Multiple path transport in quantum networks

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Refs:

[1] GA, DC, Multiple path transport (JPA 2013)

[2] DD, DC, Double path crossing (JPA 2013)

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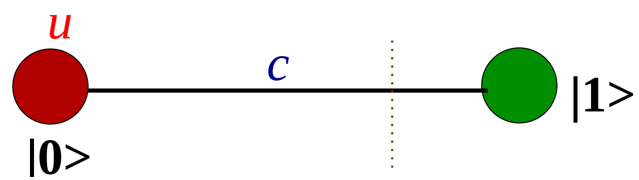
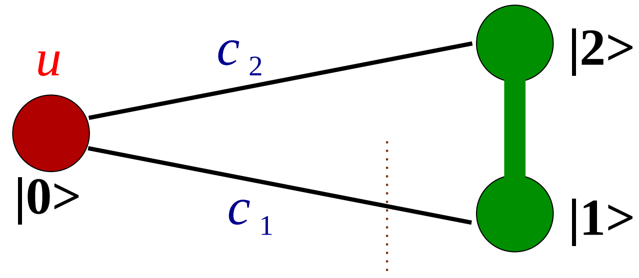
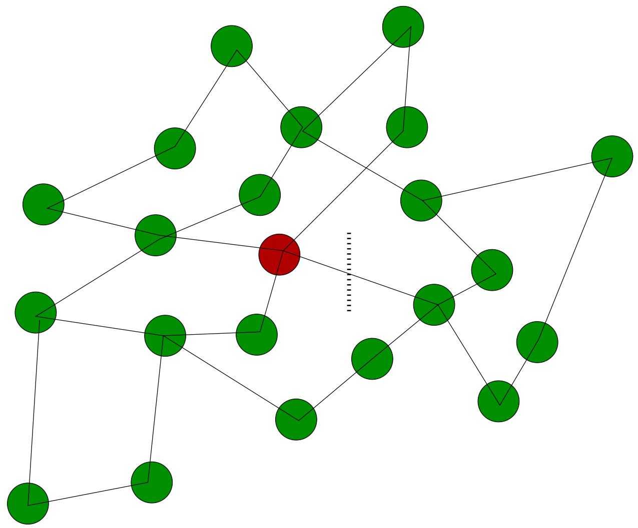






Objective

$$|0\rangle \quad = \quad \text{shuttle (chosen to be the initial state)}$$
$$|i\rangle \quad = \quad \text{network site (standard basis)}$$
$$|n\rangle \quad = \quad \text{network level (energy basis)}$$

$u(t)$ ... shuttle potential

C_i ... coupling of the shuttle to site i

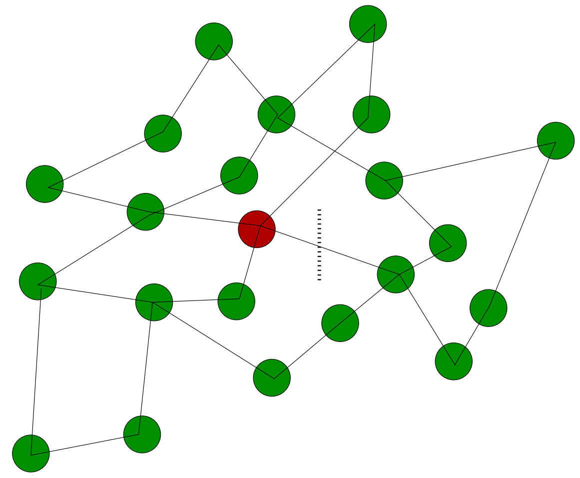
$0 \rightsquigarrow a$ ... bond of interest, coupling C_a

Questions to be addressed:

$$p(t) \quad = \quad ???$$
$$q_n(t) \quad = \quad ???$$

$$I_{0 \rightsquigarrow a}(t) \ = \ ???$$

$$Q \ = \ \int I dt \ = \ ???$$



$$\mathcal{H} \ = \ \sum_{i=0}^{N} |i\rangle \mathcal{E}_i \langle i| + \sum_{i \neq j} |i\rangle C_{ij} \langle j|$$

$$\mathcal{E}_0 \quad = \quad u(t)$$
$$C_{i0} \quad = \quad C_i$$

For single path crossing:

