrm{d}x\,\psi^{(\alpha)}_{(\mu\nu)}(x)^*\,\psi^{(\beta)}_{(\mu\nu)}(x)$$

Using

$$\int_0^{l_{\mu\nu}}\mathrm{d}x\,f_{\mu\nu}(x)^2 = \partial_E\frac{\mathrm{d}f_{\mu\nu}}{\mathrm{d}x_{\mu\nu}}(\mu)$$
$$\int_0^{l_{\mu\nu}}\mathrm{d}x\,f_{\mu\nu}(x)f_{\nu\mu}(x) = -\partial_E\frac{\mathrm{d}f_{\mu\nu}}{\mathrm{d}x_{\mu\nu}}(\nu)$$

we obtain :

$$\rho^{(\alpha,\beta)}(E) = \sum_{\mu,\nu}\psi^{(\alpha)*}_\mu\,\partial_E\left(\mathrm{i}\sqrt{E}\,M_{\mu\nu}\right)\,\psi^{(\beta)}_\nu \qquad (1)$$

$$
\begin{aligned}
\rho^{(\alpha,\beta)}(E) &= \left(\Psi^\dagger \frac{\mathrm{d}}{\mathrm{d}E}\left(\mathrm{i}\sqrt{E}\,M\right)\,\Psi\right)_{\alpha\beta} \\
&= -\frac{1}{2\mathrm{i}\pi}\left(W\frac{1}{-M+W^\mathrm{T}W}\left[2\frac{\mathrm{d}M}{\mathrm{d}E}+\frac{1}{E}M\right]\frac{1}{M+W^\mathrm{T}W}W^\mathrm{T}\right)_{\alpha\beta}
\end{aligned}
$$

since

$$
\frac{\mathrm{d}\Sigma}{\mathrm{d}E} = -2W\frac{1}{M+W^\mathrm{T}W}\frac{\mathrm{d}M}{\mathrm{d}E}\frac{1}{M+W^\mathrm{T}W}W^\mathrm{T}
$$

we obtain

$$
\rho^{(\alpha,\beta)}(E) = \frac{1}{2\mathrm{i}\pi}\left(\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}+\frac{1}{4E}(\Sigma-\Sigma^\dagger)\right)_{\alpha\beta}
$$

With a trace

$$
\sum_\alpha \int_{\mathrm{Graph}} \mathrm{d}x\,|\psi^{(\alpha)}(x)|^2 = \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\}+\frac{1}{4E}\,\mathrm{Tr}\left\{\Sigma-\Sigma^\dagger\right\}\right)
$$

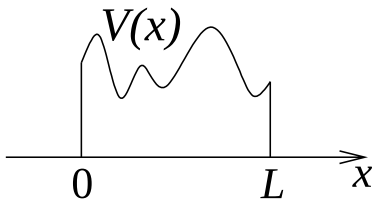
This is not always related to $\int_{\mathrm{Graph}}\mathrm{d}x\,\rho(x;E)$

The discrete part of the spectrum is not probed by scattering

FSR : Relation between spectral and scattering properties

Counting the states from Σ

THE SMITH RELATION



• One-dimensional case :

Local DoS : $\rho(x;E) = \langle\, x\,|\delta(E-H)|\,x\,\rangle$.

LDoS integrated in the scattering region :

$$\int_0^L \mathrm{d}x\,\rho(x;E) = \sum_{\alpha=L,R}\int_0^L \mathrm{d}x\,|\psi^{(\alpha)}(x)|^2$$
$$= \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\mathrm{Tr}\left\{\Sigma-\Sigma^\dagger\right\}\right)$$

• Case of graphs : $\rho(x;E) = \rho_{\mathrm{cont}}(x;E) + \rho_{\mathrm{disc}}(x;E)$

We can prove that

$$\sum_\alpha\int_{\mathrm{Graph}}\mathrm{d}x\,|\psi^{(\alpha)}(x)|^2 = \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\mathrm{Tr}\left\{\Sigma-\Sigma^\dagger\right\}\right)$$

which is $\int_{\mathrm{Graph}}\mathrm{d}x\,\rho_{\mathrm{cont}}(x;E)$, the continuous part of $\int_{\mathrm{Graph}}\mathrm{d}x\,\rho(x;E)$

