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S-matrix formalism of transmission through two quantum billiards coupled by a waveguide

Almas F Sadreev[1,2], **Evgeny N Bulgakov**[1] **and Ingrid Rotter**[3]

[1] Kirensky Institute of Physics, 660036, Krasnoyarsk, Russia

[2] Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden

[3] Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

E-mail: almsa@ifm.liu.se, almas@tnp.krasn.ru, ben@tnp.krasn.ru and rotter@mpipks-dresden.mpg.de

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Abstract

We consider a system that consists of two single-quantum billiards (QBs) coupled by a waveguide and study the transmission through this system as a function of length and width of the waveguide. To interpret the numerical results for the transmission, we explore a simple model with a small number of states which allows us to consider the problem analytically. The transmission is described in the S-matrix formalism by using the non-Hermitian effective Hamilton operator for the open system. The coupling of the single QBs to the internal waveguide characterizes the 'internal' coupling strength u of the states of the system while that of the system as a whole to the attached leads determines the 'external' coupling strength v of the resonance states via the continuum (waves in the leads). The transmission is resonant for all values of v/u in relation to the effective Hamiltonian. It depends strongly on the ratio v/u via the eigenvalues and eigenfunctions of the effective Hamiltonian. The results obtained are compared qualitatively with those from simulation calculations for larger systems. Most interesting is the existence of resonance states with vanishing widths that may appear at all values of v/u. They cause zeros in the transmission through the double QB due to trapping of the particle in the waveguide.

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1. Introduction

Recently, much interest has been devoted to the study of the transmission properties of coupled quantum dots [1–7]. A single quantum dot can be considered as an artificial atom if the energy levels can be resolved. Two or more quantum dots can be coupled to form an artificial molecule in which the electrons are shared by different sites. While in natural molecules the ground-state interatomic distance is dictated by the nature of the bonding [8], such a restriction does not exist in artificial molecules. This fact provides a large diversity for the construction of quantum dot systems.

The split gate in the middle of a double dot allows us, e.g., to control the width W of the wire that connects the two single dots. This gives the possibility of studying the transmission through the double dot as a function of the wire size and energy. Considering the wire as a stripe with the width W and the length L, we present the wire as a third quantum subsystem with the energies $\varepsilon_w \sim (m/W)^2 + (n/L)^2$, where m, n are the quantum numbers of the wire. These modes appear additionally to the eigenenergies $\varepsilon_i \propto R^{-2}$ of the single quantum dots where R is the characteristic scale of the single dot. If $L, W \ll R$ and $\varepsilon_w \gg \varepsilon_i$, the role of the wire as a third quantum subsystem is not relevant because the coupling between the dots is of tunnelling type. However, for the case $\varepsilon_w \sim \varepsilon_i$, the wire's degrees of freedom are important. In this case, the quantum system consists, indeed, of two quantum subsystems coupled by a third quantum subsystem that has an energy spectrum of its own.

The electron transmission through double quantum dots might be obscured by the Coulomb interaction, mainly by the effect of the Coulomb blockade. There is, however, an exact correspondence between the quantum mechanical description of the single electron transmission through a quantum dot and the transmission of planar electromagnetic waves through a microwave (or quantum) billiard (QB) [9]. The energy of the incident electron corresponds to the squared frequency of the microwave. Moreover, it is easy to vary the length of the internal waveguide that connects the two single QBs to a double QB and to control the transmission through the coupled system as a function of this parameter. Much more can be learned therefore from a study of the transmission through the coupled microwave billiards.

The resonant states of the coupled system depend, in a natural manner, on L and W and also on the coupling strength u by which the single QBs are coupled to the internal waveguide. Besides this internal coupling, the resonance states of an open quantum system can interact via the continuum represented by the propagating waves in the attached waveguides. This coupling is seldom considered in the literature. It causes the so-called external coupling of the resonance states which appears additionally to the other well-known coupling mechanisms.