$$Q \ = \ \sum_n q_n(\infty) \ = \ 1 - p(\infty)$$

Expression for the probability current

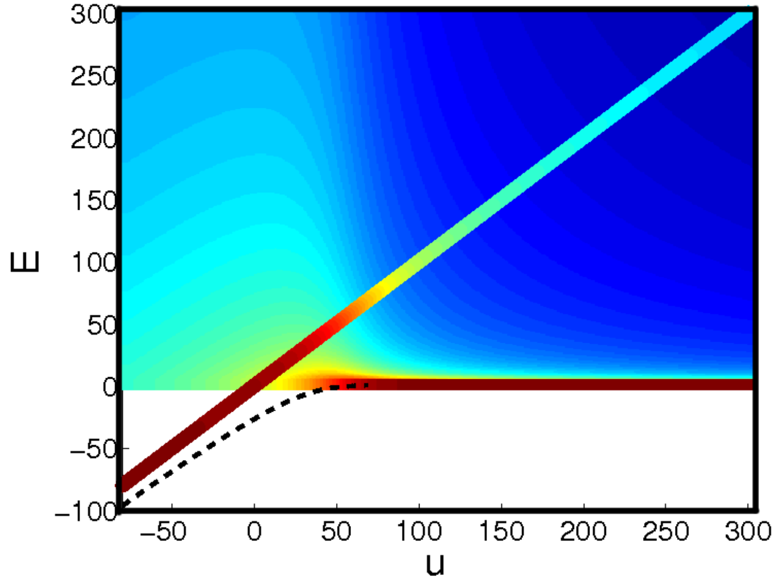
Adiabatic transport [Kubo, Thouless, Avron, Berry]:

$$I_{0 \rightsquigarrow a} = G\ \dot{u}, \qquad G(u) = 2\mathrm{Im}\left[\left\langle \frac{\partial}{\partial \phi}\Psi \middle| \frac{\partial}{\partial u}\Psi \right\rangle\right]_{\phi=0}$$

Splitting ratio picture:

$$I_{0 \rightsquigarrow a} = \frac{d}{dt}\left[\sum_n \lambda_n q_n\right]$$

$$\lambda_n = \frac{\langle n|a\rangle\ C_a}{\sum_i \langle n|i\rangle\ C_i}$$



$p(t)$ = occupation probability of the shuttle

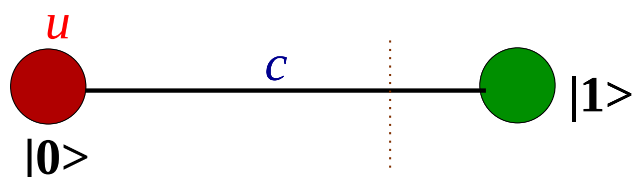
$q_n(t)$ = occupation probabilities of the network levels

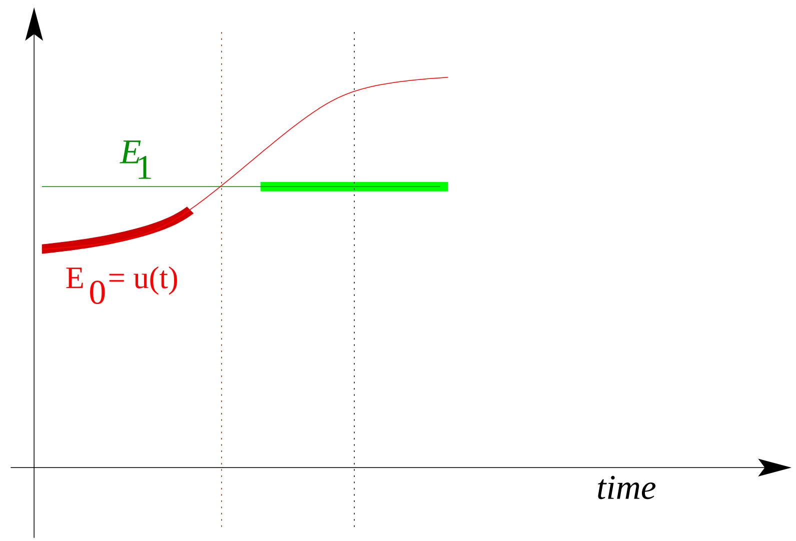
Single path crossing

$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & C \\ C & u_c \end{pmatrix}, \qquad \mathcal{I} \mapsto \begin{pmatrix} 0 & iC \\ -iC & 0 \end{pmatrix}$$

$$E(u) \;=\; \frac{1}{2}\left[(u+u_c) - \sqrt{4C^2 + (u-u_c)^2}\right]$$

$$|\Psi\rangle \;\mapsto\; \frac{1}{\sqrt{(E-u_c)^2 + C^2}} \begin{pmatrix} E-u_c \\ C\mathrm{e}^{i\phi} \end{pmatrix}$$





