Quantum dynamics and transport in a double well system

Itamar Sela and Doron Cohen
Department of Physics, Ben-Gurion University, Beer-Sheva 84005, Israel
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The simplest one-dimensional model for the studying of nontrivial geometrical effects is a ring shaped device which is formed by joining two arms. We explore the possibility to model such a system as a two-level system (TLS). Of particular interest is the analysis of *quantum stirring*, where it is not evident that the topology is properly reflected within the framework of the TLS modeling. On the technical side we provide a practical "neighboring level" approximation for the analysis of such quantum devices, which remains valid even if the TLS modeling does not apply.

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I. INTRODUCTION

In this paper we explore the possibility to model a ring shaped device [Fig. 1(a)] as a two-level system (TLS) [Fig. 1(b)]. We shall see that both technical and conceptual difficulties are involved. The model Hamiltonian is

$$\mathcal{H} = \frac{1}{2\mathbf{m}}\hat{p}^2 + V_A(\hat{x} - x_A) + V_B(\hat{x} - x_B), \tag{1}$$

with periodic boundary conditions over $x \in [-L/2,\ L/2]$ so as to have a ring geometry, as illustrated in Fig. 1(a). V_A and V_B represent high barriers, such that the ring is composed of two weakly coupled arms. We assume that we have control over some geometrical parameters of the model and in particular over the heights X_A and X_B of both barriers. Our main interest is in the current that flows in the system. The current through an arbitrary point x_0 is obtained as the expectation value of the operator

$$\mathcal{I} = \frac{1}{2\mathbf{m}}[\hat{p}\,\delta(\hat{x} - x_0) + \delta(\hat{x} - x_0)\hat{p}]. \tag{2}$$

Having defined the system and its observables we can consider various dynamical scenarios such as coherent *Bloch oscillations* between the two arms. Then we can ask whether a TLS modeling is meaningful. Of particular interest for us is the analysis of *quantum stirring*:[1] this means to induce a circulating current by periodic modulation of the potential.

We note that transport due to periodic modulations of the potential[2] has been studied mainly in the context of quantum pumping,[3–5] where the current is induced between reservoirs. The notion of quantum stirring relates to closed geometry, where the emerging physical picture is significantly different.[6,7]

The quantum stirring problem highlights an obvious topological subtlety: one wonders whether the nontrivial topology of the ring is properly reflected in the effective TLS model.

On the technical side we define the unperturbed Hamiltonian $\mathcal{H}_0$ as the $X_A = X_B = \infty$ limit. In this limit the two arms are disconnected from each other, and the diagonalization gives a set of eigenenergies E_i such that each eigenstate belongs to only one of the two arms. Then we make either X_A or X_B or both finite, and we ask what is the perturbation matrix W_{ij} in the reduced Hamiltonian

$$\mathcal{H}_{ij} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} W_{11} & W_{12} \\ W_{21} & W_{22} \end{pmatrix}. \tag{3}$$

Obviously we would like to express the perturbation using the transmission coefficients of the barriers.

II. OUTLINE

In the first part of the paper (Secs. III–V) we establish the building blocks. We derive expressions for the perturbation matrix W_{ij} and for the reduced current operator $\mathcal{I}_{ij}$ and figure out how the topology is reflected in the reduced description.

In the second part of the paper (Secs. VI and VII) we turn to the applications. We begin with the simplest problems: The coherent Bloch oscillations of a particle in a mirror symmetric device, and the Wigner decay of a particle from a short arm to a long arm. Then we continue with the quantum stirring problem and show how one can derive expressions for the geometric conductance.

In the third part of the paper (Secs. VIII–X) we address some nontrivial technical points that are associated with the analysis, thus exploring the limitations of the TLS modeling. We demonstrate that even if the TLS modeling does not apply, we still can use a *neighboring level approximation* in order to extract results for the geometric conductance.

In the summary (Sec. XIII) we highlight the practical value of our findings for the purpose of design and analysis

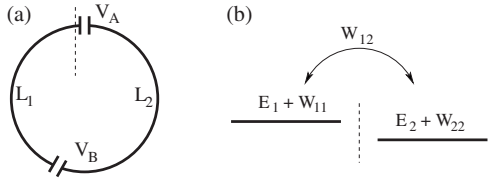

FIG. 1. Panel (a): Illustration of a ring shaped device that is divided by the barriers V_A and V_B into two arms of length L_1 and L_2. The current is measured through the dashed section near barrier A. In the quantum stirring scenario it is assumed that there is a gate control over the potential floor of each arm or over the height or the location of barrier B. Panel (b): Within the framework of the TLS modeling, the reduced Hilbert space contains two levels. The perturbation W_{ij} is due to having finite rather than infinite barriers, so it corresponds to the difference $\mathcal{H} - \mathcal{H}(\infty)$ and not to $V = \mathcal{H} - \mathcal{H}(0)$. See the text for further details.

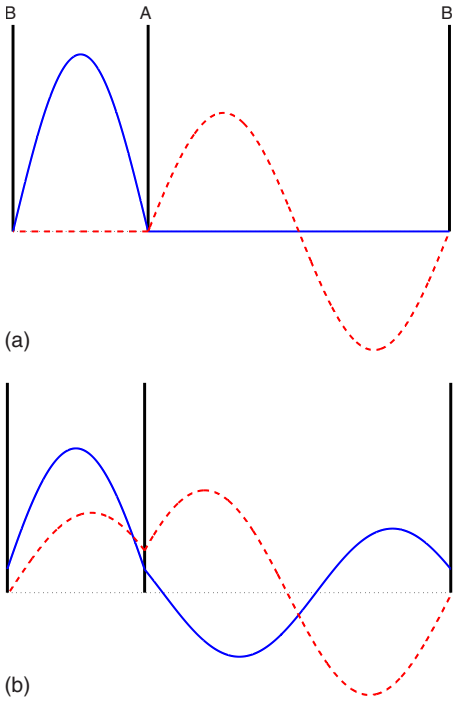

FIG. 2. (Color online) Upper panel: Two nearly degenerate eigenfunctions $\psi(x)$ of a particle in a ring with arms of lengths $L_1=1$ and $L_2=2.23$. These are the two unperturbed states of Eq. (4). Lower panel: The exact eigenfunctions assuming that the barriers are finite ($g_A \approx 0.28$ and $g_B \approx 0.06$). These do not vanish at the barriers and therefore cannot be written as a superposition of the unperturbed states. Still we explain in the text how a decent approximation for the former can be obtained using the neighboring levels approximation scheme.

of quantum stirring devices, and we briefly relate to the experimental measurement issue.