The relation between the external coupling v of the resonance states via the continuum to the direct internal coupling u of the resonance states is known to play an important role in open quantum systems [10]. The interplay between the external and internal couplings of resonance states is studied in detail in laser-induced continuum structures in atoms [11]. As a result, most interesting is the regime in which the internal and external couplings are of the same order of magnitude. Here, the widths of some states may vanish with the consequence that the states do not decay in spite of the fact that they are populated and their decay is not forbidden by any selection rule. This phenomenon is known in the literature as 'population trapping'. In coupled QBs, a similar phenomenon may lead to zeros in the transmission [12]. In QBs, the role of the external coupling at fixed internal mixing of the resonance states is studied experimentally by varying the degree of opening between the QB and the attached lead by means of a slit [13, 14]. At full opening of the QB, most resonance states decouple from the continuum (resonance trapping). The relation of this phenomenon to branch points in the complex energy plane is studied in [15], and the influence of these branch points on the transmission through small QBs is investigated in [16].

A double QB allows us to study the interplay between the external and the internal interaction of the resonance states and its influence on the transmission in a very natural manner. It is possible to control, independently of each one another, both the internal coupling

u between the two single dots and the external coupling v of the system as a whole to the attached leads. The transmission through the system can be controlled therefore by the ratio v/u.

It is the aim of the present paper to provide the equations for the transmission through a double QB and its explicit dependence on v/u. To this purpose, we use the *S*-matrix formalism together with the effective Hamilton operator that characterizes the open double QB. The equations derived by us for the effective Hamiltonian and for the transmission show that both are strongly dependent on v/u. The transmission is resonant at small as well as at large values of v/u. Transmission zeros may appear.

In section 2, we present numerical results for the transmission through a system consisting of two single QBs connected by a waveguide. The single QBs are identical, and each has many levels. The main features of the transmission are represented as a function of the length L and width W of the waveguide. In section 3, the Hamiltonian of the closed system is presented. It consists of two single QBs and a waveguide connecting them. The Hamiltonian of the closed system is, after diagonalizing, basic for deriving the effective Hamiltonian of the corresponding open system. This system has the same structure as the closed system, but two infinitely long leads are attached to it. We derive the equations for the transmission on the basis of the *S*-matrix theory by using the eigenvalues and eigenfunctions of the non-Hermitian effective Hamilton operator of the open system [17]. We provide the results for the case that the waveguide and each single QB contain one level (section 4) and two or more levels (section 5), respectively. The transmission picture shows all the characteristic features that are obtained from a direct calculation of the transmission through a double QB with a large number of levels, as discussed in section 2. In the case of more than one level in each single cavity that are identical, the widths of a few resonance states may approach zero. They cause zeros in the transmission. The scattering wavefunctions show that the particle is trapped, in these cases, in the internal waveguide that is effectively decoupled from the leads. In the last section, we conclude the present study. We underline that the theory presented here may be applied also to the transmission through a system that consists of two scattering subsystems connected by a waveguide. An example might be waveguides with two bends [18–20].

2. Transmission through double quantum billiards

Let us consider first a double QB consisting of two single QBs, for example of rectangular (or circular) shape, which are connected by a waveguide of length L and width W, as shown in figure 1. The coupling strength u between the waveguide and the two single QBs can be varied by means of a diaphragm [13, 14] (see figure 1). Similar diaphragms are located between the whole double QB system and the input and output waveguides by means of which it is possible to vary the coupling strength v.

In this section, we calculate numerically the transmission amplitudes by using two different methods: (i) we calculate directly the scattering wavefunction by discretizing the solution of the Schrödinger equation with the application of the Ando boundary conditions at the input and output waveguides [21] and (ii) we use the *S*-matrices for the individual QBs in order to calculate the transmission through the double QB [19, 22]. Ignoring in the calculations (ii) the evanescent modes in the waveguide, the transmission amplitude in the single-channel case becomes especially simple for two identical single QBs [22]:

$$t_{12} = \frac{t_1^2}{1 - r_1^2 \exp(2\mathrm{i}qL)}, \tag{1}$$

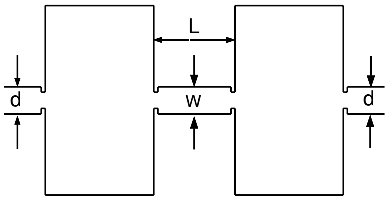

Figure 1. The double QB system consisting of two identical rectangular billiards and a waveguide that connects them. The waveguide is of length L and width W. By means of the diaphragms between the single QBs and, respectively, the waveguides and attached leads, the corresponding coupling constants can be varied.

