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Multiple path adiabatic crossing in a three-site ring

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Abstract

We find an exact expression for the current that is induced in a three-site ring during a multiple-path adiabatic crossing. The understanding of the dynamics requires us to go beyond the two-level phenomenology. In particular we highlight a prototype process, 'adiabatic metamorphosis', during which current is flowing through a non-accessible site. This helps to understand the crossover from coherent non-classical *splitting* to stochastic noisy-alike *partitioning* of the current.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Adiabatic quantum transport [1–5] is a major theme in quantum mechanics, with diverse applications, e.g. quantum Hall effect [6], dynamics of Josephson junctions [7] and the analysis of pericyclic reactions [8]. If a parameter is slowly varied in a closed system that has a non-trivial topology, say a ring-shaped device, the formalism implies that current is induced. In the absence of magnetic fields, we call such an effect 'quantum stirring' [9–12]. On the one hand, it is related to the classical problem of 'stochastic stirring' [13–16], and on the other hand, it is related to 'quantum pumping' in open systems [17–24].

Most results regarding adiabatic quantum transport are rather abstract, based on a formal mathematical approach, notably the 'Dirac monopoles picture' [4, 9]. This should be contrasted with the analysis of stochastic stirring where the phenomenology is quite mature [13]. The way to gain better physical insight is to analyze prototype model systems [11, 12] and to identify the elementary ingredients that determine the nature of the dynamics.

In this work, we would like to address the minimal model for a closed isolated quantum system that has a non-trivial topology. This is evidently the three-site ring that is illustrated in figure 1. Quite generally, in the absence of magnetic field, the stationary states of the system, and the ground state in particular, carry zero current. If we want to obtain current, we have to

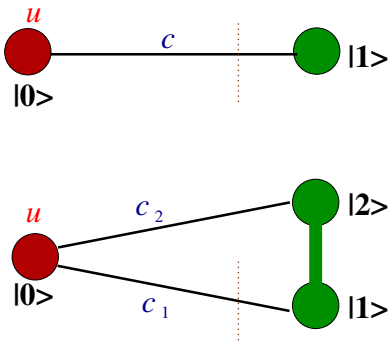

Figure 1. Two-site and three-site toy models for transport. A particle is initially positioned at the left site $|0\rangle$, called 'dot'. The dot has a potential energy u that can be controlled externally. As u is varied adiabatically from $-\infty$ to $+\infty$, currents are induced in the bonds, and the particle ends up at the right sites. In the case of a three-site system, it is a multiple-path transition through the $0 \rightsquigarrow 1$ and $0 \rightsquigarrow 2$ bonds to the lower level of the 'wire'.

drive the system by varying a parameter u in time. In the adiabatic limit, the current is given by the following formula:

$$\langle \mathcal{I} \rangle = G(u(t))\dot{u}, \tag{1}$$

where $G(u)$ is the geometric conductance

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

In the above formula, Ψ is the adiabatic ground state that depends on the parameter u, and on an auxiliary test flux ϕ through the bond of interest.

Specifically, we want to consider the following scenario, which we call 'multiple path adiabatic crossing'. Assume that a particle is placed in the 0th site, which we call 'dot'. The potential of the dot is raised slowly from $u = -\infty$ to $u = +\infty$. As a result the particle is adiabatically transferred from the dot to the other two sites. These two sites ('1' and '2') can be regarded as a two-orbital entity that we call 'wire'. At the end of the process, the particle will be found in the lower energy level of the wire. We ask what is the current through the first bond ($0 \rightsquigarrow 1$). Equivalently, we can characterize the transport by the integrated current

$$Q(u) = \int_{-\infty}^{u} G(u')\,\mathrm{d}u'. \tag{3}$$

In particular, we define $Q \equiv Q(\infty)$. If we had single-path geometry obviously the result for the latter would be $Q = 1$, reflecting 100% transition probability. But we are dealing here with a multiple path geometry.

At this point, it is important to emphasize that if we were dealing with a stochastic process the current would be *partitioned* between the paths, hence $|Q| < 1$. But the essence of 'quantum stirring' is the observation that during the driving process a circulating current is induced. Due to this circulation, the integrated current can be *any* number.

The above recipe equation (2) for calculating adiabatic currents is well known from the works on adiabatic transport, but its physical implications have not been fully recognized. In fact, the original interest in this model has been motivated by a wrong assertion that 'adiabatic pumping' in a closed system has to be quantized [27]. The fallacy of this statement has been illuminated using the 'Dirac monopoles picture' [9] and later using a two-level 'splitting ratio' phenomenology [12, 28]. The exact solution of the three-site ring has been considered as well

[9], to establish that Q of a closed driving cycle can have any value. However, the full solution of the multiple-path adiabatic crossing has not been explored. In particular, it has remained vague whether to go beyond the two-level approximation is of any physical significance.