The discrete part of the spectrum
is not probed by scattering

“Violation” of FSR in certain graphs

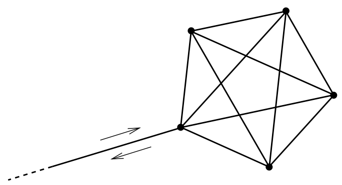
IDoS of the graph : $\mathcal{N}(E) = \int_{-\infty}^{E} \mathrm{d}E' \int_{\text{Graph}} \mathrm{d}x\, \rho(x; E')$

If $V(x) = 0 \;\Rightarrow\; \mathcal{N}_{\text{Weyl}}(E) = \frac{\mathcal{L}k}{\pi}$
where $\mathcal{L} = \frac{1}{2}\sum_{\alpha,\beta} a_{\alpha\beta} l_{\alpha\beta}$ is the “volume” of the graph

$\rightarrow$ We compare $\mathcal{N}_{\text{Weyl}}(E)$ and $\frac{1}{2\pi}\delta^f(E)$

where $\delta^f(E) = -\mathrm{i} \ln \det \Sigma$

The complete graph K_V : (highly degenerate spectrum)



IDoS :

$$\mathcal{L} = B\ell = \frac{V(V-1)}{2}\ell \Rightarrow \mathcal{N}_{\text{Weyl}}(E) = \frac{V(V-1)}{2\pi} k\ell$$

Scattering : $\Sigma = \mathrm{e}^{\mathrm{i}\delta^f}$ with

$$\mathrm{cotg}(\delta^f/2) = \cos\varphi \frac{\cos k\ell + \cos\varphi - 1}{\cos k\ell + \cos\varphi} \mathrm{cotg}(k\ell/2)$$

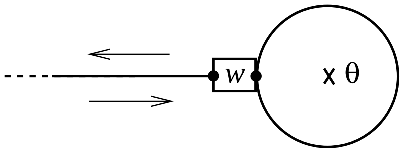
where $\cos\varphi = \frac{1}{V-1}$

$$\left(\frac{\delta^f(E)}{2\pi}\right)_{\text{Weyl}} = \frac{3k\ell}{2\pi}$$

$$\mathcal{N}_{\text{Weyl}}(E) \neq \left(\frac{\delta^f(E)}{2\pi}\right)_{\text{Weyl}}$$

The counting method from scattering misses states

Ring threaded by a flux :



isolated ring ($w=0$) :

$$S(-k^2) = \cos kl - \cos\theta$$

spectrum : $k_n^{\pm} = \frac{1}{l}\left(2n\pi \pm \theta\right)$

$$\varphi_n^{\pm}(x) = \frac{1}{\sqrt{l}}\mathrm{e}^{\mp 2\mathrm{i}\pi n x/l}$$

$\rightarrow$ Construction of the stationary scattering state :

$$\psi_{\mathrm{lead}}(x) = \frac{1}{\sqrt{4\pi k}}\left(\mathrm{e}^{-\mathrm{i}kx} + \mathrm{e}^{\mathrm{i}kx+\mathrm{i}\delta}\right)$$

where $\mathrm{cotg}(\delta/2) = \frac{w^2\sin kl}{2(\cos\theta - \cos kl)}$

$$\psi_{\mathrm{ring}}(x) = \psi_1 \frac{\mathrm{e}^{\mathrm{i}\theta x/l}}{\sin kl}\left(\sin k(l-x) + \mathrm{e}^{-\mathrm{i}\theta}\sin kx\right)$$

where where $\psi_1 = \frac{1}{\sqrt{\pi k}}\,\frac{w\sin kl}{w^2\sin kl + 2\mathrm{i}(\cos kl - \cos\theta)} = \frac{1}{w}\psi_{\mathrm{lead}}(0)$

