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)

\$ISF\$
The calculation of the induced current

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

\[ dQ = G \, du \quad \sim \quad I = G \, \dot{u} \]

\[ G(u) = 2 \text{Im} \left[ \left\langle \frac{\partial}{\partial \phi} \Psi \left| \frac{\partial}{\partial u} \Psi \right\rangle \right] \right|_{\phi=0} \]

Splitting ratio picture [MC, IS, DC]:

\[ I = \frac{d}{dt} \left[ \sum_n \lambda_n q_n \right] \]

\[ q_n(t) = \text{occupation probabilities of the network levels} \]
\[ p(t) = \text{occupation probability of the shuttle} \]

\[ p(t) + \sum_n q_n(t) = 1 \]

\( I \) [current via \( C_a \)]
Single path crossing

\[ H \mapsto \begin{pmatrix} u(t) & C \\ C & u_c \end{pmatrix}, \quad I \mapsto \begin{pmatrix} 0 & iC \\ -iC & 0 \end{pmatrix} \]

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

\[ |\Psi\rangle \mapsto \frac{1}{\sqrt{(E - u_c)^2 + C^2}} \begin{pmatrix} E - u_c \\ Ce^{i\phi} \end{pmatrix} \]

\[ I = G \dot{u}, \quad G(u) = 2\text{Im} \left[ \langle \frac{\partial}{\partial \phi} \Psi \mid \frac{\partial}{\partial u} \Psi \rangle \right]_{\phi=0} \]

\[ G = \frac{2C^2}{(4C^2 + (u - u_c)^2)^{3/2}} \quad \sim \quad I = \frac{d}{dt} q_1 \]

\[ q_1(t) = |\langle 1 | \Psi \rangle|^2 \]

A complicated way to derive the continuity equation....
Double path crossing

\[ \mathcal{H} \mapsto \begin{pmatrix} u & c_1 & c_2 \\ c_1 & 0 & c_0 \\ c_2 & c_0 & 0 \end{pmatrix}, \quad \mathcal{I} \mapsto \begin{pmatrix} 0 & ic_1 & 0 \\ -ic_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

\[ I = G \dot{u}, \quad G(u) = 2\text{Im} \left[ \left\langle \frac{\partial}{\partial \phi} \Psi \right| \frac{\partial}{\partial u} \Psi \right\rangle \bigg|_{\phi=0} \]

\[ G = \frac{d}{du} \left[ \frac{c_1^2 E^2 + 2c_0c_1c_2 E + c_0^2 c_1^2}{E^4 + (c_1^2 + c_2^2 - 2c_0^2)E^2 + 2c_0c_1c_2 E + c_0^2(c_0^2 + c_1^2 + c_2^2)} \right] \]

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

\[ I = \frac{d}{dt} \left[ \lambda_- q_- + \lambda_+ q_+ \right], \quad \text{with} \quad \lambda_\pm = \text{splitting ratio} = \frac{c_1}{c_1 \pm c_2} \]

\[ q_\pm(t) \quad \text{occupation probabilities of the network levels} \]

\[ Q_{0 \rightarrow 1} \equiv \int I \, dt = \int G \, du \quad = \quad \lambda_- = \frac{c_1}{c_1 - c_2} \quad \ldots \text{Not bounded within } [0, 1] \]
“adiabatic crossing” and “adiabatic metamorphosis” processes

\[ (c_0, c_1, c_2) = (1, 0.2, 0.15) \]

\[ Q = \frac{c_1}{c_1 - c_2} \]

\[ (c_0, c_1, c_2) = (1, 19, 15) \]

\[ Q = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} \sim Q = \frac{c_1}{c_1 - c_2} \]
Shuttle crosses an half-filled energy band

For a Fermi sea occupation we have to sum the currents of all the occupied levels.

\[ G(u) \approx \lambda_{\text{filled}} \frac{2C_{\text{eff}}^2}{(4C_{\text{eff}}^2 + (u - \epsilon_{n_0})^2)^{3/2}} \]

\[ C_a, C_b = \text{couplings to the ends of the wire} \]

\[ \kappa_{\pm} \propto (C_a \pm C_b) = \text{couplings to the levels} \]

\[ \Gamma \equiv \pi \frac{\kappa_+^2 + \kappa_-^2}{\Delta}, \quad C_{\text{eff}} \equiv \frac{2}{\pi} \frac{\kappa_+ \kappa_-}{\Delta} \]

Occupation probability of the shuttle if only \( n_0 = 250 \) were occupied:

\[ p(u) = \Delta \cdot L[u - \epsilon_{n_0}; \Gamma, \theta] \]

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

\[ \sin(\theta) \equiv (\kappa_+^2 - \kappa_-^2)/(\kappa_+^2 + \kappa_-^2) \]

Maximal \( p \) is attained away from the crossing point.
Non-adiabatic crossing of an empty quasi-continuum

A particle is loaded into the shuttle.

Standing shuttle - Wigner decay problem.