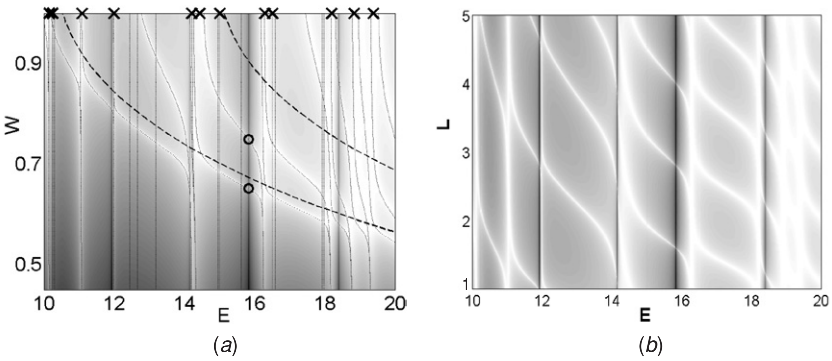

Figure 2. The logarithm of the probability $\ln(T)$ for the transmission through the double QB shown in figure 1 versus energy and width of the waveguide W (a) and length of the waveguide L (b). White corresponds to maximum and dark to minimum transmission. The eigenenergies of each single QB marked by crosses are independent of W. The eigenenergies of the internal connecting waveguide are shown by dashed lines and those of the closed double QB by thin solid lines. In the present calculation, the eigenenergies of the closed system are almost the same as the eigenenergies of the open system. The bold open circles mark two points with zero transmission (see figure 7).

where t_1 and r_1 are the complex amplitudes of the transmission and reflection for the single QBs, and q is the wave number of the connecting waveguide which is related to the energy of the transmission in the first channel by

$$E = E_0(q^2 + \pi^2/W^2), \tag{2}$$

where $E_0 = \hbar^2/2m^*$. In application to microwave waveguides the energy is the squared frequency $E = \omega^2$ and $E_0 = c^2$, c being the velocity of light.

In figure 2(a) we show the transmission probability (brightness in log-scale) versus energy E and width W of the waveguide which is calculated by the method (i). Transmission zeros (black) are independent of W, while transmission peaks (white) are strongly related to the positions of the resonance states of the double QB. In figure 2(b) we show the transmission probability as a function of the energy E and length L of the waveguide. Similar results for a system of two single QBs with another shape were obtained numerically by Pichugin [23].

The transmission probability demonstrates a few interesting features that are shown in figure 2. The first is some periodical dependence of the transmission peaks (white) on the waveguide length (or width) and on the energy. This dependence can be seen immediately in formula (1), and we will not discuss it further. The second feature is the transmission zeros (black). They do not at all depend on the waveguide sizes; see figure 2 where the transmission probability T is shown in logarithmic scale. Also this feature follows directly from (1): the zeros of the transmission probability $|t_1|^2$ through the single QB lead directly to the zeros of the total transmission probability $T = |t_{12}|^2$. The third feature concerns the peaks of the transmission probability. Figure 2 shows that the transmission peaks follow the eigenenergies of the system that consists of two single QBs connected by the internal waveguide (figure 2(a), dotted lines). These energies result from the interaction u of the states of the internal waveguide (full lines) with the states of the single QBs (marked by crosses) provided that both types of states have the same parity perpendicular to the direction of the transport. Interesting features arise at the points where the eigenenergies of the opened system (dotted lines in figure 2(a)) cross the energies of transmission zeros (two of them are shown by open circles). At these points, the widths of the resonance states vanish, i.e., the particle is trapped inside the waveguide as will be shown in section 5.