We study the weak coupling $w \to 0$ limit

• Non degenerate spectrum $\boldsymbol{\theta \neq 0}$ and $\boldsymbol{\pi}$

$$\psi_{\mathrm{ring}}(x) \underset{k\sim k_n^{\pm}}{\simeq} \frac{1}{\sqrt{\pi k}}\,\frac{\mathrm{i}w/2l}{k - k_n^{\pm} + \mathrm{i}w^2/2l}\,\mathrm{e}^{\mp 2\mathrm{i}\pi n x/l}$$

$$\int_0^l \mathrm{d}x\,|\psi_{\mathrm{ring}}(x)|^2 \underset{k\sim k_n^{\pm}}{\simeq} \frac{1}{2k}\,\frac{1}{\pi}\,\frac{w^2/2l}{(k-k_n^{\pm})^2 + (w^2/2l)^2} \underset{w\to 0}{\longrightarrow} \frac{1}{2k}\delta(k - k_n^{\pm}) = \delta(E - [k_n^{\pm}]^2)$$

which is the correct DoS of the isolated ring.

• Degenerate spectrum $\boldsymbol{\theta = 0}$

$$\psi_{\text{ring}}(x) \underset{k\sim k_n}{\simeq} \frac{1}{\sqrt{\pi k}} \frac{\mathrm{i}w/l}{k-k_n+\mathrm{i}w^2/l} \underbrace{\cos(2n\pi x/l)}_{\text{symmetric wave fct}}$$

$$\int_0^l \mathrm{d}x\,|\psi_{\text{ring}}(x)|^2 \underset{k\sim k_n}{\simeq} \frac{1}{2k}\frac{1}{\pi}\frac{w^2/l}{(k-k_n)^2+(w^2/l)^2} \underset{w\to 0}{\longrightarrow} \frac{1}{2k}\delta(k-k_n) = \delta(E-k_n^2)$$

the degeneracy 2 is missing

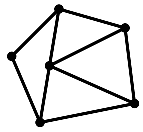
The antisymmetric wave function $\sin(2n\pi x/l)$ vanishes at the vertex
$\Rightarrow$ this state is not probed by scattering

Discontinuous behaviour of Σ as a function of certain parameters (length, fluxes,...)

4. Local quantities related to Σ

• Generalities X a physical quantity ($\mathcal{M}$, $\rho(x)$, I,...)
and f its conjugate force ($-\mathcal{B}$, $V(x)$, $-\phi$,...)

$\star$ Isolated system at equilibrium : $\varphi_n(x)$, E_n

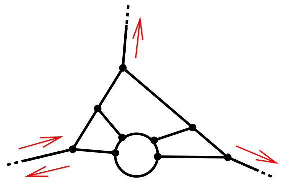


$$\langle\,\psi_n\,|X|\,\psi_n\,\rangle = \frac{\partial E_n}{\partial f}$$

$\star$ Open system out of equilibrium :

Scattering approach $\Rightarrow$ $\psi_E^{(\alpha)}(x)$, $\Sigma_{\alpha\beta}$

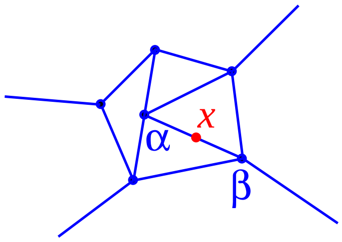
$$\langle\,\psi_E^{(\alpha)}\,|X|\,\psi_E^{(\beta)}\,\rangle = -\frac{1}{2\mathrm{i}\pi}\left(\Sigma^\dagger\frac{\partial\Sigma}{\partial f}\right)_{\alpha\beta}$$



$\boxed{\text{Local DoS, Injectivities,...}}$

How to calculate $\frac{\delta\,\Sigma}{\delta V(x)}$?

$$\Sigma[V(x') + \lambda\,\delta(x'-x)] = \Sigma[V(x')] + \lambda\frac{\delta\,\Sigma}{\delta V(x)}[V(x')] + \cdots$$