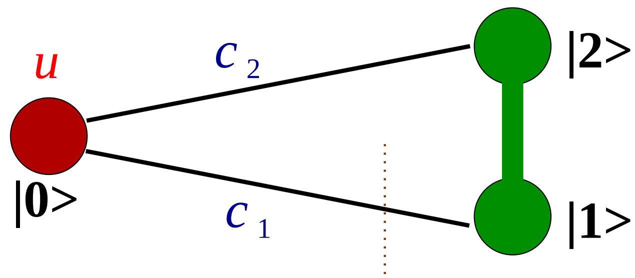
$$I = G\,\dot{u}, \qquad G(u) = 2\mathrm{Im}\left[\left\langle \frac{\partial}{\partial\phi}\Psi \middle| \frac{\partial}{\partial u}\Psi \right\rangle\right]_{\phi=0}$$

$$G = \frac{2C^2}{\left(4C^2 + (u-u_c)^2\right)^{3/2}} \quad \rightsquigarrow \quad I = \frac{d}{dt}q_1$$

A complicated way to derive the continuity equation....

Double path crossing

$$\mathcal{H} \mapsto \begin{pmatrix} u & c_1 & c_2 \\ c_1 & 0 & c_0 \\ c_2 & c_0 & 0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \begin{pmatrix} 0 & ic_1 & 0 \\ -ic_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



$$I = G\,\dot{u}, \qquad G(u) = 2\mathrm{Im}\left[\left\langle \frac{\partial}{\partial\phi}\Psi \middle| \frac{\partial}{\partial u}\Psi \right\rangle\right]_{\phi=0}$$

$$G \;=\; \frac{d}{du}\left[\frac{c_1^2E^2 + 2c_0c_1c_2E + c_0^2c_1^2}{E^4 + (c_1^2 + c_2^2 - 2c_0^2)E^2 + 2c_0c_1c_2E + c_0^2(c_0^2 + c_1^2 + c_2^2)}\right]$$

Here we are not able to deduce it from the continuity equation. But...

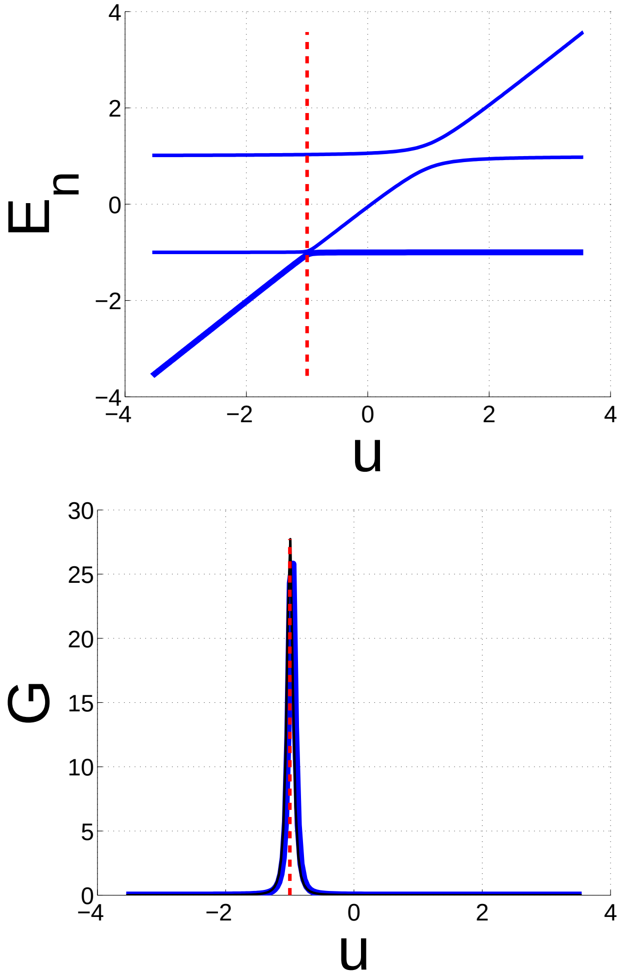
$$I \;=\; \frac{d}{dt}\Big[\lambda_+ q_+ + \lambda_- q_-\Big], \qquad \text{with} \qquad \lambda_\pm = \text{splitting ratio} = \frac{c_1}{c_1 \pm c_2}$$