In the following, we will consider these features in detail. For this purpose, we use the periodicity (first feature) of the transmission picture that allows us to restrict the investigation to the transmission properties of a simple model with only a few states. The study is based on the S-matrix theory by using the effective non-Hermitian Hamilton operator of the system opened by attaching leads to it [17, 24].

3. Closed system consisting of two single quantum billiards connected by a waveguide

The Hamiltonian of the system shown in figure 1 consists of three parts: two parts describe the two single QBs and the third one is related to the waveguide (wire). The Hamiltonian of the two single QBs is formulated in a standard way,

$$H_d = H_1 + H_2 = \sum_{n_1=1}^{N_1} \varepsilon_{n_1} |n_1\rangle\langle n_1| + \sum_{n_2=1}^{N_2} \varepsilon_{n_2} |n_2\rangle\langle n_2|, \tag{3}$$

where the indices 1, 2 stand, respectively, for the first and second single QB with the energies $\varepsilon_{n_1}, \varepsilon_{n_2}$ and the Hilbert dimensions are N_1, N_2. The waveguide is the third independent quantum mechanical subsystem described by the Hamiltonian

$$H_w = \sum_{n_w=1}^{N_w} \varepsilon_{n_w}(L) |n_w\rangle\langle n_w|. \tag{4}$$

The eigenenergies $\epsilon_{n_w}(L)$ of the waveguide depend on at least two values: on the width d and the length L of the waveguide. Without loss of generality, we can fix one of these values and vary the other one, say L as in (4). The variation of L is carried out in such a manner that the eigenenergies of the waveguide and those of the single QBs can cross. We assume further that the waveguide is coupled to, respectively, the left and the right single QB via the matrices U_1, U_2 of dimensionality $N_1 \times N_w$, $N_2 \times N_w$. Then the total Hamiltonian has the following matrix form

$$H_B = \begin{pmatrix} H_1 & U_1 & 0 \\ U_1^+ & H_w & U_2^+ \\ 0 & U_2 & H_2 \end{pmatrix}. \tag{5}$$

The Hamiltonian (5) differs from those used in the literature [25–27] for the description of a double quantum dot of similar shape by taking explicitly into account the third part (4) for the waveguide.

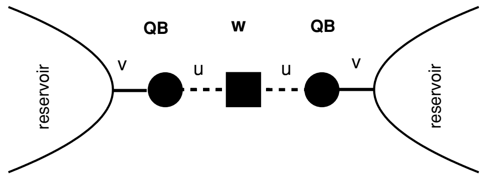

Figure 3. Two single state QBs ('QB') are connected to the waveguide ('w') with the coupling constants u and to the reservoirs with the coupling constants v.

For the simplest case $N_1 = N_w = N_2 = 1$ and equal single QBs, the total Hamiltonian takes the following form

$$H_B = \begin{pmatrix} \varepsilon_1 & u & 0 \\ u & \varepsilon_w(L) & u \\ 0 & u & \varepsilon_1 \end{pmatrix}. \tag{6}$$

The eigenvalues of this Hamiltonian are

$$E_{1,3} = \frac{\varepsilon_1 + \epsilon(L)}{2} \mp \eta, \qquad E_2 = \varepsilon_1, \tag{7}$$

$$\eta^2 = \Delta\varepsilon^2 + 2u^2, \qquad \Delta\varepsilon = \frac{\varepsilon_1 - \varepsilon_w(L)}{2} \tag{8}$$

and the eigenstates read

$$|1\rangle = \frac{1}{\sqrt{2\eta(\eta + \Delta\varepsilon)}} \begin{pmatrix} -u \\ \eta + \Delta\varepsilon \\ -u \end{pmatrix}, \qquad |2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},$$
$$|3\rangle = \frac{1}{\sqrt{2\eta(\eta - \Delta\varepsilon)}} \begin{pmatrix} u \\ \eta - \Delta\varepsilon \\ u \end{pmatrix}. \tag{9}$$

It is remarkable that one of the eigenenergies of the total system coincides with the energy ε_1 of the single QB. This fact is true also in the more general cases with higher dimensions.