$\Rightarrow$ add a vertex of weight λ at x

$$\frac{\delta\,\Sigma}{\delta V(x)} = -\frac{2\mathrm{i}}{k}W\frac{1}{M+W^{\mathrm{T}}W}K(x)K(x)^\dagger\frac{1}{M+W^{\mathrm{T}}W}W^{\mathrm{T}}$$

$$\text{with } K(x) = \begin{array}{c}\left(\begin{array}{c}\vdots\\ 0\\ f_{\alpha\beta}(x)\mathrm{e}^{-\mathrm{i}\theta_{\alpha x}}\\ f_{\beta\alpha}(x)\mathrm{e}^{-\mathrm{i}\theta_{\beta x}}\\ 0\\ \vdots\end{array}\right)\end{array}\begin{array}{l}\\ \\ \leftarrow\ \alpha\\ \leftarrow\ \beta\\ \\ \\ \end{array}$$

$\Rightarrow$ Algebraic calculations.

- Functional derivative of Σ :

$$-\frac{1}{2\mathrm{i}\pi}\frac{\delta\,\Sigma_{\alpha\beta}}{\delta V(x)} = \psi^{t.r.(\alpha)}(x)\,\psi^{(\beta)}(x)$$

where $\psi^{t.r.(\alpha)}(x;\{\theta_{\mu\nu}\}) = \psi^{(\alpha)}(x;\{-\theta_{\mu\nu}\})$ is the wave function of the "time reversed graph"

$$-\frac{1}{2\mathrm{i}\pi}\left(\Sigma^\dagger\frac{\delta\,\Sigma}{\delta V(x)}\right)_{\alpha\beta} = \psi^{(\alpha)}(x)^*\,\psi^{(\beta)}(x)$$

- Injectivities :

$$\rho(x,\alpha;E) = -\frac{1}{2\mathrm{i}\pi}\left(\Sigma^\dagger\frac{\delta\,\Sigma}{\delta V(x)}\right)_{\alpha\alpha} = |\psi_E^{(\alpha)}(x)|^2$$

- Emissivities :

$$\rho(\alpha,x;E) = -\frac{1}{2\mathrm{i}\pi}\left(\frac{\delta\,\Sigma}{\delta V(x)}\Sigma^\dagger\right)_{\alpha\alpha} = |\psi_E^{t.r.(\alpha)}(x)|^2$$

- LDoS (continuous part) :

$$\rho_{\mathrm{cont}}(x;E) = \sum_\alpha \rho(x,\alpha;E) = \sum_\alpha |\psi_E^{(\alpha)}(x)|^2$$

$$\rho_{\mathrm{cont}}(x;E) = -\frac{1}{2\mathrm{i}\pi}\frac{\delta}{\delta V(x)}\ln\det\Sigma$$

- Integration over the graph :

$$-\int_{\mathrm{Graph}}\mathrm{d}x\,\Sigma^\dagger\frac{\delta\,\Sigma}{\delta V(x)} = \Sigma^\dagger\frac{\mathrm{d}\,\Sigma}{\mathrm{d}E} + \frac{1}{4E}\left(\Sigma-\Sigma^\dagger\right)$$

Application :

Charge in a graph out of equilibrium

Charge operator :

$$\hat{Q}(t) = \int_{\text{Graph}} \mathrm{d}x\, \hat{\psi}^\dagger(x,t)\hat{\psi}(x,t)$$

where the field operator is

$\hat{\psi}(x,t) = \sum_{\alpha=1}^{L} \int_0^\infty \mathrm{d}E\, \psi_E^{(\alpha)}(x)\, \hat{a}_\alpha(E)\, \mathrm{e}^{-\mathrm{i}Et}$

DoS matrix

$$\begin{aligned}\rho^{(\alpha,\beta)}(E) &\stackrel{\text{def}}{=} \langle\, \psi_E^{(\alpha)}\, |\hat{Q}(t)|\, \psi_E^{(\beta)}\, \rangle = \int_{\text{Graph}} \mathrm{d}x\, \psi_E^{(\alpha)}(x)^*\, \psi_E^{(\beta)}(x) \\ &= \frac{1}{2\mathrm{i}\pi}\left(\Sigma^\dagger \frac{\mathrm{d}\,\Sigma}{\mathrm{d}E} + \frac{1}{4E}\left(\Sigma - \Sigma^\dagger\right)\right)_{\alpha\beta}\end{aligned}$$