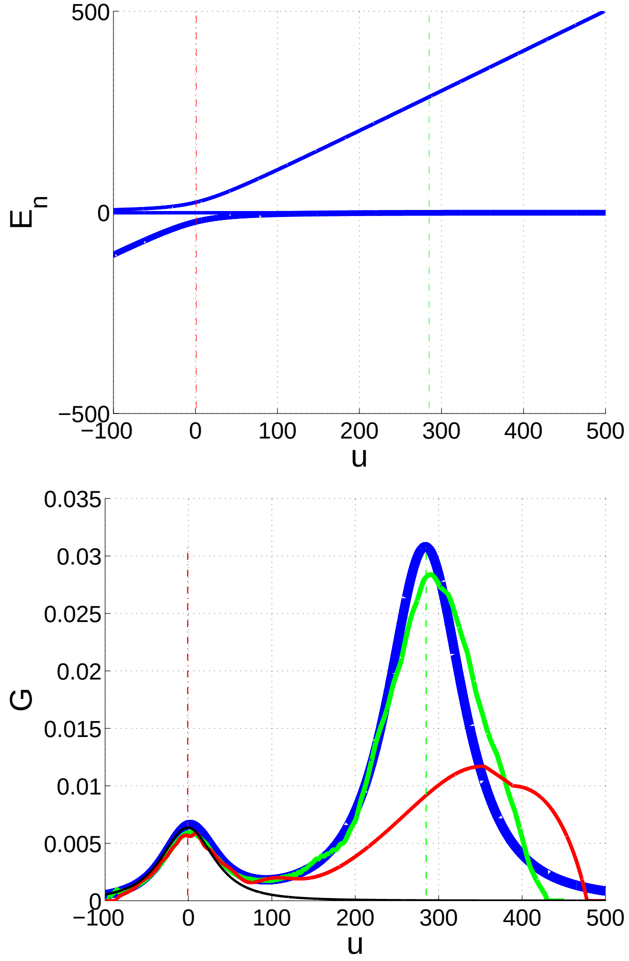
$$q_\pm(t) \;=\; \text{occupation probabilities of the network levels}$$

$$Q_{0\leadsto 1} \;\equiv\; \int I\,dt \;=\; \int G\,du \;=\; \lambda_- \;=\; \frac{c_1}{c_1 - c_2}$$

... Not bounded within $[0,1]$

“adiabatic crossing” and “adiabatic metamorphosis” processes





$$(c_0, c_1, c_2) \;=\; (1,\ 0.2,\ 0.15)$$

$$Q \;=\; \frac{c_1}{c_1 - c_2}$$

$$(c_0, c_1, c_2) \;=\; (1,\ 19,\ 15)$$

$$Q = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} \quad \rightsquigarrow \quad Q = \frac{c_1}{c_1 - c_2}$$