III. TLS MODELING SCHEME

The unperturbed eigenstates $\psi^j(x)$ are labeled as $i=1,2$, corresponding to the two arms of the ring. The associated eigenenergies are $E_i=k_i^2/(2\mathbf{m})$. We have

$$\psi^{(1)}(x)=\begin{cases}\sqrt{\dfrac{2}{L_1}}\sin(k_1x+\varphi_1) & \text{if } x\in \text{first arm}\\ 0 & \text{if } x\in \text{second arm}\end{cases} \tag{4}$$

and a similar expression for $\psi^{(2)}(x)$, where L_i is the length of the ith arm and $|\varphi|<\pi/2$. Two representative eigenstates are illustrated in Fig. 2. Note that the wave number of the particle in the ith arm is $k_i=(\pi/L_i)\times$ integer. Our interest is in a very small energy range $E_1\sim E_2\sim E$, where the wave numbers are $k_1\sim k_2\sim k_E$, corresponding to the velocity $v_E=(2E/\mathbf{m})^{1/2}$. We would like to ignore all the other levels. Later we discuss the validity conditions for this TLS modeling scheme.

Once we lower from infinity one barrier, say barrier A, the two states become coupled. In Sec. IV we consider a delta barrier and obtain the following expression for the perturbation matrix:

$$W_{ij}^A=-\frac{v_E}{2\sqrt{L_iL_j}}\sqrt{g_A}, \tag{5}$$

where g_A is the transmission of the barrier. For $i\neq j$ the minus sign is a convention that fixes the gauge (see Appendix). In Sec. V we show that essentially the same result applies to any other type of barrier, but the $i=j$ expression for the energy shift should be somewhat generalized.

If both barriers are finite the two associated perturbation terms should be added together and one obtains for the energy difference

$$\varepsilon=(E_1+W_{11}^A+W_{11}^B)-(E_2+W_{22}^A+W_{22}^B), \tag{6}$$

and for the coupling

$$\frac{\kappa}{2}=W_{12}^A+W_{12}^B=-\frac{v_E}{2\sqrt{L_1L_2}}(\sqrt{g_A}\pm^c\sqrt{g_B}). \tag{7}$$

The latter expression involves a relative sign $\pm^c$ that cannot be gauged away (see Appendix). If we had magnetic flux penetrating through the ring we could have, instead of the $\pm^c$, an arbitrary phase factor.

Using the Pauli matrices we can write the TLS Hamiltonian as

$$\mathcal{H}_{ij}=\frac{\varepsilon}{2}\boldsymbol{\sigma}_z+\frac{\kappa}{2}\boldsymbol{\sigma}_x\equiv\frac{\boldsymbol{\Omega}}{2}\,\sigma. \tag{8}$$

Defining θ as the angle between Ω and the "z" axis, with the convention $0<\theta<\pi$, the eigenstates n_0 and m_0 of this Hamiltonian are

$$|n_0\rangle=\begin{pmatrix}\mp\sin(\theta/2)\\ \cos(\theta/2)\end{pmatrix},\quad |m_0\rangle=\begin{pmatrix}\cos(\theta/2)\\ \pm\sin(\theta/2)\end{pmatrix}, \tag{9}$$

where the $\pm$ indicates the sign of κ. The energy difference between these eigenstates is

$$\Omega=\sqrt{\varepsilon^2+\kappa^2}. \tag{10}$$

If we have a symmetric well then the effective coupling between odd and even levels vanishes ($\kappa=0$), and then we can get a degeneracy provided we tune appropriately the energy-level difference ε.

The TLS description is valid if W_{12} is much smaller compared with the level spacing, namely,

$$\max\{g_A,\ g_B\}\ll L_2/L_1, \tag{11}$$

where without loss of generality we assume $L_1>L_2$.

In Sec. IX we are going to derive expressions for the current $\mathcal{I}^A$ through barrier A, as defined by Eq. (2) with $x_0=x_A$. One observes that the matrix elements of this operator in the "standard basis" of Eq. (4) vanish because the unperturbed wave functions are zero at the barriers. The more careful treatment reveals that the reduced operator that gives the net current from the first arm to the second arm is

$$\mathcal{I}_{ij}=\frac{\kappa}{2}\boldsymbol{\sigma}_y, \tag{12}$$

and it turns out that $\mathcal{I}_{ij}^A=\lambda_A\mathcal{I}_{ij}$ and $\mathcal{I}_{ij}^B=\lambda_B\mathcal{I}_{ij}$, where the splitting ratio is defined as

$$\lambda_A = \frac{W_{12}^A}{W_{12}^A + W_{12}^B} = \frac{\sqrt{g_A}}{\sqrt{g_A} \pm^c \sqrt{g_B}}, \tag{13}$$

with a similar definition for λ_B. We have $\lambda_A + \lambda_B = 1$, but contrary to the naive point of view $0 < \lambda_A < 1$ is not implied. Rather, if the two states have opposite parities, then one λ is larger than 100%, while the other λ is negative. We shall see later in Sec. XIII that the physical interpretation of the "splitting ratio" requires recognition in the existence of induced circulating current in the system. Thus the multiple path topology of the system is reflected in the TLS modeling via λ.

IV. EXPRESSION FOR W_{ij} FOR A DELTA BARRIER

Let us assume that barrier B is infinitely high, while barrier A is modeled as a delta function. In other words, we consider the simplest possibility of having an infinite well $[(-L/2) < x < (L/2)]$ which is divided at $x = x_A$ by a delta function

$$V_A(x - x_A) = X_A \delta(x - x_A). \tag{14}$$

The total perturbation is obtained from a sequence of infinitesimal variations in the barrier height

$$\mathcal{H}(X_A) = \mathcal{H}(\infty) - \int_{X_A}^{\infty} \frac{\partial \mathcal{H}}{\partial X} dX \tag{15}$$

$$\equiv \mathcal{H}(\infty) + W^A. \tag{16}$$

For any value of X the Hilbert space of the system is spanned by a set of (real) eigenfunction labeled by n. The matrix elements for an infinitesimal variation in the barrier height is

$$\left(\frac{\partial \mathcal{H}}{\partial X} \right)_{nm} = \psi^{(n)}(x_A) \psi^{(m)}(x_A). \tag{17}$$