The case of two identical single QBs with each having $N > 1$ states is similar to the $N = 1$ case if the waveguide is a straight one. The case $N = 2$ is considered in section 5.

4. *S*-matrix for the transmission through double-quantum billiards: single billiards with one state

Knowledge of the eigenstates of the closed quantum system allows us to formulate the S-matrix and the effective Hamiltonian in the manner described in [17, 24]. Let us consider first the most simple case of the Hamiltonian (6). For the transmission through this system, we have two leads coupled to the reservoirs with the strength v, as shown in figure 3. The coupling matrix has the following general form [17, 24]

$$V = \sum_m \sum_{C=l,r} \int \mathrm{d}E\, V_m(E, C)|E, C\rangle\langle m| + \text{h.c.}, \tag{10}$$

where $|m\rangle$ are the eigenstates of the closed system given in the present case by (9), and C enumerates the reservoirs with the states $|E, C\rangle$ normalized by

$$\langle E, C|E', C'\rangle = \delta(E - E')\delta_{C,C'}.$$

Obviously,

$$V_m(E,C) = \langle E, C|V|m\rangle = \sum_j \sum_{j_C} \psi_C(j_C)\psi_m(j)\langle j_C|V|j\rangle, \tag{11}$$

where j runs over the QB system, j_C runs over the two reservoirs C (left and right), $\psi_C(j)$ are the eigenfunctions of the half-infinite leads, and $\psi_m(j)$ are the eigenfunctions of the closed double QB system. j and j_C both run over those sites at which the lead C is attached to the QB [17]. In our model we choose the couplings, that are shown in figure 3 by solid lines, to be fixed at some points: at $j = 1, 3$ of the left and the right single QD and at some points x_C which belong to the reservoirs. Moreover, we describe for simplicity the reservoirs as half-infinite one-dimensional waveguides in the tight-binding approach [17]. As in [17], we take the connection points of the coupling to the reservoirs at the edges of the one-dimensional leads. Then the matrix elements (11) take the following form

$$\begin{aligned} V_m(E,l) &= v\psi_{E,l}(x_L)\psi_m(j=1) = v\sqrt{\frac{\sin k}{2\pi}}\psi_m(1), \\ V_m(E,r) &= v\psi_{E,r}(x_r)\psi_m(j=3) = v\sqrt{\frac{\sin k}{2\pi}}\psi_m(3), \end{aligned} \tag{12}$$

where k is the wave vector related to energy by $E = -2\cos k$. In the long-wave approximation, the last equality is simply $E \approx -2 + k^2$. The effective Hamiltonian can be written as [17, 24]

$$H_{\text{eff}} = H_B + \sum_{C=l,r} V_{BC}\frac{1}{E^+ - H_C}V_{CB}, \tag{13}$$

where H_C is the Hamiltonian of the reservoir C and $E^+ = E + \text{i}0$. Substituting (12) into (13) we obtain for the matrix elements of the effective Hamiltonian

$$\begin{aligned} \langle m|H_{\text{eff}}|n\rangle &= E_m\delta_{mn} + \sum_{C=l,r}\frac{1}{2\pi}\int_{-2}^{2}\text{d}E'\frac{V_m(E',C)V_n(E',C)}{E+\text{i}0-E'} \\ &= E_m\delta_{mn} - v^2(\psi_m(1)\psi_n(1) + \psi_m(3)\psi_n(3))\,\text{e}^{\text{i}k}, \end{aligned} \tag{14}$$

where the states $\psi_n(j)$ are given in (9) and the indices $j = 1, 3$ mean, respectively, the left single QB ($j = 1$) and the right single QB ($j = 3$). Substituting (9) into (14) we obtain

$$H_{\text{eff}} = \begin{pmatrix} E_1 - \dfrac{v^2u^2\,\text{e}^{\text{i}k}}{\eta(\eta+\Delta\varepsilon)} & 0 & \dfrac{v^2u\,\text{e}^{\text{i}k}}{\sqrt{2}\eta} \\ 0 & E_2 - v^2\,\text{e}^{\text{i}k} & 0 \\ \dfrac{v^2u\,\text{e}^{ik}}{\sqrt{2}\eta} & 0 & E_3 - \dfrac{v^2u^2\,\text{e}^{\text{i}k}}{\eta(\eta-\Delta\varepsilon)} \end{pmatrix}. \tag{15}$$