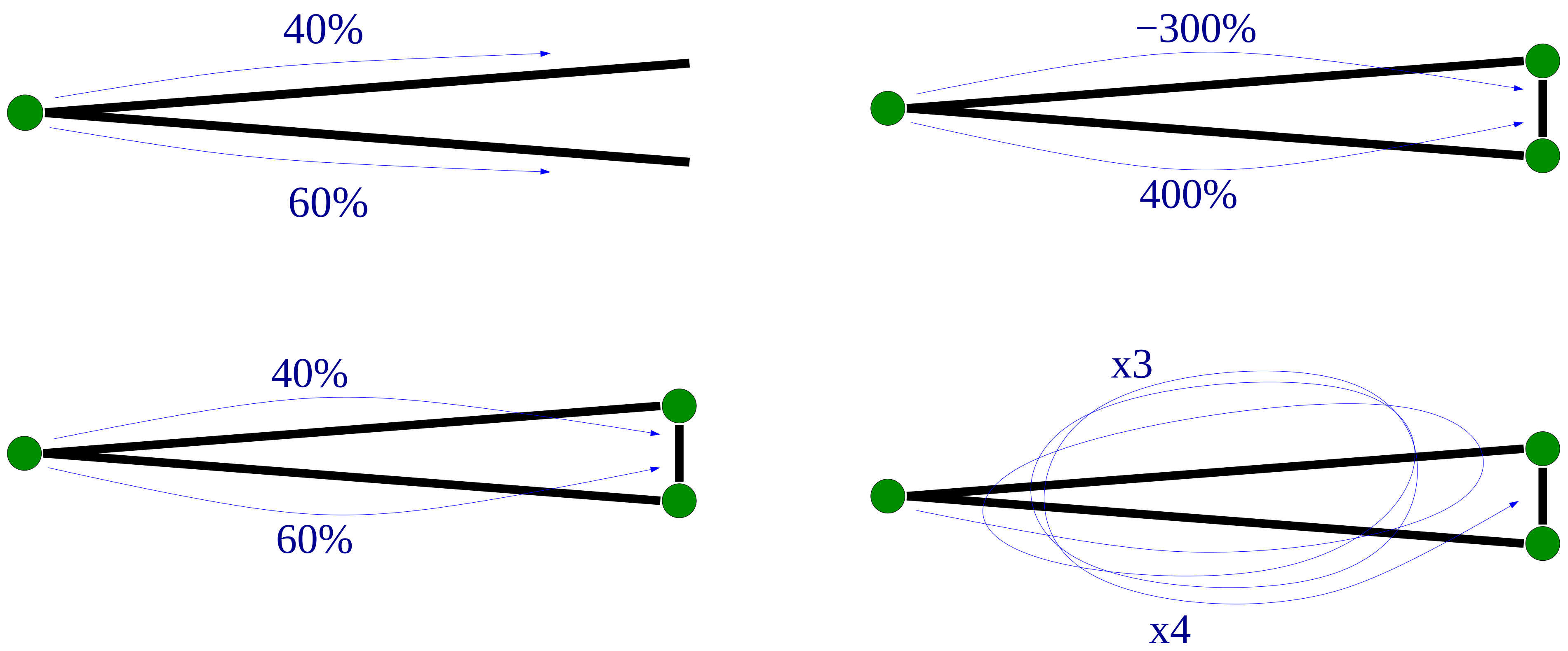
Splitting and stirring

The scattering point of view:

The particle has two paths to its destination.

The stirring point of view:

A circulating current is induced due to the driving.



The splitting ratio approach to quantum stirring

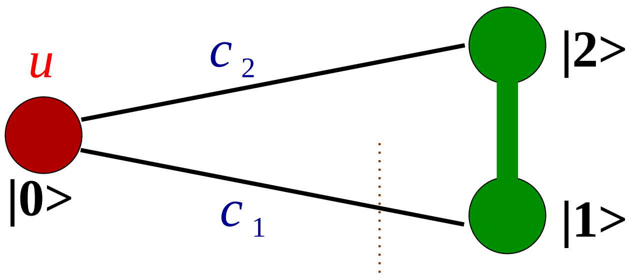
Half cycle:

$$\langle \mathcal{N} \rangle = p$$

$$\langle \mathcal{Q} \rangle = \lambda p$$

$$\mathrm{Var}(\mathcal{Q}) = \lambda^2 (1-p)p$$

$$\neq (1-\lambda p)\lambda p$$



Full cycle:

$$\langle \mathcal{N} \rangle \approx \left| \sqrt{P_{\mathrm{LZ}}^{\circlearrowleft}} - \mathrm{e}^{i\varphi}\sqrt{P_{\mathrm{LZ}}^{\circlearrowright}} \right|^2$$

$$\langle \mathcal{Q} \rangle \approx \lambda_{\circlearrowleft} - \lambda_{\circlearrowright}$$

$$\mathrm{Var}(\mathcal{Q}) \approx \left| \tilde{\lambda}_{\circlearrowleft}\sqrt{P_{\mathrm{LZ}}^{\circlearrowleft}} + \mathrm{e}^{i\varphi}\lambda_{\circlearrowright}\sqrt{P_{\mathrm{LZ}}^{\circlearrowright}} \right|^2$$

[Interference of two LZ transitions]

Counting statistics for a coherent transition, Maya Chuchem and DC (PRA 2008)
Counting statistics in multiple path geometries, Maya Chuchem and DC (JPA 2008)
Quantum stirring of electrons in a ring, Itamar Sela and DC (PRBs 2008)

In the classical context a similar approach has been independently proposed:
current decomposition formula, S.Rahav, J.Horowitz, and C.Jarzynski1 (PRL 2008).

Motivation

Brouwer [PRB 1998], following BPT - calculation of Q in open geometry

Shutenko, Aleiner, Altshuler [PRB 2000] - Wrong conception of Q quantization

DC [arXiv 2002, PRB 2003] - Kubo approach to quantum pumping - too formal

Moskalets, Buttiker [PRB 2003] - Problem to apply scattering approach in Q calculation

DC [PRB (R) 2003] - from closed to open systems - too formal

with Maya Chuchem and Itamar Sela [JPA, PRA, PRB 2008] - splitting ratio approach

Open issues that have motivated the present work:

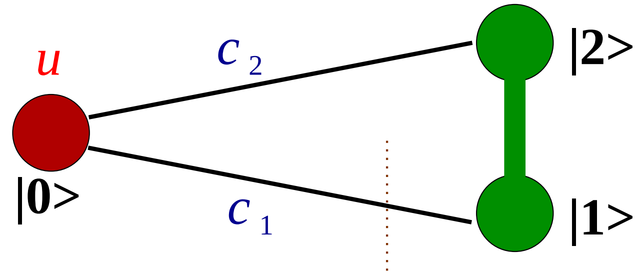
- Originally derived in the context of adiabatic transport.
- Originally based on a two level approximation scheme.
- Not clear what happens in a multi-level network (effect of strong mixing).
- Not clear what happens in the non-adiabatic case.