Using the matching conditions for a delta potential at $x = x_A$ we can express the wave function by its derivative

$$\psi^{(n)}(x_A) = \frac{1}{2\mathbf{m} X_A} [\partial \psi^{(n)}(x_A + 0) - \partial \psi^{(n)}(x_A - 0)]. \tag{18}$$

A more elegant way of writing this relation is

$$\psi^{(n)}(x_A) = \frac{1}{2\mathbf{m} X_A} \sum_{a=1,2} \partial_a \psi^{(n)}(x_A), \tag{19}$$

where ∂_a is defined as the *radial* derivative in the direction of the ath arms that stretch out of the junction at $x = x_A$. Defining the total radial derivative as $\partial = \partial_1 + \partial_2$ we get

$$\left(\frac{\partial \mathcal{H}}{\partial X} \right)_{nm} = \frac{1}{(2\mathbf{m} X_A)^2} \partial \psi^{(n)}(x_A) \, \partial \psi^{(m)}(x_A). \tag{20}$$

For a large barrier with small transmission

$$g_A \approx \left(\frac{v_E}{X_A} \right)^2 \ll 1, \tag{21}$$

the nth and mth states remain similar to some unperturbed ith and jth states. Accordingly, upon integration we get from Eq. (15) the result

$$W_{ij}^A = -\frac{1}{4\mathbf{m}^2 X_A} [\partial \psi^{(i)}(x_A)][\partial \psi^{(j)}(x_A)]. \tag{22}$$

Note that in the last equation the contribution to the total derivative ∂ comes from one term only because each unperturbed wave function $\psi^{(i)}(x)$ is nonzero only in one box. Using Eq. (21) we get Eq. (5).

V. EXPRESSION FOR W_{ij} FOR A GENERAL BARRIER

It is possible to deduce an expression for W_{ij} without assuming a specific form of potential barrier. For the purpose of this calculation we describe the barrier at $x = x_A$ by a general scattering matrix

$$S = e^{i\gamma} \begin{pmatrix} i\sqrt{1-g}\, e^{i\alpha} & -\sqrt{g} \\ -\sqrt{g} & i\sqrt{1-g}\, e^{-i\alpha} \end{pmatrix}. \tag{23}$$

Regarding the barrier as a *junction* it can be embedded either in a *closed* ring geometry with the two *arms* attached or in an *open* one-dimensional geometry with two infinite *leads* attached. In both cases the differential representation of W should be the *same* because W is local in space. In other words W_{ij}^A should come out the same for the wave functions $\psi^{(i)}(x)$ and $\psi^{(j)}(x)$ of the ring, if in the vicinity of $x = x_A$ they are identical with $\Psi^{(i)}(x)$ and $\Psi^{(j)}(x)$ of the scattering geometry.

In the scattering geometry it is conventional to label the two leads by $a = 1, 2$ and to define a radial coordinate $r = |x - x_A|$. The flux normalized scattering states of the junction (assuming outgoing waves) are $\Psi^{(i+)}$. By definition we have

$$\Psi^{(1+)} = \begin{cases} \frac{1}{\sqrt{v_E}} [e^{-ik_E r} - S_{11} e^{ik_E r}] & \text{if } r \in \text{first lead} \\ \frac{1}{\sqrt{v_E}} [-S_{21} e^{ik_E r}] & \text{if } r \in \text{second lead}. \end{cases} \tag{24}$$

A similar expression holds for $\Psi^{(2+)}$. If the leads are not coupled, the scattering matrix becomes S_0 with $g = 0$. In the vicinity of $x = x_A$ the unperturbed scattering states coincide with those of Eq. (4) up to normalization. Namely, in the vicinity of $x = x_A$ we have the relation

$$\Psi^{(i)}(x) = -i \left(\frac{2L_i}{v_E} \right)^{1/2} e^{i\varphi_i} \psi^{(i)}(x), \tag{25}$$

where

$$\varphi_i = \frac{1}{2} \left(\gamma_0 + \frac{\pi}{2} \pm \alpha_0 \right), \tag{26}$$

with $\pm$ sign for $i = 1, 2$, respectively.

The relation between the scattering matrix and the perturbation matrix W can be deduced via the T matrix formalism. The S matrix is related to the T matrix through $S = (1 - iT) S_0$, or more explicitly

$$[S S_0^{-1}]_{ij} = \delta_{ij} - i \langle \Psi^{(i)} | T | \Psi^{(j)} \rangle. \tag{27}$$

In leading order T equals W so we have

$$\langle \Psi^{(i)}|W|\Psi^{(j)}\rangle \approx i(S-S_0)S_0^{-1}, \tag{28}$$

where

$$S-S_0 = e^{i\gamma_0}\begin{pmatrix} e^{i\alpha_0}(\delta\gamma+\delta\alpha) & \sqrt{g} \\ \sqrt{g} & e^{-i\alpha_0}(\delta\gamma-\delta\alpha) \end{pmatrix}. \tag{29}$$

Thus

$$\langle \Psi^{(i)}|W|\Psi^{(j)}\rangle = -\begin{pmatrix} \delta\gamma+\delta\alpha & \sqrt{g}e^{i\alpha_0} \\ \sqrt{g}e^{-i\alpha_0} & \delta\gamma-\delta\alpha \end{pmatrix}. \tag{30}$$

Using Eq. (25) we deduce that each element of $\langle \psi^{(i)}|W|\psi^{(j)}\rangle$ involves multiplication by $v_E/(4L_iL_j)^{1/2}$, while the α_0 is canceled out. This leads to Eq. (5) for the $i\neq j$ coupling and a generalized expression for the energy-level shifts.

VI. WIGNER DECAY AND BLOCH OSCILLATIONS

If the two arms of the ring have exactly the same length $L_1=L_2=L/2$, then the coherent Bloch oscillations of a wave packet in such a symmetric double well are characterized by the frequency

$$\Omega_{\text{Bloch}} = 2|W_{12}| = \frac{v_E}{L_1}|\sqrt{g_A}+\sqrt{g_B}|. \tag{31}$$

If one arm of the ring (L_1) is very long and the other arm (L_2) is short, then a particle placed initially at the short arm will decay into the quasicontinuum of the long arm. The decay rate is given by the Fermi golden rule

$$\Gamma = \frac{2\pi}{\Delta}|W_{12}|^2, \tag{32}$$

where $\Delta=(\pi/L)v_E$ is the mean level spacing. If the arms are coupled through barrier A while barrier B is infinitely high, then the decay rate is

$$\Gamma = \frac{v_E}{2L_2}g_A. \tag{33}$$

This result agrees with the well-known Gamow formula: the decay rate is given by the attempt frequency multiplied by the probability to cross the barrier.