Average charge

$$\langle \hat{Q}(t) \rangle = \sum_\alpha \int \mathrm{d}E\, f_\alpha(E)\, \rho^{(\alpha,\alpha)}(E)$$

$\rightarrow$The concept of injectivity is necessary to describe the out of equilibrium situation

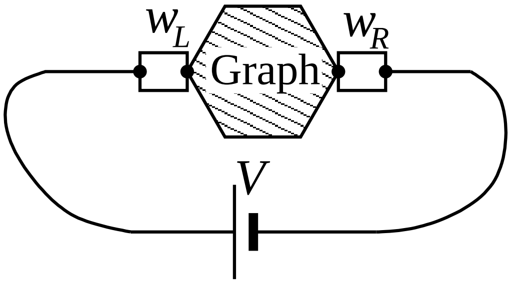
Charge fluctuations

$$S_{QQ}(\omega) \stackrel{\text{def}}{=} \int \mathrm{d}t\, \left(\langle \hat{Q}(t)\, \hat{Q}(0)\rangle - \langle \hat{Q}(t)\rangle\langle \hat{Q}(0)\rangle\right)\, \mathrm{e}^{\mathrm{i}\omega t}$$

$$S_{QQ}(\omega = 0) = 2\pi \sum_{\alpha,\beta} \int \mathrm{d}E\, f_\alpha(1 - f_\beta)\, \rho^{(\alpha,\beta)}(E)\, \rho^{(\beta,\alpha)}(E)$$

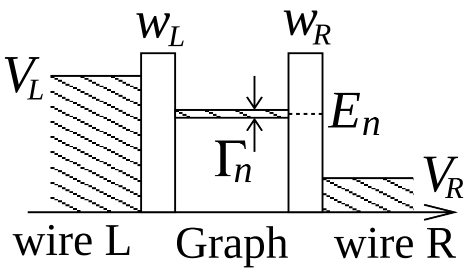
Example :

A graph with two leads



For one resonant level E_n of width $\Gamma_n = \Gamma_{n,L} + \Gamma_{n,R}$

$$\Gamma_{n,\alpha} = w_\alpha^2 \sqrt{E_n}\, |\varphi_n(\alpha)|^2.$$



$$\langle \hat{Q}(t) \rangle \simeq \frac{\Gamma_{n,L}}{\Gamma_n}$$

$$S_{QQ}(\omega = 0) \simeq \frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n^3}$$

Compare to the average current :

$\langle I \rangle \simeq 2\frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n}$

and the shot noise :

$S_{II}(\omega = 0) \simeq 2\frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n^3}(\Gamma_{n,R}^2 + \Gamma_{n,L}^2).$

$\rightarrow$ Finite frequency :

$$S_{QQ}(\omega) \simeq S_{QQ}(0)\frac{1}{1 + (\omega/2\Gamma_n)^2} \quad \text{for } \omega \ll V$$

Current distribution inside a graph

⋆ Current in the external wires :

average currents : conductances

correlations : shot noise

⋆ Current in the internal wires :

→ At equilibrium

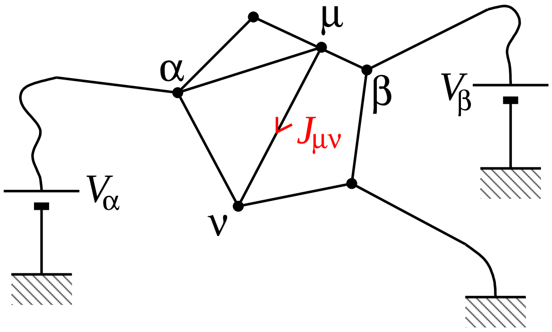
Relation between persistent current and scattering matrix :

Akkermans *et al.*, 1991

Correlation function :

Taniguchi, 2001

What about the out of equilibrium situation ?