Possible application:

Electronic Quantum Fluxes during Pericyclic Reactions
[Andrae, Barth, Bredtmann, Hege, Manz, Marquardt, Paulus]

Original derivation - based on Two-level approximation

Standard site (i) basis:



$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & c_1 & c_2 \\ c_1 & 0 & c_0 \\ c_2 & c_0 & 0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \begin{pmatrix} 0 & ic_1 & 0 \\ -ic_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Energy level (n) basis:

$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & \kappa_- & \kappa_+ \\ \kappa_- & -c_0 & 0 \\ \kappa_+ & 0 & c_0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \frac{c_1}{\sqrt{2}} \begin{pmatrix} 0 & i & i \\ -i & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

$$\kappa_\pm \equiv \frac{c_1 \pm c_2}{\sqrt{2}}$$

Two level approximation:

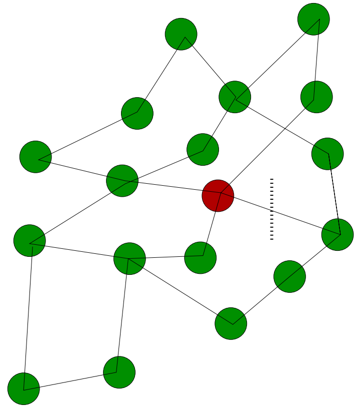
$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & \kappa_- \\ \kappa_- & -c_0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \frac{c_1}{c_1 - c_2} \begin{pmatrix} 0 & i\kappa_- \\ -i\kappa_- & 0 \end{pmatrix}$$

Formally the same as single path crossing with $\mathcal{I} := \lambda \mathcal{I}$

General derivation - embarrassingly simple

We assume that we know to how to find the level occupations:

$$q_n(t) \quad = \quad |\psi_n(t)|^2$$

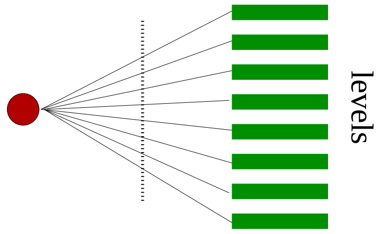


Continuity equation for star geometry:

$$\dot{q}_n \quad = \quad \kappa_n \ \mathrm{Im}[\psi_n^* \psi_0]$$

Getting site amplitudes from level amplitudes:

$$\Psi_a(t) \quad = \quad \sum_n \langle a|n\rangle \ \psi_n(t)$$



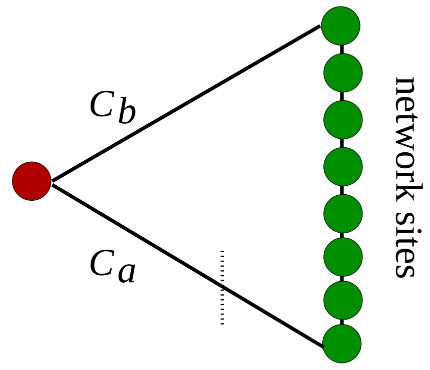
Expression for the current in the bond of interest:

$$I_{0 \rightsquigarrow a} \quad = \quad C_a \ \mathrm{Im}\left[\Psi_a(t)^* \ \Psi_0(t)\right] \quad = \quad C_a \ \mathrm{Im}\left[\sum_n \langle n|a\rangle \ \psi_n(t)^* \ \psi_0(t)\right] \quad = \quad \frac{d}{dt}\left[\sum_n \lambda_n q_n\right]$$

with $\qquad \lambda_n \quad = \quad \dfrac{\langle n|a\rangle \ C_a}{\kappa_n} \quad = \quad \dfrac{\langle n|a\rangle \ C_a}{\sum_i \langle n|i\rangle \ C_i}$

Application to dot-wire geometry

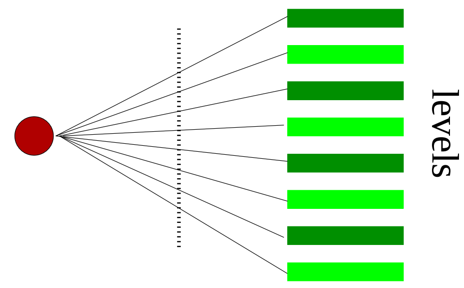
$$Q_{0 \rightsquigarrow a} \;=\; \sum_n \Big[q_n(\text{final}) - q_n(\text{initial}) \Big] \; \lambda_n$$