If both barriers are finite, it is important to notice that the quasicontinuum of the long arm is composed of odd and even states. The state of the short arm, which is either even or odd, is coupled to states of the same parity with a plus sign in the expression of Eq. (7) and to states of the opposite parity with a minus sign. Accordingly, the decay rate is the sum of the decay rate to states of the same parity and the decay rate to states of the opposite parity

$$\Gamma = \sum_{\pm}\frac{2\pi}{\Delta_{\pm}}\left|\frac{v_E}{2\sqrt{L_1L_2}}(\sqrt{g_A}\pm^c\sqrt{g_B})\right|^2 = \frac{v_E}{2L_2}(g_A+g_B), \tag{34}$$

where $\Delta_{\pm}=2\Delta$ is the mean level spacing for states with the same parity. So in spite of the parity considerations we still get the naive result that agrees with Gamow formula.

VII. QUANTUM STIRRING

We assume that we have control over geometrical parameters of the device, such as the potential floor in each arm, the barriers heights, their location, or any other gate controlled feature of the potential landscape. With a control parameter X we associate a generalized force operator

$$\mathcal{F} = -\frac{\partial \mathcal{H}}{\partial X}. \tag{35}$$

Quantum stirring means to induce a circulating current by changing the parameter X. We assume that the parametric variation is adiabatic, so we have a linear relation $\langle I\rangle=-G\dot{X}$, where G is known as the geometric conductance.[8] The Kubo formalism implies that G equals to the Berry curvature[9–11]

$$G = \sum_{m(\neq n)}\frac{2\,\text{Im}[\mathcal{I}_{nm}]\mathcal{F}_{mn}}{(E_m-E_n)^2}, \tag{36}$$

where n is the level in which the particle is prepared and m are the other levels.

Within the framework of the TLS modeling the sum in Eq. (36) contains only one term which involves the states n_0 and m_0 of Eq. (9). For the matrix element of the current operator we get

$$\mathcal{I}_{n_0m_0} = \left[\lambda\frac{\kappa}{2}\boldsymbol{\sigma}_y\right]_{n_0m_0} = i\lambda\frac{\kappa}{2}, \tag{37}$$

where λ is the appropriate splitting ratio. The matrix element of the generalized force operator is calculated using Eqs. (9) and (35),

$$\mathcal{F}_{m_0n_0} = -\frac{1}{2}\left[\frac{\partial\varepsilon}{\partial X}\boldsymbol{\sigma}_z+\frac{\partial\kappa}{\partial X}\boldsymbol{\sigma}_x\right]_{m_0n_0}, \tag{38}$$

$$= \pm\frac{1}{2}\sin(\theta)\frac{\partial\varepsilon}{\partial X}-\frac{1}{2}\cos(\theta)\frac{\partial\kappa}{\partial X}, \tag{39}$$

$$= \frac{1}{2\Omega}\left(\kappa\frac{\partial\varepsilon}{\partial X}-\varepsilon\frac{\partial\kappa}{\partial X}\right), \tag{40}$$

where we used $\pm\sin(\theta)=\kappa/\Omega$ and $\cos(\theta)=\varepsilon/\Omega$. This leads to the following result for the geometric conductance:

$$G = \frac{\lambda\kappa}{2\Omega^3}\left[\kappa\frac{\partial\varepsilon}{\partial X}-\varepsilon\frac{\partial\kappa}{\partial X}\right]. \tag{41}$$

In the analysis of the operation of a stirring device we typically have a well defined region where the potential is being varied. We may call this segment "the pump." It is convenient to measure the current elsewhere, where the potential is fixed. If barrier A is not part of the "pump" then we can measure the current at $x_0=x_A$. Then it follows from the definitions of λ and κ that the product $\lambda\kappa$ does not change with time, even if barrier B is modulated. Then we can rewrite the above formula as

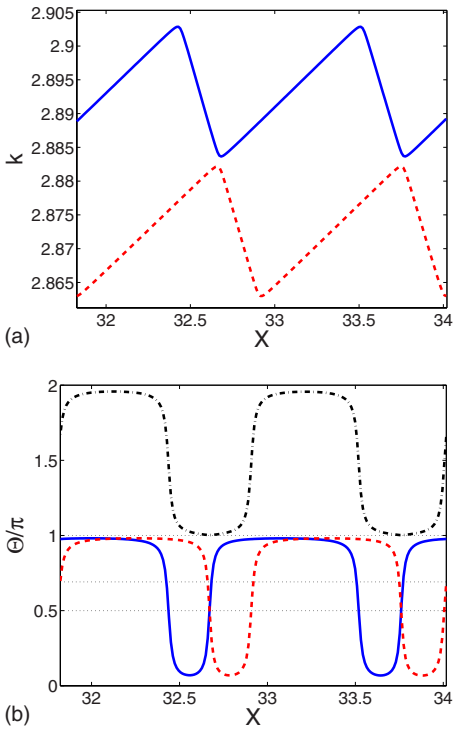

FIG. 3. (Color online) We consider a particle of mass $\mathbf{m}=1$ in a ring of length $L=151.43$. The position of barrier B is X, so we have $L_1=X$ and $L_2=L-X$. We calculate numerically k_n and $\Theta^{(n)}$ for two neighboring levels (solid and dashed lines). The sum $\Theta^{(m)}+\Theta^{(n)}$ is plotted as a dash-dotted line. We have high barriers with $g_A \sim 10^{-2}$ and $g_B \sim 10^{-5}$. Accordingly we expect TLS modeling to be valid. The dotted lines indicate the values $\Theta=\pi/2$ (expected crossing point) and $\Theta=\pi$ (expected sum). For the sake of comparison there is a third dotted line that indicates the value of Θ that corresponds to equal amplitudes $C_1=C_2$.