Outline.–We first derive an exact expression for $Q(u)$. This is quite straightforward, but as usual the exact expression is not very illuminating physically. We therefore try to derive approximations that are based on a two-level phenomenology. Then we realize that there are different regimes depending on the ratio between the inter dot-wire and the intra-wire couplings. In particular, we find a regime where the crossing process involves an 'adiabatic metamorphosis' stage, during which current is flowing through the energetically non-accessible dot.

2. $G(u)$ for a two-site system

We start with the analysis of a single-path crossing in a two-site system. The Hamiltonian and the associated current operator are

$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & C^* \\ C & u_c \end{pmatrix}, \qquad \mathcal{I} \mapsto \lambda \begin{pmatrix} 0 & \mathrm{i}C^* \\ -\mathrm{i}C & 0 \end{pmatrix}, \tag{4}$$

where $u(t)$ is the potential of the dot, u_c is the level that is crossed and C is the dot-level coupling. The extra parameter $\lambda = 1$ is reserved for later. Without loss of generality, we assume C to be real and positive $C > 0$. For the purpose of defining the current operator $\mathcal{I} \equiv -\partial\mathcal{H}/\partial\phi$, and later using equation (2), one should substitute $C \mapsto C\mathrm{e}^{\mathrm{i}\phi}$.

For a given value of u the energy of the adiabatic ground state is

$$E(u) = \tfrac{1}{2}[(u + u_c) - \sqrt{4C^2 + (u - u_c)^2}]. \tag{5}$$

The corresponding eigenstate is

$$|\Psi\rangle \mapsto \frac{1}{\sqrt{S}} \begin{pmatrix} E - u_c \\ C\mathrm{e}^{\mathrm{i}\phi} \end{pmatrix} \tag{6}$$

where the normalization factor for zero flux is

$$S = (E - u_c)^2 + C^2. \tag{7}$$

Using equation (2) we obtain

$$G(u) = C^2 \frac{\partial}{\partial u} \left[\frac{1}{S} \right] \tag{8}$$

leading to

$$G(u) = \lambda \frac{2C^2}{(4C^2 + (u - u_c)^2)^{3/2}}, \tag{9}$$

where $\lambda = 1$. It is easily verified that upon integration $Q = \lambda$, hence $Q = 1$, as implied by the continuity equation for a single-path adiabatic crossing.

3. $G(u)$ for a three-site system

We now use the same procedure for the analysis of the double-path crossing in a three-site system. The Hamiltonian and the associated current operator are

$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & c_1^* & c_2^* \\ c_1 & 0 & c_0^* \\ c_2 & c_0 & 0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \begin{pmatrix} 0 & \mathrm{i}c_1^* & 0 \\ -\mathrm{i}c_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{10}$$

We assume the cs to be real (no magnetic field) but for the purpose of defining the current through the $0 \rightsquigarrow 1$ bond, and later using equation (2), we substitute $c_1 \mapsto c_1 e^{i\phi}$.

The secular equation for the eigenvalues is

$$E_n^3 - uE_n^2 - \left(c_0^2 + c_1^2 + c_2^2\right)E_n + c_0^2 u - 2c_0 c_1 c_2 \cos(\phi) = 0 \tag{11}$$

with the solution

$$E_n = \frac{u}{3} + 2\sqrt{Q}\cos\left(\frac{\theta}{3} + n\frac{2\pi}{3}\right), \quad n = 0, \pm 1, \tag{12}$$

where

$$\cos(\theta) \equiv \frac{\mathcal{R}}{\sqrt{\mathcal{Q}^3}} \tag{13}$$

$$\mathcal{Q} \equiv \frac{1}{9}u^2 + \frac{1}{3}\left(c_0^2 + c_1^2 + c_2^2\right) \tag{14}$$

$$\mathcal{R} \equiv \frac{1}{27}u^3 + \frac{1}{6}\left(c_1^2 + c_2^2 - 2c_0^2\right)u + c_0 c_1 c_2 \cos(\phi). \tag{15}$$

As u is varied from $-\infty$ to $+\infty$, the angle θ varies from π to 0, and the ground state energy E_1 goes from $-u$ to $-c_0$. The corresponding eigenstates are

$$|n(u)\rangle \mapsto \frac{1}{\sqrt{S_n}}\begin{pmatrix} E_n^2 - |c_0|^2 \\ c_1 E_n + c_0^* c_2 \\ c_2 E_n + c_0 c_1 \end{pmatrix}. \tag{16}$$