Moving shuttle - a variant of Wigner decay problem:

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

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

Regimes:
- Adiabatic \( \dot{u} \ll \kappa^2 \)
- Slow \( \kappa^2 \ll \dot{u} \ll \Gamma^2 \)
- Fast \( \dot{u} \gg \Gamma^2 \)

\( \kappa = \) coupling to the levels

\( \Gamma = 2\pi \frac{\kappa^2}{\Delta} \)
Adiabatic vs non-adiabatic crossing - results for $Q$

$$Q_{0\rightarrow a} = \sum_n \left[ q_n(\text{final}) - q_n(\text{initial}) \right] \lambda_n$$

Starting with an occupied shuttled, adiabatic case:

occupation $q_1$ of lower network level changes from zero to unity

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

Starting with an occupied shuttled, non-adiabatic case:

many levels are occupied

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

$$Q_{0\rightarrow a} = \text{WeightedAverage} \left[ \lambda_+, \lambda_- \right] = \frac{|C_a|^2}{|C_a|^2 + |C_b|^2}$$

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

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

for even/odd parity level:

$$\lambda_n = \frac{C_a}{C_a \pm C_b}$$
The splitting ratio formula - general network

\[ |0\rangle = \text{shuttle site} \]
\[ |i\rangle = \text{network site (standard basis)} \]
\[ |n\rangle = \text{network level (energy basis)} \]

Splitting ratio:

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

Generalized continuity equation:

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

For a single path crossing:

\[ Q \equiv \int_0^{\infty} I dt = \sum_n q_n(\infty) = 1 - p(\infty) \]

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

\[ \mathcal{E}_0 = u(t) = \text{shuttle potential} \]
\[ C_{i0} = C_i = \text{coupling of the shuttle to site } i \]
Original derivation - based on Two-level approximation

Standard site \((i)\) basis:
\[
\mathcal{H} \mapsto \begin{pmatrix} u(t) & c_1 & c_2 \\ c_1 & 0 & c_0 \\ c_2 & c_0 & 0 \end{pmatrix}, \quad \mathcal{I} \mapsto \begin{pmatrix} 0 & ic_1 & 0 \\ -ic_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}
\]

Energy level \((n)\) basis:
\[
\mathcal{H} \mapsto \begin{pmatrix} u(t) & \kappa_- & \kappa_+ \\ \kappa_- & -c_0 & 0 \\ \kappa_+ & 0 & c_0 \end{pmatrix}, \quad \mathcal{I} \mapsto \frac{c_1}{\sqrt{2}} \begin{pmatrix} 0 & i & i \\ -i & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}
\]

Two level approximation:
\[
\mathcal{H} \mapsto \begin{pmatrix} u(t) & \kappa_- \\ \kappa_- & -c_0 \end{pmatrix}, \quad \mathcal{I} \mapsto \frac{c_1}{c_1 - c_2} \begin{pmatrix} 0 & i\kappa_- \\ -i\kappa_- & 0 \end{pmatrix}
\]

Formally the same as single path crossing with \(\mathcal{I} := \lambda \mathcal{I}\)
General derivation - embarrassingly simple

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

\[ q_n(t) = |\psi_n(t)|^2 \]

Continuity equation for star geometry:

\[ \dot{q}_n = \kappa_n \operatorname{Im}[\psi^*_n \psi_0] \]

Getting site amplitudes from level amplitudes:

\[ \Psi_a(t) = \sum_n \langle a|n \rangle \psi_n(t) \]

Expression for the current in the bond of interest:

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

with

\[ \lambda_n = \frac{\langle n|a \rangle C_a}{\kappa_n} = \frac{\langle n|a \rangle C_a}{\sum_i \langle n|i \rangle C_i} \]
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.

\[ x_3 \]

\[ x_4 \]
The splitting ratio approach to quantum stirring

**Half cycle:**

\[
\langle \mathcal{N} \rangle = p
\]

\[
\langle Q \rangle = \lambda p
\]

\[
\text{Var}(Q) = \lambda^2 (1 - p)p
\]

\[
\neq (1 - \lambda p) \lambda p
\]

**Full cycle:**

\[
\langle \mathcal{N} \rangle \approx \left| \sqrt{P_{\text{LZ}}} - e^{i\varphi} \sqrt{P_{\text{LZ}}} \right|^2
\]

\[
\langle Q \rangle \approx \lambda \left| \sqrt{P_{\text{LZ}}} - e^{i\varphi} \sqrt{P_{\text{LZ}}} \right|^2
\]

\[
\text{Var}(Q) \approx \left| \tilde{\lambda} \sqrt{P_{\text{LZ}}} + e^{i\varphi} \lambda \sqrt{P_{\text{LZ}}} \right|^2
\]

[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:

Motivation

Brouwer [PRB 1998], following BPT - calculation of $Q$ in open geometry
Shutenko, Aleiner, Altshuler [PRB 2000] - Wrong conception of $Q$ quantization
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]
Main messages

- The splitting ratio approach: a simple way to calculate 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 \( \text{Var}(Q) \).

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

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

- Exact analysis of shuttling in dot-wire geometry.