$$G=\frac{\lambda_0\kappa_0}{2\Omega^3}\left[\kappa\frac{\partial\varepsilon}{\partial X}-\varepsilon\frac{\partial\kappa}{\partial X}\right], \tag{42}$$

where λ_0 and κ_0 are that values at some arbitrary moment of time. Typically the variation in X leads to a sequence of level crossings if κ is disregarded. These become avoided crossings if κ is taken into account. At the vicinity of a crossing we typically can use a linear approximation

$$\varepsilon=\dot{\varepsilon}\times(X-X_0), \tag{43}$$

$$\kappa=\kappa_0+\dot{\kappa}\times(X-X_0). \tag{44}$$

The amount of probability $dQ=Idt$ which is being transported equals $-GdX$. For an individual crossing the dX integration over G can be performed using

$$\int_{-\infty}^{+\infty}\frac{a(b+cx)\ dx}{(a^2x^2+(b+cx)^2)^{3/2}}=\frac{2a}{b\sqrt{a^2+c^2}}, \tag{45}$$

$$\int_{-\infty}^{+\infty}\frac{c\ ax\ dx}{(a^2x^2+(b+cx)^2)^{3/2}}=-\frac{2c^2}{ab\sqrt{a^2+c^2}}. \tag{46}$$

Then we get the result

$$Q=\pm\lambda_0\sqrt{1+(\dot{\kappa}/\dot{\varepsilon})^2}, \tag{47}$$

where the $\pm$ is determined according to the sign of $\dot{\varepsilon}$. We observed that in order to get the "quantized" value $Q=1$ there should be neither topological splitting ($\lambda=1$) nor barrier modulation ($\dot{\kappa}=0$) during the transition.

VIII. NEIGHBORING LEVEL APPROXIMATION SCHEME

A major interest is in systems with zero-temperature Fermi occupation. In such a case Eq. (36) has to be summed over n up to the Fermi energy. It turns out[1] that the result is dominated by the contribution that comes from the coupling between the last occupied level and its neighboring empty level. This suggests adopting a neighboring level approximation scheme that holds irrespective of the validity of the TLS modeling and coincides with it if the condition of Eq. (11) is satisfied. The key idea is to characterize each eigenstate by a mixing parameter

$$\Theta\equiv 2\arctan\left(\sqrt{\frac{\mathrm{Prob}(x\in 2)}{\mathrm{Prob}(x\in 1)}}\right), \tag{48}$$

such that $\Theta=0$ for states that belong to the first arm and $\Theta=\pi$ for states that belong to the second arm. Numerical examples are presented in Figs. 3 and 4. If we are given Θ then we can construct the eigenstate using a procedure that we describe below. If the TLS modeling applies then Θ becomes essentially the same as θ.

Let us see how we construct the wave function given the energy $E=E_n$, the mixing parameter $\Theta=\Theta_n$, and the parity $\pm^a$ with respect to (say) barrier A, as defined in the Appendix. Consequently it is convenient to set the origin such that $x_A=0$ and write the nth eigenstate of the ring as

$$\psi^{(n)}(x)=\begin{cases}\pm^a C_1\sin(k_1x+\varphi_1) & \text{if } x\in\text{first arm}\\ C_2\sin(k_2x+\varphi_2) & \text{if } x\in\text{second arm},\end{cases} \tag{49}$$

where $C_i>0$ and $|\varphi|<\pi/2$. Assuming $k_EL\gg 1$, the amplitudes satisfy the normalization condition

$$\frac{1}{2}L_1C_1^2+\frac{1}{2}L_2C_2^2\approx 1. \tag{50}$$

It follows that

$$C_1\approx\sqrt{\frac{2}{L_1}}\cos\left(\frac{\Theta}{2}\right), \tag{51}$$

$$C_2\approx\sqrt{\frac{2}{L_2}}\sin\left(\frac{\Theta}{2}\right). \tag{52}$$

We still have to say what are the wave numbers k_1 and k_2 and the phase shifts φ. Let us see first how they are determined within the framework of the TLS modeling and then how they can be found irrespective of the TLS modeling.

Naively the $|n_0\rangle$ and $|m_0\rangle$ eigenstates, within the framework of the TLS modeling, are the superposition of the basis states of Eq. (4) and accordingly

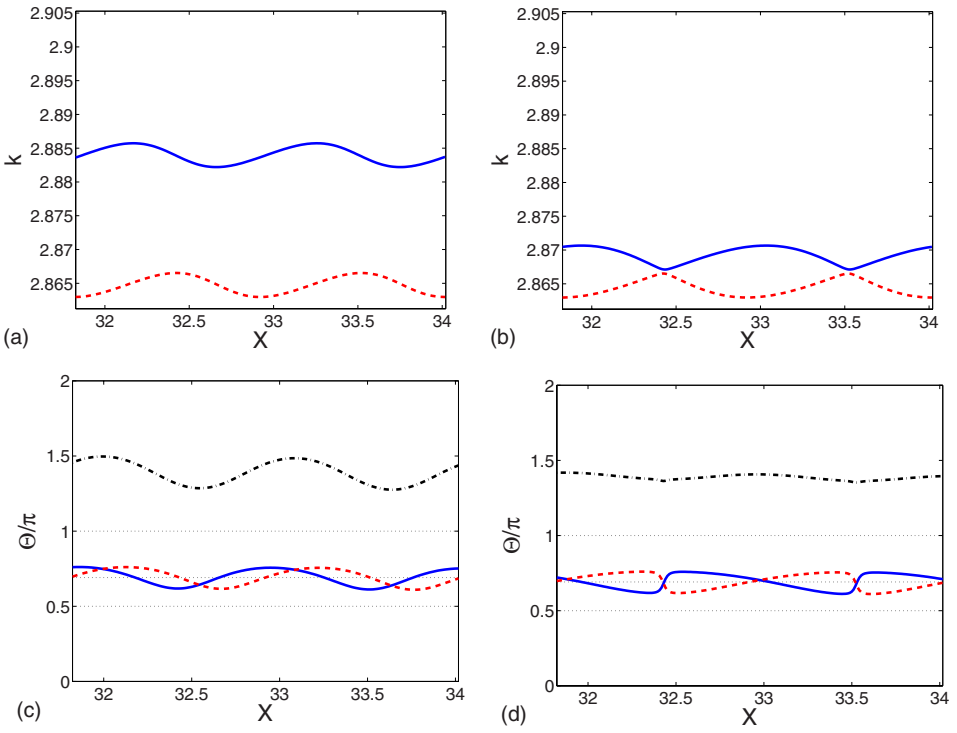

FIG. 4. (Color online) The same as the previous figure, but here the TLS modeling does not apply. In the (a) and (c) one barrier is high ($g_A \sim 10^{-2}$) and one barrier is low ($g_B \sim 0.9$), while in (b) and (d) both barriers are low ($g_A \sim g_B \sim 0.9$).