The normalization factor for zero flux is

$$S_n = \left(E_n^2 - c_0^2\right)^2 + (c_1 E_n + c_0 c_2)^2 + (c_2 E_n + c_0 c_1)^2 \tag{17}$$

$$= E_n^4 + \left(c_1^2 + c_2^2 - 2c_0^2\right)E_n^2 + 2c_0 c_1 c_2 E_n + c_0^2\left(c_0^2 + c_1^2 + c_2^2\right). \tag{18}$$

If we placed the test flux at the c_0 bond we would obtain from equation (2) the result that had been derived in [9] for the current in the $1 \rightsquigarrow 2$ bond, namely

$$G_{1\rightsquigarrow 2}(u) = c_0^2\left(c_1^2 - c_2^2\right)\frac{\partial}{\partial u}\left[\frac{1}{S_1}\right]. \tag{19}$$

But our interest is in the current that goes through the $0 \rightsquigarrow 1$ bond. Accordingly, we have placed the test flux at c_1 and obtain

$$G = 2\left[c_1^2 E_1 + c_0 c_1 c_2\right]\frac{1}{S_1}\frac{\partial E_1}{\partial u} - \left[c_1^2 E_1^2 + 2c_0 c_1 c_2 E_1 + c_0^2 c_1^2\right]\frac{1}{S_1^2}\frac{\partial S_1}{\partial u} \tag{20}$$

$$= \frac{\mathrm{d}}{\mathrm{d}u}\left[\frac{c_1^2 E_1^2 + 2c_0 c_1 c_2 E_1 + c_0^2 c_1^2}{E_1^4 + \left(c_1^2 + c_2^2 - 2c_0^2\right)E_1^2 + 2c_0 c_1 c_2 E_1 + c_0^2\left(c_0^2 + c_1^2 + c_2^2\right)}\right]. \tag{21}$$

4. The integrated current

On the basis of equation (21) one observes that for any $c_0 \neq 0$ the integrated current equation (3) at the end of the process is

$$Q = \left.\frac{c_1^2 E_1^2 + 2c_0 c_1 c_2 E_1 + c_0^2 c_1^2}{E_1^4 + \left(c_1^2 + c_2^2 - 2c_0^2\right)E_1^2 + c_0 \cdots}\right|_{E_1 = -c_0} = \frac{c_1}{c_1 - c_2}. \tag{22}$$

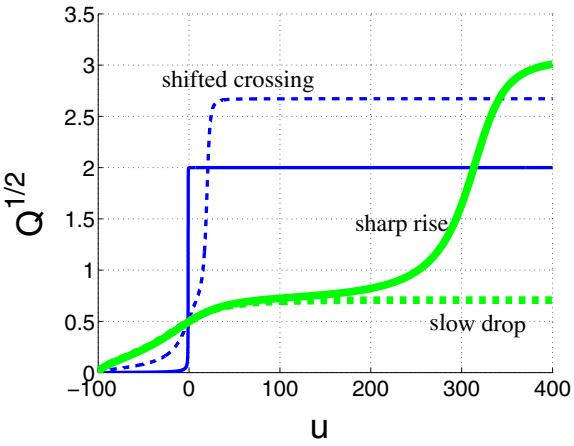

Figure 2. An initially loaded level crosses the other two levels of a three-site network. We plot the parametric variation of the integrated current $Q(u)$ in representative cases. For graphical purpose, the horizontal axis is $Q^{1/2}$. The parameters are $c_0 = 1$ and (c_1, c_2) as follows: solid blue $(0.2, 0.15)$ is like a simple two-level crossing; dashed blue $(5.0, 4.3)$ exhibits a shifted two-level crossing; solid green $(19, 17)$ features a sharp metamorphosis; dashed green $(19, -17)$ features a gradual metamorphosis.

Strangely enough, this does not depend on the value of c_0. But for $c_0 = 0$, based on the *same* expression, the result is quite different

$$Q = \left.\frac{c_1^2}{E_1^2 + \left(c_1^2 + c_2^2\right)}\right|_{E_1=0} = \frac{|c_1|^2}{|c_1|^2 + |c_2|^2}. \tag{23}$$

It is therefore required to explain what happens *physically* if c_0 is very very small but not zero. In figure 2, we illustrate $Q(u)$ for several representative cases. If c_0 is large $Q(u)$ rises monotonically in a step-like fashion to the value that is predicted by equation (22). However, if c_0 is small one observes two stages in the parametric evolution: first $Q(u)$ rises to the value that is predicted in equation (23), and only after that it re-adjust to the value of equation (22). In Section 9, we shall use the term 'adiabatic metamorphosis' in order to describe this re-adjustment of the occupations. We shall see that it involves a much larger parametric scale $u_m \propto 1/c_0$ that diverges in the limit $c_0 \to 0$. Hence, for $c_0 = 0$, we are left with equation (23) instead of equation (22). A closer inspection of the metamorphosis stage (dashed versus solid green curves in figure 2) reveals that it can be either a gradual or a sharp transition, depending on the relative sign of c_1 and c_2.