Current operator :

$$\hat{J}(x,t) = \frac{1}{\mathrm{i}}\left[\hat{\psi}^{\dagger}(x,t)\,\mathrm{D}_x\hat{\psi}(x,t) - \mathrm{D}_x^{*}\hat{\psi}^{\dagger}(x,t)\,\hat{\psi}(x,t)\right]$$

Current density matrix in arc $\mu\nu$

$$\begin{aligned} j_{\mu\nu}^{(\alpha,\beta)}(E) &\stackrel{\text{def}}{=} \langle\, \psi_E^{(\alpha)} \,|\hat{J}(x \in \ \mu\nu, t)|\, \psi_E^{(\beta)}\,\rangle \\ &= \frac{1}{\mathrm{i}}\psi^{(\alpha)}(x)^{*}\,\mathrm{D}_x\psi^{(\beta)}(x) + \ \mathrm{c.c.} \qquad \text{for } x \in \ \text{arc } \mu\nu \end{aligned}$$

Using : $\frac{\mathrm{d}\Sigma}{\mathrm{d}\theta_{\mu\nu}} = -2W\frac{1}{M+W^{\mathrm{T}}W}\frac{\mathrm{d}M}{\mathrm{d}\theta_{\mu\nu}}\frac{1}{M+W^{\mathrm{T}}W}W^{\mathrm{T}}$ we obtain :

$$j_{\mu\nu}^{(\alpha,\beta)}(E) = \frac{1}{2\mathrm{i}\pi}\left(\Sigma^{\dagger}\frac{\mathrm{d}\Sigma}{\mathrm{d}\theta_{\mu\nu}}\right)_{\alpha\beta}$$

→ We can also give a more general arc formulation.

Average current in the arc $\mu\nu$

$$\langle \hat{J}_{\mu\nu}(t)\rangle = \sum_{\alpha}\int \mathrm{d}E\, f_{\alpha}(E)\, j_{\mu\nu}^{(\alpha,\alpha)}(E)$$

Current correlations

$$S_{J_{\mu\nu}J_{\mu'\nu'}}(\omega=0) = 2\pi\sum_{\alpha,\beta}\int \mathrm{d}E\, f_{\alpha}(1-f_{\beta})\, j_{\mu\nu}^{(\alpha,\beta)}(E)\, j_{\mu'\nu'}^{(\beta,\alpha)}(E)$$

At equilibrium :

$$S_{J_{\mu\nu}J_{\mu'\nu'}}(0) = \frac{1}{2\pi}\int \mathrm{d}E\, f(E)(1-f(E))\ \mathrm{Tr}\left\{\frac{\mathrm{d}\Sigma}{\mathrm{d}\theta_{\mu\nu}}\frac{\mathrm{d}\Sigma^{\dagger}}{\mathrm{d}\theta_{\mu'\nu'}}\right\}$$

→We computed the contribution of the continuous spectrum to the current.

5. Summary

- Construction of Σ using arc matrices

- if the wave function is continuous at vertices
  $\Rightarrow$ we expressed Σ with vertex matrices and generalized
  $$\Sigma = -1 + 2\,W\left(M + W^{\mathrm{T}}W\right)^{-1}W^{\mathrm{T}}$$
  to the case of graphs with potential

- How tunable couplings can be easily introduced

- LDoS of a graph : $\rho(x;E) = \rho_{\mathrm{cont}}(x;E) + \rho_{\mathrm{disc}}(x;E)$
  The Friedel sum rule only mesures the continuous spectrum.
  $\Rightarrow$ The state counting method fails if states remain localized in the graph.
  (This is related to some discontinuous behaviour of Σ as a function of certain parameters as lengths, fluxes,...)

- Relation between Σ and local quantities for graphs out of equilibrium : LDoS, emissivities,...
  charge distribution,
  current distribution.
  $\rightarrow$ derivations within the vertex AND the arc formulations.
  $\rightarrow$ All quantities can be calculated with algebraic calculations.