$$\Theta = \theta, \quad \pi - \theta, \tag{53}$$

$$k_1 = \text{corresponds to the unperturbed } E_1, \tag{54}$$

$$k_2 = \text{corresponds to the unperturbed } E_2, \tag{55}$$

$$\varphi_1 = \text{same as the unperturbed}, \tag{56}$$

$$\varphi_2 = \text{same as the unperturbed}, \tag{57}$$

while the true eigenstates are with (see Fig. 2)

$$\Theta \approx \theta, \quad \pi - \theta, \tag{58}$$

$$k_1 = \text{corresponds to } E_n, \tag{59}$$

$$k_2 = \text{corresponds to } E_n, \tag{60}$$

$$\varphi_1 = \text{shifted}, \tag{61}$$

$$\varphi_2 = \text{shifted}. \tag{62}$$

To be more specific, we have $\Theta^{(m_0)} \approx \theta$ and $\Theta^{(n_0)} \approx \pi - \theta$ and hence $\Theta^{(m_0)} + \Theta^{(n_0)} \approx \pi$ if the TLS modeling is valid (see Fig. 4). We note that from Eqs. (51) and (52) it follows that within the framework of the TLS approximation we have

$$C_i^{(m_0)} C_i^{(n_0)} \approx \frac{1}{L_i} \sin(\theta). \tag{63}$$

This will be used later on in order to obtain simplified expressions for the matrix elements of various operators.

Whether k_1 and k_2 in Eqs. (54) and (55) correspond to the same energy or not is not a big difference for us because we assume $k_1 \sim k_2 \sim k_E$ in any case. The main problem with the naive version is related to the phase shifts, as demonstrated in Fig. 2. The variation in the phase shift as the barriers are lowered reflects that there is a nonzero probability to find the particle in the region of the barriers. In particular if the phases φ_i remained the same it would imply that all the matrix elements of I^A and I^B would be zero. It is essential to take the variation in φ into account in order to get a nonzero result for the geometrical conductance. We shall discuss the calculation of the matrix elements $\mathcal{I}_{nm}$ and $\mathcal{F}_{nm}$ in the next sections. First we would like to discuss how the required information on the variation in the phases φ can be extracted.

In order to express φ by Θ, we write the wave function of Eq. (49) as ingoing and outgoing waves and set the origin $x=0$ at either one of the barriers, for example, barrier A. We match the wave functions of the two bonds by the barrier scattering matrix

$$\begin{pmatrix} \pm^a C_1 e^{+i\varphi_1} \\ C_2 e^{+i\varphi_2} \end{pmatrix} = \boldsymbol{S}_A \begin{pmatrix} \pm^a C_1 e^{-i\varphi_1} \\ C_2 e^{-i\varphi_2} \end{pmatrix} \tag{64}$$

and get closed equations for the phase shifts

$$\sqrt{1-g}\sin(2\varphi_1 - \alpha - \gamma) = 1 - \frac{g}{2}\left[1 + \left(\frac{C_2}{C_1}\right)^2\right], \tag{65}$$

$$\sqrt{1-g}\sin(2\varphi_2 + \alpha - \gamma) = 1 - \frac{g}{2}\left[1 + \left(\frac{C_1}{C_2}\right)^2\right]. \tag{66}$$

So far everything is exact. So once we have Θ we can find the phases and construct the wave function. We would like to focus in the rest of this section in the regime where the TLS modeling applies. Assuming that Θ is determined by θ we want to find what are φ_1 and φ_2, so as to construct a proper wave function. Neglecting terms of order g and expanding $\arcsin(1-x)$ as $\pi/2 \pm \sqrt{2x}$ we obtain

$$\varphi_1 \approx \frac{\gamma+\alpha}{2} + \frac{\pi}{4} \pm^a \frac{\sqrt{g}}{2} \sqrt{\frac{L_1}{L_2}} \tan\left(\frac{\Theta}{2}\right), \tag{67}$$

where the $\pm^a$ sign should be the same as in Eq. (64), which can be established by direct substitution. A similar expression can be obtained for φ_2. We note that within the framework of this TLS approximation we have

$$\varphi_1^{(m_0)} - \varphi_1^{(n_0)} = \pm \sqrt{g_A} \left(\frac{L_1}{L_2}\right)^{1/2} \frac{1}{\sin(\theta)}, \tag{68}$$

where the sign is the same as that of κ. We now have all the building blocks needed for the calculation of the matrix elements.

IX. EXPRESSION FOR $\mathcal{I}_{nm}$

If we adopt the TLS point of view, we can postulate a self-consistent definition of the current operator based on the continuity equation. For this purpose we define the occupation operator $\mathcal{N}$ for one of the arms as

$$\mathcal{N} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{69}$$

and deduce the definition of the current operator from

$$\frac{d}{dt}\mathcal{N} = i[\mathcal{H}, \mathcal{N}] \equiv \mathcal{I}, \tag{70}$$

where $\mathcal{I}$ is given by Eq. (12). If we turn off the coupling at barrier A we get the same expression multiplied by λ_B, while if we turn off the coupling at barrier B we get the same expression multiplied by λ_A.

The above reasoning bypasses the confrontation which is involved in carrying out a direct calculation, and hence contains an uncontrolled error which is associated with the assumption that a TLS description of Hilbert space is valid. If we revert to the original definition of Eq. (2), then the matrix elements are given by

$$\mathcal{I}_{nm} = i\frac{1}{2\mathbf{m}}(\partial\psi^{(n)}\psi^{(m)} - \psi^{(n)}\,\partial\,\psi^{(m)})\big|_{x=x_0}. \tag{71}$$

For the calculation of $\mathcal{I}^A_{nm}$ we set $x_0 = x_A = 0$. As was already pointed out, in order to get a nontrivial result, we have to take into account the phase shifts φ which were calculated in in Sec. VIII. Substituting the wave function of Eq. (49) we get

$$\mathcal{I}^A_{nm} = -i\frac{1}{2\mathbf{m}} C_1^{(m)} C_1^{(n)} \left[\frac{k_m + k_n}{2} \sin(\varphi_1^{(m)} - \varphi_1^{(n)}) + \frac{k_n - k_m}{2} \sin(\varphi_1^{(m)} + \varphi_1^{(n)}) \right]. \tag{72}$$

Whenever the TLS modeling applies we can substitute Eqs. (63) and (68) into Eq. (72). Neglecting the second term we get

$$\mathcal{I}^A_{n_0 m_0} \approx \mp i \frac{v_E}{2\sqrt{L_1 L_2}} \sqrt{g_A}, \tag{73}$$

where the sign is the same as that of $-\kappa$. One notices that the expression for $\mathcal{I}^A_{n_0 m_0}$ can be written as Eq. (37) where κ and λ are given by Eqs. (7) and (13).