Next we calculate the (complex) eigenvalues of the effective Hamiltonian (15) that are related to the poles of the S-matrix. The result is

$$\begin{aligned} z_2(L) &= \varepsilon_1(L) - v^2\,\text{e}^{\text{i}k}, \\ z_{1,3}(L) &= \frac{\varepsilon_1(L)+\varepsilon_w(L)-v^2\,\text{e}^{\text{i}k}}{2} \mp \sqrt{\left(\frac{\varepsilon_w(L)-\varepsilon_1(L)+v^2\,\text{e}^{\text{i}k}}{2}\right)^2 + 2u^2}. \end{aligned} \tag{16}$$

The eigenvalues depend on both the internal coupling strength u and the external coupling strength v. For $v \to 0$, they coincide with the eigenvalues E_k of the closed system, equation (7). For $u \to 0$, the eigenvalues z_k are completely different from the E_k. They are $z_{1,2}(L) = \varepsilon_1(L) - v^2\,\text{e}^{\text{i}k}$, $z_3(L) = \varepsilon_w(L)$. The eigenvalue $z_3(L) = \varepsilon_w(L)$ means that the waveguide has no other connection to the reservoirs than that via the single QBs.

In order to calculate the S-matrix we need the eigenstates of the effective Hamiltonian [17]

$$H_{\mathrm{eff}}|\lambda) = z_\lambda|\lambda), \tag{17}$$

where $(\lambda| = |\lambda)^c$, $\lambda = 1, 2, 3$, c means transposition, and $(\lambda|\lambda') = \delta_{\lambda,\lambda'}$ is the biorthogonality relation for the eigenfunctions of the non-Hermitian Hamiltonian H_{eff} [10]. Then it follows from (15) (for $u \neq 0$):

$$|1) = \begin{pmatrix} a \\ 0 \\ b \end{pmatrix}, \qquad |2) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |3) = \begin{pmatrix} b \\ 0 \\ -a \end{pmatrix} \tag{18}$$

with

$$a = -\frac{f}{\sqrt{2\xi(\xi+\omega)}}, \qquad b = \sqrt{\frac{\xi+\omega}{2\xi}} \tag{19}$$

and

$$f = \frac{v^2 u\, \mathrm{e}^{\mathrm{i}k}}{\sqrt{2}\eta}, \qquad \omega = -\eta + \frac{\Delta\varepsilon v^2\, \mathrm{e}^{\mathrm{i}k}}{2\eta}, \qquad \xi^2 = \omega^2 + f^2. \tag{20}$$

Knowledge of the eigenvalues and eigenstates of the effective Hamiltonian opens large room for further analytical studies of many interesting properties of open quantum systems. An example is the study of the branch points in the complex plane where $z_1 = z_3$ [16, 28, 29]. The amplitude for the transmission through the double QB can be written in the simple form [17]

$$t = -2\pi\mathrm{i}\sum_\lambda \frac{\langle l|V|\lambda)(\lambda|V|r\rangle}{E - z_\lambda}. \tag{21}$$