The values (c_1, c_2) for the illustrations in figure 2 are indicated in the diagram of figure 3. In the following sections, we would like to illuminate the different regions in this diagram by attempting a two-level approximation scheme.

5. The two-level approximation

Let us try to reduce the three-level dynamics to a two-level crossing problem. For this purpose, we switch to the following basis:

$$|0\rangle = \text{the dot state} \tag{24}$$

$$|+\rangle = \tfrac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = \text{the upper (even) wire state} \tag{25}$$

$$|-\rangle = \tfrac{1}{\sqrt{2}}(|1\rangle - 2\rangle) = \text{the lower (odd) wire state.} \tag{26}$$

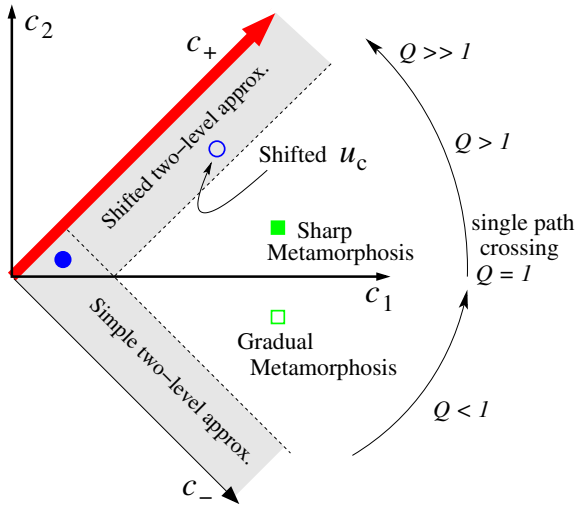

Figure 3. A schematic diagram that shows the different regimes in the analysis of the adiabatic double-path crossing. Setting $c_0 = 1$ the parameters that define the three-site system are the couplings c_1 and c_2. Without loss of generality, we relate to one quarter where both c_+ and c_- are positive. Gray shading indicates the regime where a two-level approximation scheme can be used, either $c_- \ll c_0$ or $c_+ \ll c_0$, as discussed in the text. In each regime, the $G(u)$ has a different looking lineshape. Blue and green symbols indicate the representative illustrations that have been displayed in figure 2.

In the new basis, the Hamiltonian and the current operator equation (10) take the following form:

$$\mathcal{H} \mapsto \begin{pmatrix} u(t) & c_+ & c_- \\ c_+ & c_0 & 0 \\ c_- & 0 & -c_0 \end{pmatrix}, \qquad \mathcal{I} \mapsto \tfrac{c_1}{\sqrt{2}} \begin{pmatrix} 0 & \mathrm{i} & \mathrm{i} \\ -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{pmatrix} \tag{27}$$

with couplings

$$c_\pm = \tfrac{1}{\sqrt{2}}(c_1 \pm c_2). \tag{28}$$

Without loss of generality, we focus on the strongest bond, meaning that we assume $|c_1| > |c_2|$, and by appropriate gauge we arrange that $c_1 > 0$, hence both $c_\pm$ are positive numbers. We shall see that a two-level approximation scheme is useful for the treatment of three cases that are indicted in figure 3, namely

$$|c_+| \ll c_0 \tag{29}$$

$$|c_-| \ll c_0 \tag{30}$$

$$c_0 = 0. \tag{31}$$

In all these cases, we can fit the exact result equation (21) to the two-level expression equation (9), with some effective values for C, u_c and λ. The remaining case of having a relatively *small but finite* c_0 is excluded, because it cannot be treated within the framework of a two-level approximation. This last case will be considered separately.

6. The simple two-level approximation $|c_+| \ll c_0$

We first consider the very simple case, in which the third (upper) level can be ignored. The condition for that is $|c_+| \ll c_0$. Taking the relevant block from the 3×3 Hamiltonian of