X. STIRRING BY BARRIER MODULATION

In this section we calculate the geometric conductance as determined by the matrix elements of the generalized force that is associated with modulation of a delta barrier. The motivation is to verify the results of the reduced description against the direct full Hilbert-space calculation. The potential barrier is given by

$$V_B(\hat{x}) = X_B \delta(\hat{x} - x_B). \tag{74}$$

The stirring is induced by variation in the barrier height X_B. The associated generalized force is

$$\mathcal{F} = -\frac{\partial \mathcal{H}}{\partial X_B} = -\delta(\hat{x} - x_B), \tag{75}$$

with the matrix elements

$$\mathcal{F}_{mn} = -\psi^{(n)}\psi^{(m)}. \tag{76}$$

For the wave-function amplitudes we use Eq. (63) and for the phase shifts Eq. (67). We also substitute the scattering matrix parameters that describe a delta barrier

$$\gamma_B \approx -\pi/2 + \sqrt{g_B}, \tag{77}$$

$$\alpha_B = 0, \tag{78}$$

where the approximation is valid for $g_B \ll 1$ and the relation of g_B and X_B is given in Eq. (21). With the above approximations we get

$$\mathcal{F}_{m_0 n_0} \approx g_B \frac{L_2 - L_1}{4L_1 L_2} \sin(\theta) \mp \frac{g_B}{2\sqrt{L_1 L_2}} \cos(\theta), \tag{79}$$

where the sign should be the same as that of $\mp^c\kappa$. In order to verify the consistency with the TLS expression, we differentiate Eqs. (6) and (7),

$$\frac{\partial \varepsilon}{\partial X_B} = g_B \frac{L_2 - L_1}{2L_1 L_2}, \tag{80}$$

$$\frac{\partial \kappa}{\partial X_B} = \pm^c \frac{g_B}{\sqrt{L_1 L_2}}, \tag{81}$$

and substitute into Eq. (38). Indeed we obtain the same result for $\mathcal{F}_{m_0 n_0}$ as above.

The geometric conductance of Eq. (36) involves the multiplication of $\mathcal{F}_{m_0 n_0}$ with $\mathcal{I}_{n_0 m_0}$ leading to

$$G = \frac{1}{4} v_E^2 \frac{L_2 - L_1}{(L_1 L_2)^2} \frac{g_A g_B \pm^c g_A^{1/2} g_B^{3/2}}{\Omega^3} \mp^c \frac{1}{4} v_E^2 \frac{L_2 + L_1}{(L_1 L_2)^2} \frac{g_A g_B + g_A^{1/2} g_B^{3/2}}{\Omega^3}. \tag{82}$$

The calculation of the transport proceeds as in Sec. VII.

XI. STIRRING BY BARRIER TRANSLATION

In complete analogy with Sec. X we would like to calculate the geometric conductance as determined by the matrix elements of the generalized force which is associated with the translation of the barrier

$$\mathcal{F} = -\frac{\partial \mathcal{H}}{\partial x_B} = X_B \delta'(\hat{x} - x_B). \tag{83}$$

One obtains

$$\mathcal{F}_{mn} = -X_B (\overline{\partial \psi^{(n)}} \psi^{(m)} + \overline{\partial \psi^{(m)}} \psi^{(n)}), \tag{84}$$

where $\overline{\partial \psi}$ is the average derivative on both sides of the barrier. We simplify this expression by using Eq. (19),

$$\mathcal{F}_{mn} = \frac{1}{2\mathbf{m}} [\partial \psi_1^{(n)} \, \partial \, \psi_1^{(m)} - \partial \psi_2^{(n)} \, \partial \, \psi_2^{(m)}]_{x=x_B}. \tag{85}$$

Assuming high barriers we get in leading order

$$\mathcal{F}_{mn} \approx -\frac{1}{2} \mathbf{m} v_E^2 (C_1^{(m)} C_1^{(n)} + C_2^{(m)} C_2^{(n)}), \tag{86}$$

which together with Eq. (63) leads to

$$\mathcal{F}_{m_0 n_0} \approx -\frac{1}{2} \mathbf{m} v_E^2 \frac{L_1 + L_2}{L_1 L_2} \sin(\theta). \tag{87}$$

In order to compare the above result for $\mathcal{F}_{m_0 n_0}$ with the TLS result of Eq. (38) we calculate the variation in the potential floor by taking in Eq. (6) the energies of infinite wells with $L_1 = x_B$ and $L_2 = L - x_B$. We get

$$\frac{\partial \varepsilon}{\partial x_B} = -\mathbf{m} v_E^2 \frac{L_1 + L_2}{L_1 L_2} + \mathcal{O}(\sqrt{g}), \tag{88}$$

$$\frac{\partial \kappa}{\partial x_B} = v_E \frac{L_2 - L_1}{(L_1 L_2)^{3/2}} (\sqrt{g_A} \pm^c \sqrt{g_B}). \tag{89}$$

Substitute into Eq. (38) indeed leads to the same result for $\mathcal{F}_{m_0 n_0}$ as above. Note that in this case (unlike Sec. X) the second term in Eq. (38) which involves the variation in κ is of higher order in g_B and therefore should be excluded.

The geometric conductance of Eq. (36) involves the multiplication of $\mathcal{F}_{m_0 n_0}$ with $\mathcal{I}_{n_0 m_0}$ leading to

$$G = -\frac{1}{2} \sqrt{g_A} \mathbf{m} v_E^4 \frac{L_1 + L_2}{(L_1 L_2)^2} \frac{\sqrt{g_A} \pm^c \sqrt{g_B}}{\Omega^3}. \tag{90}$$

The calculation of the transport proceeds as in Sec. VII. One realizes that a translation of the barrier is effectively equivalent to the variation in the potential floor difference as long as it does not involve modulation of its transmission (which is assumed to be small).

