

Multiple path transport in quantum networks

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Abstract. A shuttle site that crosses through a band of network levels induces currents. If the process were re-cycled this would be regarded as “pumping” or “stirring”. We show that the analysis reduces to that of calculating time dependent probabilities, as in the stochastic formulation, but with splitting (branching) ratios that are not bounded within $[0, 1]$. Our approach allows to address the adiabatic regime, as well as the Slow and Fast non-adiabatic regimes, on equal footing. We emphasize aspects that go beyond the familiar picture of sequential Landau-Zener crossings, taking into account Wigner-type multilevel mixing due to the crossing shuttle.

1. Introduction

Transport in quantum networks is a theme that emerges in diverse contexts, including quantum Hall effect [1], Josephson arrays [2], quantum computation models [3], quantum internet [4], and even in connection with photosynthesis [5]. For some specific models there are calculations of the induced currents in the adiabatic regime [6, 7, 8, 9, 10] for both open and closed systems, so called “quantum pumping” [11, 12, 13, 14, 15, 16, 17, 18] and “quantum stirring” [19, 20, 21, 22, 23] respectively. In the latter context most publications focus on 2-level [24, 25] and 3-level dynamics, while the larger perspective is rather abstract, notably the “Dirac monopoles picture” [9, 19, 21, 22]. This should be contrasted with the analysis of stochastic stirring where the theory is quite mature [26, 27, 28, 29].

Considering (e.g.) the unidirectional rotation of a molecular rotor [27], it is possibly allowed to be satisfied with a stochastic picture [26] that relates the currents, via a “decomposition formula”, to rates of change of occupation probabilities. Once we turn (e.g.) to the analysis of pericyclic reactions [30] this is no longer possible. In the latter case the method of calculating electronic quantum fluxes had assumed that they can be deduced from the continuity equation. Such procedure is obviously not applicable for (say) a ring-shaped molecule: due to the multiple path geometry there is no obvious relation between currents and time variation of probabilities.

In this work we would like to analyze the following prototype problem. Consider a network that consists of N interconnected sites, with on-site energies \mathcal{E}_i , and couplings C_{ij} . Additionally there is a shuttle ($i = 0$), where the on-site energy $\mathcal{E}_0 = u(t)$ is varied monotonically from $u = -\infty$ to $u = \infty$. Accordingly the Hamiltonian is

$$\mathcal{H} = \sum_{i=0}^N |i\rangle \mathcal{E}_i \langle i| + \sum_{i \neq j} |i\rangle C_{ij} \langle j| \quad (1)$$

$$\mathcal{E}_0 = u(t), \quad C_{i0} = C_i \quad (2)$$

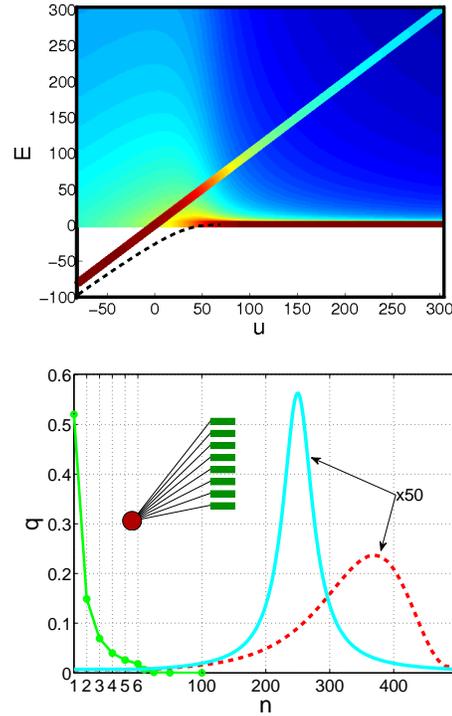


Figure 1. *Upper panel:* an initially loaded shuttle is crossing a band that contains $N = 500$ levels. The occupation probabilities of the shuttle (p) and of the levels (q_n) are imaged as a function of time. The vertical axis is the energy, and the horizontal axis is $u(t)$. We assume star geometry with level spacing $\Delta=1$, and identical couplings $c_n=3$. The dashed line illustrates the energy of the lowest adiabatic level. *Lower panel:* plot of q_n vs n in several cases. Green line with markers - the adiabatic scenario of the upper panel at $u = 60$. Cyan solid line - after decay from a standing shuttle ($\dot{u}=0$). Red dashed line - after decay from a fast shuttle ($\dot{u}=5000$).