The matrix elements $\langle L|V|\lambda)$ and $(\lambda|V|R\rangle$ are obtained by using (12), (18) and correspondingly (9),

$$\begin{aligned}
\langle l|V|2) &= \sum_m \langle E, l|V|m\rangle\langle m|2) = \frac{v}{2}\sqrt{\frac{\sin k}{\pi}}, \\
(2|V|r\rangle &= \sum_m (2|m\rangle\langle m|V|E, r\rangle = -\frac{v}{2}\sqrt{\frac{\sin k}{\pi}}, \\
\langle l|V|1) &= (1|V|r\rangle = v\sqrt{\frac{\sin k}{2\pi}}(\psi_1(1)a + \psi_3(1)b), \\
\langle l|V|3) &= (3|V|r\rangle = v\sqrt{\frac{\sin k}{2\pi}}(\psi_1(1)b - \psi_3(1)a),
\end{aligned} \tag{22}$$

where the eigenstates $\psi_m(j)$ are given in (9). The expression (21) shows that the transmission is resonant in any case. Nevertheless, it depends on the coupling strengths u and v since the effective Hamiltonian (15) and its eigenvalues z_λ, equation (16), and eigenfunctions $|\lambda)$, equation (18), depend explicitly on u and v. The transmission probability is $T = |t|^2$.

The typical behaviour of the transmission probability $T = |t(E, L)|^2$ versus energy E and length L is shown in figure 4. The waveguide eigenenergies are $\varepsilon_{mn_w}(L, W) = (m/W)^2 + (n/L)^2$ in terms of $E_0 = \frac{\hbar^2}{2m^* d^2}$, where L is the length and $W = d$ the width of the waveguide, and m, n are quantum numbers. For $W \ll L$, we can restrict ourselves to $m = 1$ and have $\varepsilon_{n_w}(L) = \mathrm{const} + (n/L)^2$. However, this specific form does not play any role. The

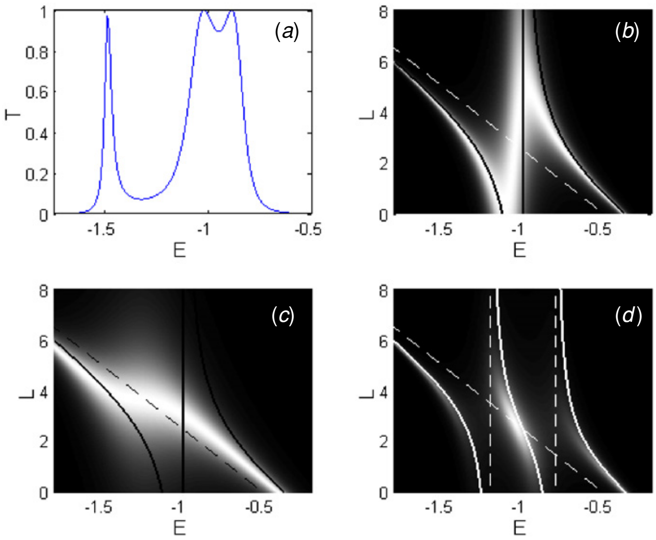

Figure 4. The transmission probability T through the double QB shown in figure 3. White corresponds to maximal transmission probability and dark to minimal one. (a) Two identical single QBs with the eigenenergy $\varepsilon_1 = 1$ and $v = 0.3, u = 0.2, L = 4$.(b) The same as (a) but the length L is not fixed. (c) The same as (b) but $v = 0.6$.(d) The same as (b) but two different single QBs with the eigenenergies $\varepsilon_L = 0.8, \varepsilon_R = 1.2$ and $v = 0.2$. The eigenenergies $E_k(L), k = 1, 2, 3$, of H_B (closed system) are shown by full lines while the energies of the waveguide, $\varepsilon_w(L) = 20/(L+1)^2$, and of the single QBs are given by dashed lines.

only condition for the concrete choice of the L dependence of ε_w in our calculations is that ε_w crosses the eigenenergies of the single QBs at a certain value of L for $u = 0$.

The results presented in figure 4 follow from the simple model which describes the double QB system by two single-state QBs connected by a waveguide, and the waveguide is characterized by the only energy $\varepsilon_w(L)$. When the coupling strength v of the double QB to the reservoir is relatively weak (meaning that the ratio v/u is relatively small as in figures 4(a), (b), (d)), the transmission probability follows the eigenenergies of the closed double QB. According to the usual definition, we have resonant transmission in this case.