XII. ERROR ESTIMATES AND LIMITATIONS

If we vary a parameter X then the energy levels $E_n(X)$ form a "spaghetti" which is characterized by a mean level spacing Δ and possibly by narrow avoided crossings with splitting Δ_0. For the ring system that we are considering it follows from the estimate of κ that

$$\frac{\Delta_0}{\Delta} \sim \min\{1, \sqrt{bg}\}, \tag{91}$$

where $b = L_1/L_2$ and $g = \max\{g_A, g_B\}$. The condition Eq. (11) for the applicability of the TLS modeling ensures that $\Delta_0 \ll \Delta$. In such circumstances Eq. (36) for the geometric conductance, which in essence is a sum of the type $\Sigma_{n=0}^{\infty} (\Delta_0 + n\Delta)^{-2}$, implies that the error that is involved in the neighboring level approximation is

$$\frac{\text{error}(G)}{G} \sim \left(\frac{\Delta_0}{\Delta} \right)^2 \sim bg \ll 1. \tag{92}$$

Once the TLS modeling fails the error becomes of order unity. This sounds bad, but in fact it is not so bad. The good news is that the far levels contribute to G a correction which is of the same order as the leading term. Therefore with the neighboring level approximation we can still get a realistic estimate disregarding numerical prefactors of order unity.

Having $b \gg 1$ is very interesting because then we have a nontrivial intermediate regime $1/b \ll g \ll 1$ where neither first order perturbation theory with respect to "zero" height barriers nor first order perturbation theory with respect to "infinite" barriers applies. This is the regime where each level of the small arm forms a distinct Wigner resonance with the quasicontinuum states of the long arm. Obviously the TLS modeling is not applicable in this regime, but the neighboring level approximation still provides a decent starting point for a calculation. We shall explore this Wigner regime in a future work.

One may also wonder whether the specific results that we have obtained for stirring using a *delta* barrier apply also for a *thick* barrier. On physical grounds it is quite obvious that the induced current is determined by the scattering matrix of the modulated barrier. Consequently if the $S(E)$ of the modulated barrier is E independent within the energy range of interest, it can be regarded as representing a delta function, and the results should come out the same.

Finally one may wonder about the implications of finite temperature or nonadiabatic driving. These aspects are complementary to the theme of the present paper. Namely, as discussed in Ref. 1, at finite temperatures the statistics of the occupation should be taken into account. So we have to average (so to say) over the level that we have labeled as n_0 with an appropriate weight as implied by the Fermi function. On the other hand the nonadiabatic effects require to introduce in the denominator of the Kubo formula Eq. (36) a term that represents the "width" of the Fermi-golden-rule transi-

tions. Then the weight of the neighboring level in the sum becomes smaller compared with the total weight of the far levels.

XIII. SUMMARY

We have developed a practical procedure for the analysis of a one-dimensional double well system which is both powerful and illuminating. The procedure assumes that we have a way to find the eigenenergies E_n of the device and the mixing ratio Θ_n of each of them. Given the transmissions of the barriers we further characterize the device by the splitting ratio λ. With these ingredients in hand we can analyze any stirring process and obtain explicit expressions for the geometric conductance G. The calculation simplifies if the TLS modeling applies because then the mixing ratio can be determined form the diagonalization of a 2×2 matrix.

In particular we obtain explicit expressions for G due to either barrier translation (generalizing a result that was obtained in Ref. 1) or barrier modulation (generalizing a result that was obtained in Ref. 7) and verify that they agree with the naive self-consistent TLS calculation. We see that whenever the TLS modeling applies the proper calculation in the full Hilbert space gives the same result as the naive calculation in the TLS Hilbert space.

As a by product of the TLS analysis we find that the pumped "charge" during an avoided crossing is not quantized [see Eq. (47)] not only because of the topological splitting effect but also due to a dynamical effect that arises if the barrier is modulated.

The practical importance of the TLS modeling in condense matter physics is obvious. On the other hand the specific application to the study of quantum stirring deserves a few words regarding the measurement procedure and the experimental relevance. As explained in Ref. 1 it should be clear that the measurement of current in a closed circuit requires special techniques.[12–14] These techniques are typically used in order to probe persistent currents, which are zero-order (conservative) effects, while in the present paper we were discussing driven currents, which are a first-order (geometric) effects. It is of course also possible to measure the dissipative conductance (as in Ref. 12). During the measurement the coupling to the system should be small. These are so-called *weak measurement* conditions. More ambitious would be to measure the counting statistics, i.e., also the second moment of Q as discussed in Refs. 15 and 16 which is completely analogous to the discussion of noise measurements in open systems.[17,18] Finally it should be pointed out that the formalism above, and hence the results, might apply to experiments with superconducting circuits (see Ref. 19).

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APPENDIX: CONVENTIONS AND NOTATIONS

Consider two segments that are connected at points that are labeled as x_A and x_B. In the absence of coupling each segment is regarded as a one-dimensional box. The unperturbed eigenstates are labeled by i (or optionally by j). In the TLS scheme $i=1,2$. If the coupling is nonzero the exact eigenstates are labeled by n (or optionally by m). Within the framework of the neighboring level approximation scheme we focus on two levels that we label as $n=n_0$ and $m=m_0$. If the TLS modeling applies then the states n_0 and m_0 are regarded as linear combinations of $i=1,2$.

The unperturbed states $i=1,2$ are characterized by their parities $\pm^1$ and $\pm^2$, respectively. The relative sign $\pm^c$ in Eq. (7) equals the product of $\pm^1$ and $\pm^2$. Inverting the arbitrary gauge sign of either $\psi^{(1)}(x)$ or $\psi^{(2)}(x)$ would multiply the expression in Eq. (5) by a global minus sign, while the relative sign $\pm^c$ remains unchanged. The gauge-invariant relative sign is due to the fact that the unperturbed states are either odd or even: we have plus sign if both states have the same parity and minus sign if they have opposite parity.

Each exact eigenfunction n, as written in Eq. (49), is characterized by what we call the parity $\pm^a$ with respect to barrier A. Positive parity means that the radial derivatives as defined in Eq. (19) have both the same sign. Optionally we can define $\pm^b$ as the parity with respect to barrier B. This parity $\pm^a$ is not a symmetry related quantum number, but it is merely required in order to define the wave function of Eq. (49) in a unique way given the energy and the mixing ratio. If the TLS modeling applies then for positive (negative) κ the state n_0 of Eq. (9) has negative (positive) parity, while the m_0 state has positive (negative) parity. Within this framework the parity $\pm^b$ with respect to barrier B is $\pm^a$ multiplied by $\pm^c$.

We have verified that the various $\pm$ signs through the paper are consistent, which is not always evident in a superficial look.

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