Our interest is in the induced current $I(t)$ that flows through a tagged connecting bond C_a . In the adiabatic limit this current is determined by the so-called geometric conductance G as follows [6, 7, 8, 9, 10, 19, 20, 21, 22, 23]:

$$I = G\dot{u}, \quad G = 2\text{Im} \left[\left\langle \frac{\partial}{\partial \phi} \Psi \left| \frac{\partial}{\partial u} \Psi \right\rangle \right]_{\phi=0} \quad (3)$$

Here ϕ is a test flux through the bond of interest, namely $C_a \mapsto C_a e^{i\phi}$, and Ψ is the wave-function of the adiabatic eigenstate.

Specific shuttling scenarios to be considered below are: **(i) Injection** - the shuttle is initially filled with a particle that later is transferred to the network; **(ii) Induction** - one of the levels of the network is initially filled, and later a current is induced via the crossing shuttle. The occupation dynamics in the first scenario is illustrated in Fig. 1, which will be further discussed later. For a non-interacting many-body occupation, results could be obtained by simple summation.

Outline.— We find explicit expression for the current I that is induced either in adiabatic or non-adiabatic shuttling process. We first consider a “star geometry” (inset in Fig. 1) and later a “ring geometry” (inset of Fig. 2). For the analysis we introduce the *splitting ratio* phenomenology.

2. Star geometry

Let us consider the special geometry of a network that consists of sites $\mathcal{E}_n = \epsilon_n$, and connections $C_{n0} = c_n$, while all the other couplings are zero, as illustrated in the inset of Fig. 1. An adiabatic eigenstate $|\Psi\rangle$ is represented by a column vector $\Psi_n = \langle n|\Psi\rangle$ that satisfies the following set of equations:

$$u\Psi_0 + \sum_{n=1}^N c_n^* \Psi_n = E\Psi_0 \quad (4)$$

$$c_n\Psi_0 + \epsilon_n\Psi_n = E\Psi_n, \quad n = 1, 2, \dots, N \quad (5)$$

It follows from Eq. (5) that it can be written as:

$$|\Psi\rangle = \sqrt{p}|0\rangle + \sqrt{p} \sum_{n=1}^N \frac{c_n}{E - \epsilon_n} |n\rangle \quad (6)$$

where \sqrt{p} is a normalization constant. We define

$$g(E; c_1, \dots, c_N) = \sum \frac{|c_n|^2}{E - \epsilon_n} \quad (7)$$

Substitution of the Ψ_n of Eq. (6) into Eq. (4) leads to the secular equation $g(E) = E - u$ for the adiabatic eigen-energies. We focus our attention on a particular root $E(u)$. As u is swept from $-\infty$ to $+\infty$, the energy $E(u)$ increases monotonically from ϵ_{n_0} to ϵ_{n_0+1} , where n_0 is the starting level. From Eq. (6) it follows that p is the probability to find the particle in the shuttle. It can be written as

$$p(u) = |\Psi_0|^2 = \left[1 - g'(E(u))\right]^{-1} \quad (8)$$

For the following derivation note that $1/p$ is a quadratic form in c_n , and that the occupation probabilities of the network levels $n = 1, 2, 3\dots$ are

$$q_n(u) = |\Psi_n|^2 = \left| \frac{c_n}{E(u) - \epsilon_n} \right|^2 p(u) \quad (9)$$

Using Eq. (3) we get after differentiation by parts that the current through c_n is

$$\begin{aligned} G &= \frac{|c_n|^2}{(E - \epsilon_n)^2} \left(\frac{\partial p}{\partial u} \right) - 2p \frac{|c_n|^2}{(E - \epsilon_n)^3} \left(\frac{\partial E}{\partial u} \right) \\ &= \frac{\partial}{\partial u} \left[\left(\frac{1}{2} \frac{\partial(1/p)}{\partial c_n} c_n \right) p \right] = \frac{\partial}{\partial u} [q_n] \end{aligned} \quad (10)$$

We further discuss and generalize this trivial result below.