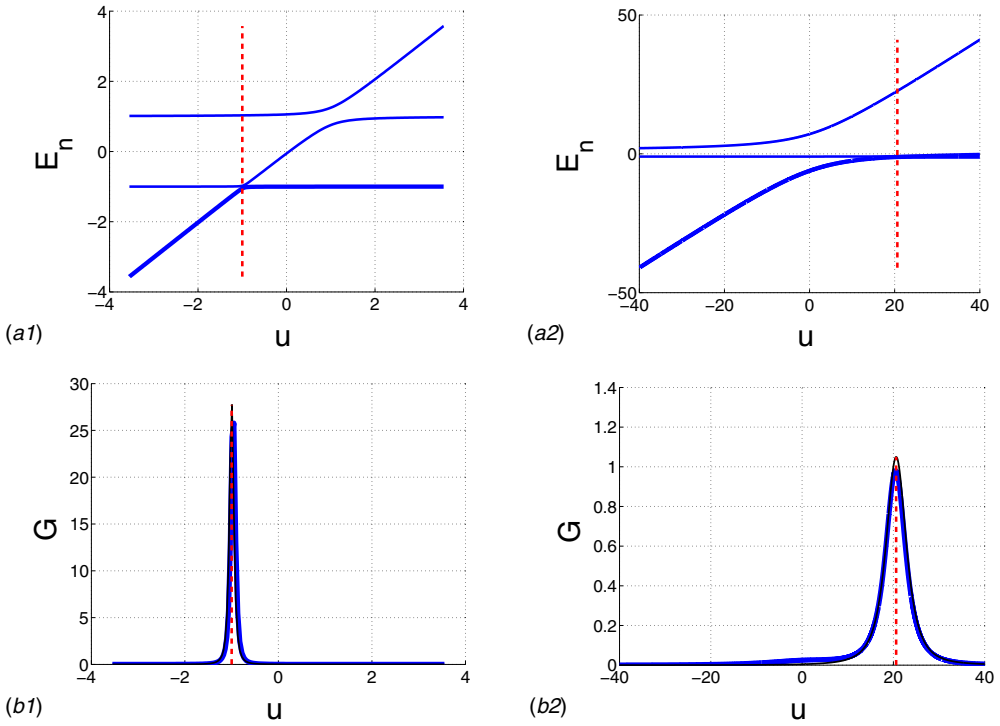

Figure 4. An initially loaded level crosses the other two levels of a three-site network. (*a*) The adiabatic energies $E_n(u)$ as a function of the dot potential. (*b*) The geometric conductance $G(u)$ during this sweep process, reflecting the current through the c_1 bond. The thick blue line is the exact solution equation (21). We use units such that $c_0 = 1$. The parameters in set (1) are $c_1 = 0.2$ and $c_2 = 0.15$, corresponding to the regime $|c_+| \ll c_0$, where the simple two-level approximation (thin black line) applies. Vertical dashed line indicates the dot-wire crossing point. The parameters in set (2) are $c_1 = 5.0$ and $c_2 = 4.3$, corresponding to the regime $|c_-| \ll c_0$, where a shifted two-level approximation (thin black line) applies. Vertical dashed line indicates the *shifted* crossing point. *Note*: the agreement is so good that the thin black lines almost cannot be resolved.

equation (27) one obtains a reduced 2×2 Hamiltonian that is given by equation (4) with the effective parameters

$$\lambda = \frac{c_1}{c_1 - c_2}, \qquad C = \frac{c_1 - c_2}{\sqrt{2}}, \qquad u_c = -c_0. \tag{32}$$

Hence, we deduce that $G(u)$ of equation (9) can be used as an approximation for the exact result. This expectation is confirmed in figure 4.

The presence of λ reflects that the flow is via two bonds instead of via only a single bond, unlike the case of the two-site model. In other words, the particle 'splits' and flows through both bonds. We note that the integrated current $Q = \lambda$ can have a manifestly non-classical value: it can be either larger than 1 or negative. In fact, if it is larger than 1 in one bond it has to be negative in the other bond, since the total corresponds to 100% probability of being adiabatically transferred. The non-classical value of λ reflects a circulating current that is induced during the transition. In a semi-classical language, it means that the particle is looping several rounds through the ring before ending up in the wire.

7. The shifted two-level approximation $|c_-| \ll c_0$

The simple two-level approximation of the previous section is not valid if $|c_+| > c_0$. Still if $|c_-| \ll c_0$, we can obtain a result that looks like equation (9). The solution procedure involves two steps. In the first step, we switch to a new basis:

$$|\theta\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|+\rangle \tag{33}$$

$$|\bar{\theta}\rangle = -\sin(\theta/2)|0\rangle + \cos(\theta/2)|+\rangle \tag{34}$$

$$|-\rangle = \text{the lower (odd) wire state,} \tag{35}$$

where

$$\theta(u) = \arctan\left(\frac{2c_+}{u - c_0}\right). \tag{36}$$

In this basis, the block of the Hamiltonian equation (27) that contains the strongly interacting states $|0\rangle$ and $|+\rangle$ becomes diagonal. Now it is possible to neglect the upper level $|\theta\rangle$ and we obtain a two-level crossing problem that involves the 'dressed' dot level $|\bar{\theta}\rangle$ and the lower (odd) wire level $|-\rangle$. The adiabatic energy of the former is

$$E_{\bar{\theta}} = \tfrac{1}{2}[(u + c_0) - \sqrt{4c_+^2 + (u - c_0)^2}] \tag{37}$$

while that of the latter is $E_- = -c_0$. Accordingly the shifted crossing point is

$$u_c = \left[-1 + \frac{1}{2}\left(\frac{c_+}{c_0}\right)^2\right] c_0. \tag{38}$$

The stronger the coupling c_+ to the upper level, the larger is the shift of u_c.