Starting with an occupied shuttled, adiabatic case:

occupation q_1 of lower network level changes from zero to unity

$$Q_{0 \rightsquigarrow a} \;=\; \lambda_- \;=\; \frac{C_a}{C_a - C_b}$$ [if ground-state is odd]



Starting with an occupied shuttled, non-adiabatic case:

many levels are occupied

$$q_n \;\propto\; |\kappa_\pm|^2 \;=\; |C_a \pm C_b|^2$$

$$Q_{0 \rightsquigarrow a} \;=\; \text{WeightedAverage}\Big[\lambda_+, \lambda_-\Big] \;=\; \frac{|C_a|^2}{|C_a|^2 + |C_b|^2}$$

Starting with an occupied level n, adiabatic case:

occupation q_n of even level changes from unity to zero

occupation q_{n+1} of odd level changes from zero to unity

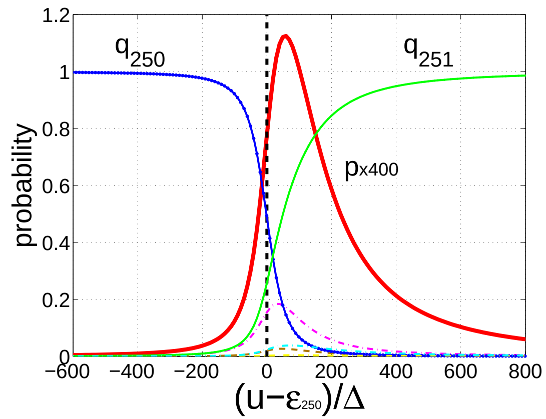
$$Q_{0 \rightsquigarrow a} \;=\; \lambda_- - \lambda_+ \;=\; \frac{2C_aC_b}{|C_a|^2 - |C_b|^2}$$

for even/odd parity level:

$$\lambda_n \;=\; \frac{C_a}{C_a \pm C_b}$$

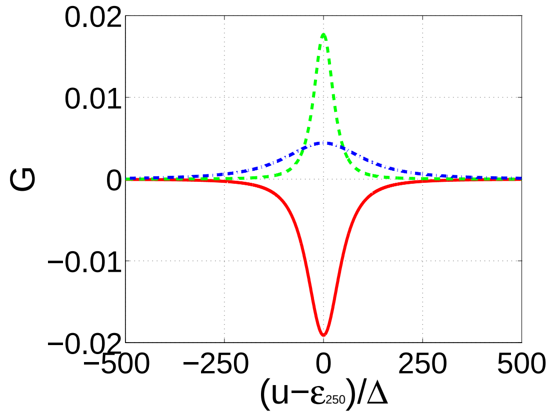
Expression for the current

For a Fermi sea occupation we have to sum the currents of all the occupied levels. Here we focus on the current that is induced if the initially occupied level is $n_0 = 250$.



$$p(u) \;=\; \Delta \cdot \mathrm{L}\left[u - \epsilon_{n_0};\; \Gamma, \theta\right], \qquad\qquad q_n(u) \;=\; [...]$$

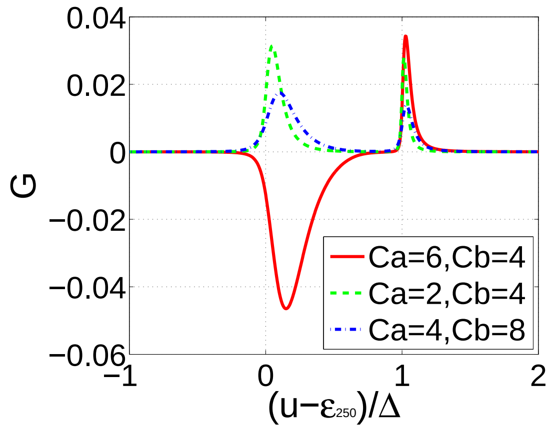
$$G(u) \;\approx\; (\lambda_- - \lambda_+) \frac{2{C_{\mathrm{eff}}}^2}{\left(4{C_{\mathrm{eff}}}^2 + (u - \epsilon_{n_0})^2\right)^{3/2}}$$



$$\Gamma \;\equiv\; \pi \frac{\kappa_+^2 + \kappa_-^2}{\Delta}, \qquad\qquad C_{\mathrm{eff}} \;\equiv\; \frac{2}{\pi}\frac{\kappa_+ \kappa_-}{\Delta}$$

$$\sin(\theta) \;\equiv\; \frac{\kappa_+^2 - \kappa_-^2}{\kappa_+^2 + \kappa_-^2},$$

$$\mathrm{L}\left[x; \Gamma; \theta\right] \;=\; \frac{1}{\pi}\left[1 + \frac{\sin\theta\; x}{\sqrt{x^2 + \cos^2\theta\;(\Gamma/2)^2}}\right]^{-1} \frac{\cos^2\theta\;(\Gamma/2)}{x^2 + \cos^2\theta\;(\Gamma/2)^2}$$



Maximal p is attained away from the crossing point.