3. Multiple path geometry

Needless to say that we do not really need Eq. (3) in order to get the expression for G in the case of a star graph. We could simply deduce Eq. (10) from conservation of probability, i.e. from the continuity equation $I = \dot{q}_n$. This is no longer the case

if we have a multiple path geometry: probability conservation alone cannot tell us how the current is split between the different paths. Furthermore, we would like to go beyond the adiabatic transport formalism, and obtain a formula that applies also in non-adiabatic circumstances.

4. Splitting ratio approach

Let us first see what is the expression for G in the case of a general network. It is natural to switch from the \mathcal{E}_i basis to an ϵ_n basis that diagonalize the network Hamiltonian in the absence of the shuttle. Consequently getting a star geometry with $c_n = \sum_i \langle n|i \rangle C_i$. Our interest is in the current through a tagged bond C_a . We define the “splitting ratio” of the current that flows in the n th levels as

$$\lambda_n[\text{splitting}] = \frac{\langle n|a \rangle C_a}{c_n} = \frac{\langle n|a \rangle C_a}{\sum_{i=1}^N \langle n|i \rangle C_i} \quad (11)$$

A straightforward generalization of the derivation that leads to Eq. (10) implies that the current through C_a is

$$I = \frac{\partial}{\partial t} \left[\sum_n \lambda_n q_n \right] \quad (12)$$

The physical simplicity of Eq. (12) suggests that it can be derived without assuming adiabaticity, where $q_n(t) = |\Psi_n(t)|^2$ is obtained from the solution of the *time dependent* Schrodinger equation. Indeed this is the case. We just have to remember that quite generally

$$I = C_a \text{Im}[\Psi_a(t)^* \Psi_0(t)] \quad (13)$$

Substitution of $\Psi_a = \sum_n \langle a|n \rangle \psi_n$, and using the definition Eq. (11) of the splitting ratio, and the identification $\dot{q}_n = c_n \text{Im}[\psi_n^* \psi_0]$, we get Eq. (12) with Eq. (11). This very simple, and yet very general result, has far reaching consequences as described below.

5. The integrated current

As the simplest example for the application of the splitting ratio approach we consider a process in which a particle has been transferred from the shuttle to the “wire” in the network of Fig. 2. In this model the splitting ratio of the even-parity levels is $\lambda_n = \lambda_+ = C_a/(C_a + C_b)$, while for the odd-parity levels we have $\lambda_n = \lambda_- = C_a/(C_a - C_b)$. From Eq. (12) it follows that the integrated current is $Q = \text{average}(\lambda_n)$, where the weighted average is determined by the final occupation of wire levels. For an adiabatic *injection* scenario, in which the particle ends up at the lower wire level, say it is odd, we get

$$Q[\text{injection}] = \lambda_- = \frac{C_a}{C_a - C_b} \quad (14)$$

Unlike the case of a stochastic transition this value is not bounded within $[0, 1]$. rather it may have any value, depending on the relative sign of the amplitudes C_a and C_b . For an adiabatic *induction* scenario, the particle is prepared (say) in an even wire-level,

and is adiabatically transferred, due to the shuttling, into the adjacent odd wire-level. Then we get

$$Q[\text{induction}] = \lambda_- - \lambda_+ = \frac{2C_a C_b}{|C_a|^2 - |C_b|^2} \quad (15)$$

However, if the process is not adiabatic, the probability is distributed over both the odd and the even levels with probabilities that are proportional to $|C_a \pm C_b|^2$ respectively. Then we get from the weighted average a stochastic-like result, namely

$$Q[\text{fast}] = \text{average}(\lambda_n) = \frac{|C_a|^2}{|C_a|^2 + |C_b|^2} \quad (16)$$

We now turn to give a detailed account with regard to the time dependence of I , considering in particular the adiabatic limit $I = G(u)\dot{u}$, where it depends parametrically on u via $G(u)$.