In order to estimate the effective parameters of the shifted two-level crossing, we have to write the Hamiltonian and the current operator in the new basis. In the vicinity of the crossing point, we set $\theta_c = \theta(u_c)$, obtaining

$$\mathcal{H} \mapsto \begin{pmatrix} [u\sin^2(\theta_c/2) + c_0\cos^2(\theta_c/2) - c_+\sin(\theta_c)] & -c_-\sin(\theta_c/2) \\ -c_-\sin(\theta_c/2) & -c_0 \end{pmatrix} \tag{39}$$

and

$$\mathcal{I} \mapsto \lambda \begin{pmatrix} 0 & -\mathrm{i}c_-\sin(\theta_c/2) \\ \mathrm{i}c_-\sin(\theta_c/2) & 0 \end{pmatrix}, \tag{40}$$

where λ is the same as in the previous section. It is important to realize that up to constant the effective dot potential equals αu with $\alpha = \sin^2(\theta_c/2)$. It is not difficult to see that this implies the replacement

$$G(u) \mapsto \alpha G(\alpha u). \tag{41}$$

Hence, within the framework of the two-level approximation the effective C in equation (9) is not $-c_-\sin(\theta/2)$ but rather it should be divided by α. So eventually we deduce that the $G(u)$ can be approximated by equation (9) with an effective coupling parameter

$$C = -\left[\sin\left(\frac{\theta_c}{2}\right)\right]^{-1} c_-. \tag{42}$$

This expectation is confirmed in figure 4. Note again that λ is the same as in the simple two-level approximation, and that we evaluate θ_c at the crossing point using equation (36) with equation (38).

8. Adiabatic crossing for $c_0 = 0$

In the previous versions of the two-level approximation, the intra-wire coupling c_0 was large in some sense. Now we go to the other extreme limit of having $c_0 = 0$. This resembles the standard setup that is used in the analysis of stimulated Raman adiabatic passage. In fact, we can adopt here the same 'dark state' picture in order to reduce the problem to a two-level crossing. Namely, for this purpose we switch to the following basis:

$$|0\rangle = \text{the dot state} \tag{43}$$

$$|C\rangle = \frac{1}{\sqrt{c_1^2 + c_2^2}}(c_1|1\rangle + c_2|2\rangle) \tag{44}$$

$$|D\rangle = \frac{1}{\sqrt{c_1^2 + c_2^2}}(c_2|1\rangle - c_1|2\rangle) = \text{dark state.} \tag{45}$$

In the new basis $|D\rangle$ state decouples, and hence we end up again with a reduced 2×2 Hamiltonian that is given by equation (4) with the effective parameters

$$\lambda = \frac{c_1^2}{c_1^2 + c_2^2}, \qquad C = \sqrt{c_1^2 + c_2^2}, \qquad u_c = 0. \tag{46}$$

Hence we deduce that $G(u)$ of equation (9) with the above set of effective parameters coincides in this case with the exact result.

It should be clear that for $c_0 = 0$, we no longer have a non-trivial geometry, and hence a circulating current cannot be induced. For this reason, it is *a priori* expected to obtain an effective two-level description with $\lambda \in [0, 1]$. In fact, we got for λ a stochastic look-alike expression that reflects the relative transmission of the two bonds.

9. Adiabatic metamorphosis

Let us contrast the $c_0 = 0$ case with the $c_0 \to 0$ case. The two cases give very different results. We would like to better clarify what really happens if c_0 is very small. We first recall the optional bases for the representation of the system. The standard basis is $|0\rangle, |1\rangle, |2\rangle$. The wire-eigenstates basis is $|0\rangle, |+\rangle, |-\rangle$, and the $c_0 = 0$ basis is $|0\rangle, |C\rangle, |D\rangle$. For the instantaneous eigenstates, we shall use the notations $|E_g\rangle$, $|E_d\rangle$ and $|E_e\rangle$.