Lower figure is for $\Delta \gg C_a, C_b$.

Non-adiabatic spreading

A particle is loaded into the shuttle.
Standing shuttle - Wigner decay problem.
Moving shuttle - a variant of Wigner decay problem:

$$q_n(t) \quad = \quad \left| \kappa_n \int_0^t d\tau \;\; \exp\left(i\epsilon_n\tau - i\frac{\dot{u}}{2}\tau^2 - \frac{\Gamma}{2}\tau \right) \right|^2$$

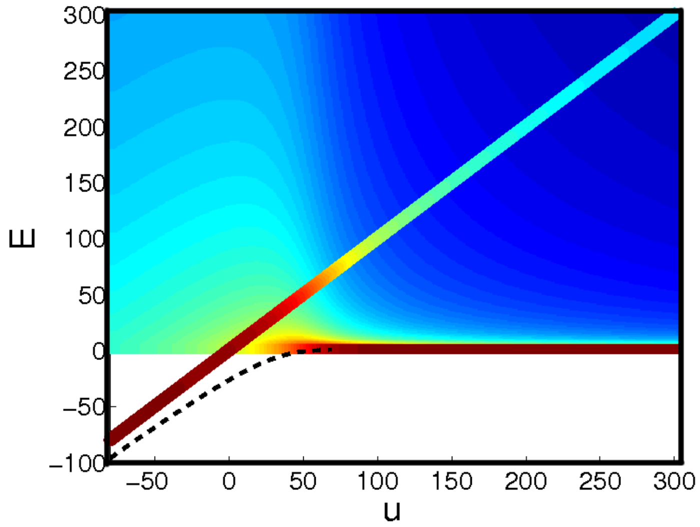
Competition between two time scales: $1/\Gamma$ and $\Gamma/\dot{u}$

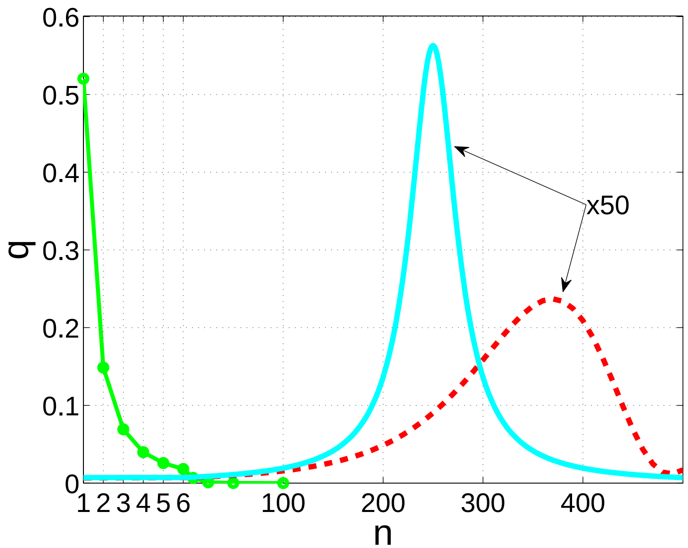
Regimes:

- Adiabatic $\quad \dot{u} \ll c^2$
- Slow $\quad c^2 \ll \dot{u} \ll \Gamma^2$
- Fast $\quad \dot{u} \gg \Gamma^2$

$$c \quad = \quad \text{coupling}$$

$$\Gamma \quad = \quad 2\pi \frac{c^2}{\Delta}$$





Main messages

- The splitting ratio approach:
  a simple way to calculated currents in a driven network.
  $I(t)$ is deduced from $p(t)$ and $q_n(t)$.

- Regimes: adiabatic; slow; fast.

- Counting statistics, in particular Q and $\mathrm{Var}(\mathcal{Q})$.

- Beyond the two level approximation:
  metamorphism and mixing processes.

- Exact analysis of stirring in a 3-site model.

- Exact analysis of shuttling in dot-wire geometry.