6. The parametric variation of the current

The results for the integrated current give the impression that the size of the coupling c_n compared with the levels spacing Δ is of no importance. But this is a wrong impression. Once we get deeper into the analysis it becomes clear that the familiar two level approximation for the adiabatic current I , requires the coupling c_n to be very small compared with the level spacing Δ . Our interest below is focused in the case of having a quasi-continuum, meaning that the c_n are larger than Δ , hence many levels are mixed as the shuttle goes through.

Before discussing the quasi-continuum case it is useful to note that the 3 site ($N = 2$) ring system has been solved exactly in [23]. It has been found that if the c_n are not smaller compared with Δ , the shuttle-induced mixing of the levels modifies the functional form of $G(u)$ in a non-trivial way.

7. Adiabatic mixing

We turn to treat the ring system for $N \gg 1$. The energy levels of the wire that has length $L = N + 1$, are $\epsilon_n = -2c_0 \cos(k_n)$, where $k_n = (\pi/L)n$. The respective couplings to the shuttle are

$$c_n = \left[\left(\frac{2}{L} \right)^{1/2} \sin(k_n) \right] (C_a \pm C_b) \quad (17)$$

where the \pm reflects the parity of the level. We focus on levels with energy $\epsilon_n \sim E$, such that their spacing Δ can be regarded as constant. Then it is convenient to absorb the factor $[(2/N)^{1/2} \sin(k)]$ into the definition of C_a and C_b . The couplings $c_n = c_{\pm}$ to the energy levels in the sum Eq. (7) are distinguished by their odd/even parity, hence after summation we get two terms:

$$g(E) = \left(\frac{\pi}{2\Delta} \right) \left[c_-^2 \cot \left(\pi \frac{E}{2\Delta} \right) - c_+^2 \tan \left(\pi \frac{E}{2\Delta} \right) \right] \quad (18)$$

The secular equation $g(E) = E - u$ becomes a quadratic equation for $\cot()$, and can be solved explicitly:

$$\cot \left(\pi \frac{E}{2\Delta} \right) = \frac{\Delta}{\pi c_-^2} \left[(E-u) \pm \sqrt{(E-u)^2 + \left(\frac{\pi c_+ c_-}{\Delta} \right)^2} \right]$$

where the \pm refers to the parity that is alternating for subsequent levels. Then it is straightforward to get an explicit expression for the shuttle occupation probability $p(u)$ via Eq. (8), and for the level occupations $q_n(u)$ via Eq. (9). The expressions are quite lengthy but can be simplified in the regime of interest as described below.

Of interest is the case of a quasi-continuum, meaning that the couplings c_n are larger compared with Δ , hence a two level approximation is out of the question, while a Wigner-type approximation is most appropriate. For this purpose we find it useful to define parameters that describe the effective coupling of the shuttle to the quasi-continuum, and its asymmetry:

$$C_{\text{eff}} \equiv \frac{\pi}{2} \frac{c_+ c_-}{\Delta} \quad (19)$$

$$\Gamma \equiv \pi \frac{c_+^2 + c_-^2}{\Delta} \quad (20)$$

$$\sin(\theta) \equiv \frac{c_+^2 - c_-^2}{c_+^2 + c_-^2} \quad (21)$$

Here and below we assume without loss of generality that the particle starts in an even-parity level. Using these notations we get after some algebra an approximation that should be valid in the quasi-continuum case:

$$p(u) \approx \Delta \cdot L[u - E; \Gamma, \theta] \quad (22)$$

The distorted Lorentzian $L[x; \Gamma; \theta]$ is

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

In the expression above E is the energy in which the particle has been prepared. In the regime of interest, where the levels are treated as quasi-continuum, this energy can be regarded as a constant. Some further straightforward algebra leads to

$$\begin{aligned} G(u) &= C_a \frac{\partial}{\partial u} \left[p \sum_n \frac{c_n^* \langle n|a \rangle}{(E - \epsilon_n)^2} \right] \quad (23) \\ &= C_a \frac{\partial}{\partial u} \left[\frac{\frac{c_-}{\sin^2(\pi \frac{E}{2\Delta})} + \frac{c_+}{\cos^2(\pi \frac{E}{2\Delta})}}{\left(\frac{2\Delta}{\pi}\right)^2 + \frac{c_-^2}{\sin^2(\pi \frac{E}{2\Delta})} + \frac{c_+^2}{\cos^2(\pi \frac{E}{2\Delta})}} \right] \\ &\approx \frac{\partial}{\partial u} C_a \left[\frac{c_+ + c_- \cot^2\left(\pi \frac{E}{2\Delta}\right)}{c_+^2 + c_-^2 \cot^2\left(\pi \frac{E}{2\Delta}\right)} \right] \\ &= (\lambda_- - \lambda_+) \frac{2C_{\text{eff}}^2}{(4C_{\text{eff}}^2 + (u - E)^2)^{3/2}} \quad (24) \end{aligned}$$

Disregarding the splitting-ratio factor, this expression has surprisingly the same functional form as that of crossing a single level ($N = 1$), see e.g. [23], but with an effective coupling constant C_{eff} that reflects the density of states.

The functions $p(u)$ and $G(u)$ are plotted in Fig. 2 and in Fig. 3. In the latter we contrast with the $c_n \ll \Delta$ case, for which the dynamics can be regarded as a sequence of two $N = 1$ crossings.

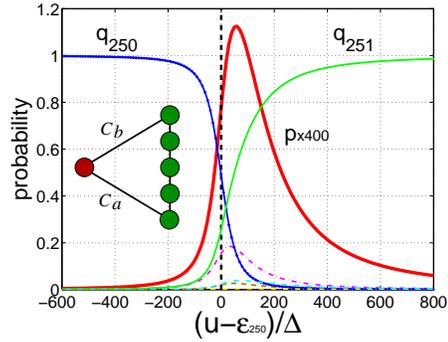


Figure 2. The variation of the occupation probabilities as a function of u for an adiabatic shuttling process. The particle initially has been placed at $n_0 = 250$. The level spacing is $\Delta = 1$, and the couplings are $C_a = 6$ and $C_b = 4$. The red thick line is p . The other solid lines are q_{250} , and q_{251} . The dashed lines from up to down are q_{249} and q_{253} and q_{247} and q_{252} .

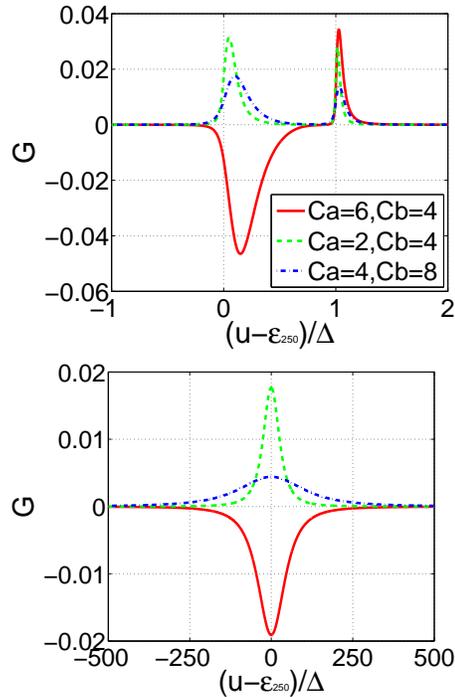


Figure 3. Flow of the current from the shuttle to the wire through the C_a bond, for the same scenario as in Fig. 2. The parameters are indicated in the legend. The raw calculation is done using Eq. (23) with Eq. (8). In the upper panel $\Delta = 200$, hence a two level approximation is satisfactory. In the lower panel $\Delta = 1$, hence the explicit result Eq. (24) can be optionally used in order to describe the multi-level crossing.