Recall that for $c_0 = 0$ the dark state $|D\rangle$ decouples, meaning that $|E_d\rangle = |D\rangle$, while the other two eigenstates $|E_g\rangle$ and $|E_e\rangle$ are superpositions of $|0\rangle$ and $|C\rangle$. At the end of an adiabatic process, the system will be found in the degenerate $|E_g\rangle = |C\rangle$ state. However, if c_0 is non-zero, the system ends up in the non-degenerate $|E_g\rangle = |-\rangle$ state.

It is therefore clear that for very small but finite c_0 the adiabatic ground state changes from $|C\rangle$ to $|-\rangle$. We call this 'adiabatic metamorphosis'. We define u_m as the value of u at which this metamorphosis occurs. Close to u_m the dot level is energetically far above, hence the lower states $|1\rangle$ and $|2\rangle$ form a two-level system with virtual coupling through the distant dot level. The reduced Hamiltonian is determined by second-order perturbation theory:

$$\mathcal{H} \mapsto \begin{pmatrix} \dfrac{c_1^2}{u} & c_0 - \dfrac{c_1 c_2}{u} \\ c_0 - \dfrac{c_1 c_2}{u} & \dfrac{c_2^2}{u} \end{pmatrix}. \tag{47}$$

By inspection of this Hamiltonian it is clear that for large enough u the direct coupling c_0 takes over, and then the metamorphosis to $|E_g\rangle = |-\rangle$ is finalized. In particular, it is interesting

to consider the case in which $c_2 \sim c_1$. Then the metamorphosis crossing point is sharply defined

$$u_m = \frac{c_1 c_2}{c_0}, \quad \text{[for sharp metamorphosis]} \tag{48}$$

which is demonstrated in figure 5. Otherwise the metamorphosis is a gradual process, as was illustrated in figure 2. Note that for sharp metamorphosis, at $u = u_m$, all the probability is concentrated in one site of the wire, namely, in the site that is more strongly connected to the dot. This is demonstrated in panel (c) of figure 5.

10. Beyond the adiabatic limit

In order for the process to be adiabatic the probability distribution should change slowly with time. This implies that the current cannot be very large. Let us see what is the precise statement. Specifically, for a two level Landau–Zener crossing the adiabatic condition is

$$\dot{u} \ll C^2, \tag{49}$$

where C is the coupling between the dot and the crossed level. This implies that

$$I_{\max} \sim G(u_c)\dot{u}_{\max} \sim C. \tag{50}$$

One observes that the maximal current reflects the coupling. Furthermore, also the integrate current cannot be too large. It is simply bounded by unity ($|Q| < 1$) reflecting that the maximum transfer is 100%.

If we consider multiple path geometry, it is easy to show that the conclusion regarding the maximal current still holds. However, as was clarified in previous sections, the integrated current $Q = \lambda$ becomes arbitrarily large if $c_1 \sim c_2$, rather than being bounded. A large value $|Q| > 1$ reflects the existence of a circulating current that is induced in the system during the driving process. It should be clear that in order to witness $|Q| \gg 1$ one has to satisfy a very demanding adiabatic condition, because the effective coupling that enters into equation (49) is $C = (c_1 - c_2)\sqrt{2}$.

Within the conventional framework of the two-level approximation, the implication of non-adiabaticity is to have less than 100% probability to cross from the dot to the wire, as implied by the Landau–Zener expression [25, 26]. But for very small c_0, such that the metamorphosis scenario applies, the implications of non-adiabaticity are more interesting as explained below. For finite $\dot{u}$ there is a finite range of small c_0 values for which the result for Q is approximately the same as for $c_0 = 0$. The complementary statement is as follows: for a given c_0, if $\dot{u}$ is large enough, the system does not have enough time to realize that it is coupled to a 'dark state'. Roughly this non-adiabatic condition takes the form $\dot{u} > c_0^2$. Thus, we have an intermediate 'diabatic' regime $c_0^2 \ll \dot{u} \ll C^2$ where the dynamics is 'adiabatic' with regard to the crossing, but 'sudden' with regard to the metamorphosis. The bottom line of the above discussion is illustrated in figure 5. One observes that for mild values of $\dot{u}$ the metamorphosis stage is not expressed, and the dynamics looks like that of $c_0 = 0$ system.

11. Discussion

Transport in quantum networks is a theme that emerges in diverse contexts. The simplest network that has non-trivial topology is the three-site system that we have considered in this paper. It can be regarded as composed of 'dot' and 'wire' segments. The most elementary process that has to be understood is an adiabatic sweep of the potential energy of a selected site (the dot), leading to the transfer of the probability to the other sites (the wire). Unlike

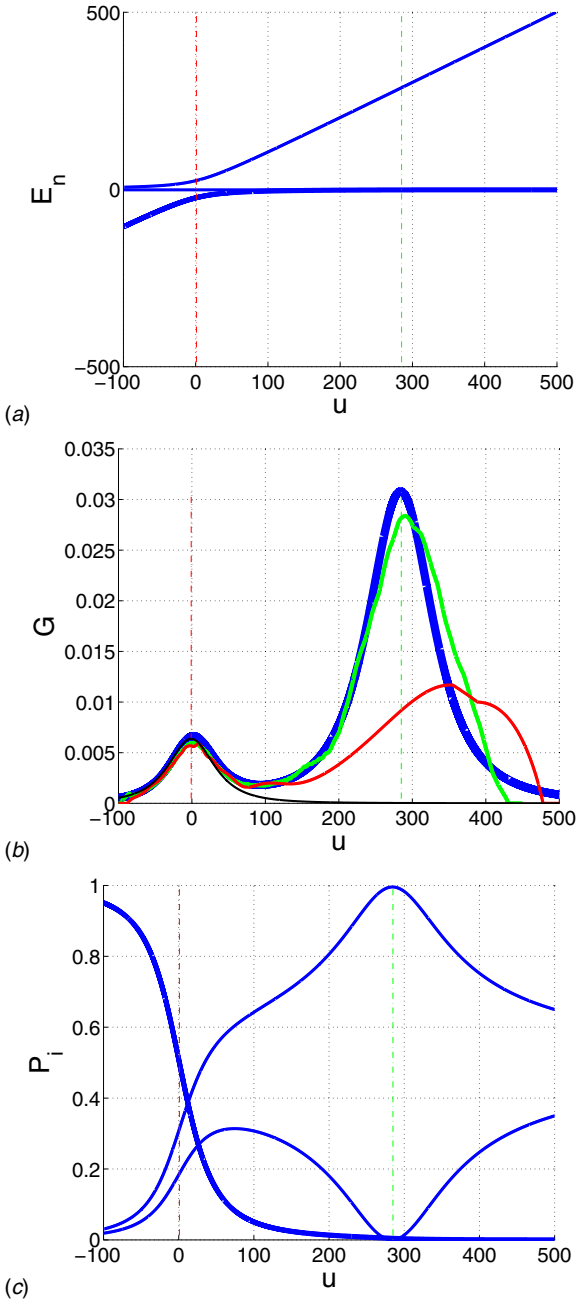

Figure 5. The same as in figure 4 but with $c_1 = 19$ and $c_2 = 15$, illustrating a sharp metamorphosis. The additional panel (c) shows the parametric variation of the occupation probabilities. In (b) the black line is the $c_0 = 0$ solution. The thinner (green) and the thinnest (red) lines are $I/\dot{u}$ for $\dot{u} = 2$ and for $\dot{u} = 50$, as determined by numerical simulation. The left and right vertical lines indicate the dot-wire crossing point, and the metamorphosis point, with separation $(u_m - u_c) = 286$. During the adiabatic metamorphosis, a current is flowing through the energetically distant dot. Mild non-adiabaticity spoils the metamorphosis without affecting the dot occupation.

stochastic process in which the probability current is partitioned with branching ratios that are bounded within [0, 1], here the splitting ratio λ can be any number reflecting a quantum stirring effect.

The detailed analysis of the three-site model allows us to highlight several essential ingredients in the analysis of quantum transport. In particular, it was important to clarify what is the way in which the two-level approximation breaks down. Strangely enough, the splitting ratios are independent of the intra-wire coupling, but still the $G(u)$ line shape is strongly influenced.

In particular, we have distinguished between two types of processes: inter dot-wire 'adiabatic crossing' processes and intra-wire 'adiabatic metamorphosis' processes. In the former, probability is transported between the dot and the wire, while in the latter the changes in the occupation are exclusively within the wire. During the metamorphosis stage the dot level is very far from the wire levels, but still current flows through the inter-connecting bonds, without being accumulated in the dot.

We believe that the processes that we have illuminated are of much relevance, and might shed new light, on the analysis of pericyclic reactions [8]. In this context, the method of calculating electronic quantum fluxes had assumed that the latter 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.

Furthermore, it is important to understand how non-adiabaticity and decoherence affect adiabatic transport. Possibly the most dramatic demonstration concerns the suppression of metamorphosis processes by mild non-adiabaticity. Then we obtain instead of coherent splitting, stochastic-like partitioning of the current. The reason for this crossover can be optionally explained using a very general paradigm. Namely, once the intra-wire couplings are introduced, there is a protecting 'gap' that becomes effective if the rate of the sweep is slow enough; this protecting gap forces the particle to be in a definite superposition at any moment. It follows that coherent splitting, unlike 'partitioning' of current is not a noisy process. This observation has implications on the calculation of 'counting statistics' and 'shot noise' [29, 28].

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