8. Regimes

The results for the integrated current give another wrong impression: it looks as if we are dealing with two regimes: either the process is adiabatic or non-adiabatic. A more careful inspection reveals that depending on \dot{u} we have 3 regimes: Adiabatic, Slow and Fast. For star geometry with comb-like quasi continuum of levels, the Slow regime is defined by the condition

$$c^2 < \dot{u} < \Gamma^2, \quad \Gamma \equiv 2\pi \frac{c^2}{\Delta} \quad (25)$$

For simplicity we assume here comb-like quasi continuum with identical couplings $c_n = c$. The left inequality in Eq. (25) means that the adiabatic condition is violated, while the right inequality implies that a first-order perturbative approximation is violated as well. The identification of this intermediate Slow regime parallels the notion of Wigner or FGR or Kubo regime in past studies of time dependent dynamics [19].

Some illustrations for energy spreading are presented in Fig. 1. If $c < \Delta$ the transport of probability from the shuttle to the network levels would be described using a two-level approximation. But the illustration in the upper panel assumes $c > \Delta$, hence many levels are mixed within a parametric range Γ . The time during which this mixing takes place is Γ/\dot{u} . In the opposite limit of Fast shuttling, which we further discuss below, the decay time of the probability to the quasi-continuum is $1/\Gamma$.

9. Non adiabatic spreading

The calculation of I in the non-adiabatic regime requires knowledge of $q_n(t)$. For star geometry this calculation is a variant of the Wigner decay problem, and hence can be solved analytically: instead of a *fixed* level that decays into a quasi-continuum we have a *moving* shuttle. The usual textbook procedure is followed [31] leading to the following set of equations

$$\partial_t \Psi_0 = \left[-iu(t) - (\Gamma/2) \right] \Psi_0 \quad (26)$$

$$\partial_t \Psi_n = -i\epsilon_n \Psi_n - ic_n \Psi_0 \quad (27)$$

With $u(t) = \dot{u}t$ one obtains the solution

$$q_n(t) = \left| c_n \int_0^t d\tau \exp \left(i\epsilon_n \tau - i\frac{\dot{u}}{2} \tau^2 - \frac{\Gamma}{2} \tau \right) \right|^2 \quad (28)$$

By inspection one observes that going from the Slow to the Fast regime, the spreading line shape changes from Lorentzian-type to Fresnel-type, as illustrated in the lower panel of Fig. 1.

10. Summary

We have found, using elementary considerations, without the need to rely on a complicated transport formalism, that it is possible to replace Eq. (3) by the general expression Eq. (12), that holds both in adiabatic and non-adiabatic circumstances. Hence the problem of calculating currents is reduced to that of calculating time dependent probabilities $q_n(t)$ as in the stochastic formulation [26].

Our result Eq. (12) is quite general. We have demonstrated its use in the very simple case of “ring geometry”, but it can be applied to any network configuration, and for any $u(t)$ time dependence. In particular one can use it in order to analyze a multi-cycle stirring process. Furthermore, the application of Eq. (12) to a many-body system of non-interacting particles follows trivially, with $q_n(t)$ that represent the actual occupations of the levels.

It is important to realize that the “splitting ratio” Eq. (11) unlike the stochastic “partitioning ratio” [26] is not bounded within $[0, 1]$. This observation has implications on the calculation of “counting statistics” and “shot noise” [32, 33, 34].

We have emphasized aspects that go beyond the familiar two-level approximation phenomenology, related to the scrambling of the network levels during the shuttling process. This shuttle-induced mixing process is reflected in the time dependence of the currents, but not in Q .

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