Comparing figures 4(b)–(d) with figure 2, we see that the simple model, basic to figure 4, is able to explain the peaks of the transmission probability. That means, the main features of the transmission pictures 2 are, at small v, related to the avoided crossings of the levels of the single QBs with the level of the waveguide.

We can further learn from figure 4 that the transmission through the system consisting of two QBs that are connected by a waveguide is characterized by the ratio v/u, i.e., by the ratio between the external and internal couplings of the states of the double QB system via, respectively, the reservoir and the waveguide. In figure 4(b), (d), the ratio v/u is small and the transmission probability completely follows the eigenenergies of the closed double QB system. In figure 4(c), the coupling strength v between the double QB and the reservoirs exceeds essentially the coupling strength u of the two single QBs to the waveguide. In this case, the transmission is mainly given by the resonant transmission through the waveguide, and the two single QBs become parts of the reservoirs, as can be seen directly from (16).

All the results obtained for a double QB with one-site single QBs do not show any transmission zeros between the transmission peaks. This can be understood in the following manner. The model underlying the results of figure 4 has a one-dimensional architecture,

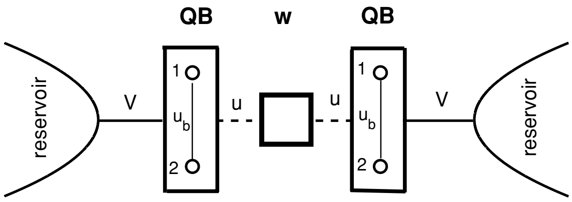

Figure 5. The double QB system is connected to the reservoirs by the coupling constants v. The two single QBs ('QB') are coupled to the waveguide ('w') by the coupling constants u.

i.e., the one-dimensional leads are connected at a single point to the single QBs that have only one state each. The absence of transmission zeros in this case is in complete agreement with the consideration by Lee [30] that odd and even resonance levels alternate in energy in one-dimensional systems so that zeros in the transmission probability cannot appear. The results of figure 4 agree also with those obtained from consideration of a simple two-site system [17, 27]. It has been shown for these systems that an architecture of the couplings between system and reservoirs, which *violates* the true one dimensionality of the closed system, gives rise to a zero in the transmission probability at a certain energy. This is a consequence of the unitarity of the S-matrix: each lead is attached to only one single QB. Unitarity of the S-matrix leads therefore to a zero in the transmission between every two states of a *single* QB [12]. It cannot cause any zero when each single QB has only one state.

5. *S*-matrix for the transmission through double quantum billiards: single billiards with many states

Here, we consider the transmission through a double QB when each single QB of the system has two states as shown in figure 5. For simplicity we assume that all the coupling constants between the waveguide and the single QBs are the same and are given by the constant value u. Then the Hamiltonian (5) of the closed double QB consisting of the two single QBs and the waveguide is

$$H_B = \begin{pmatrix} \varepsilon_1 & 0 & u & 0 & 0 \\ 0 & \varepsilon_2 & u & 0 & 0 \\ u & u & \varepsilon_w(L) & u & u \\ 0 & 0 & u & \varepsilon_2 & 0 \\ 0 & 0 & u & 0 & \varepsilon_1 \end{pmatrix}. \tag{23}$$

The Hamiltonian (23) is written in the energy representation (3), (4). In order to specify the connection between the reservoirs and the single QBs, we have however to know the eigenstates of (23) also in the site representation. The Hamiltonian of the single QB in the site representation is

$$H_b = \begin{pmatrix} \varepsilon_0 & u_b \\ u_b & \varepsilon_0 \end{pmatrix}. \tag{24}$$

The hopping matrix elements u_b are shown in figure 5 by thin solid lines. The eigenfunctions and eigenvalues are the following

$$\langle j|\varepsilon_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \langle j|\varepsilon_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \qquad \varepsilon_{1,2} = \varepsilon_0 \mp u_b. \tag{25}$$

We introduce the projection operators

$$P_1 = \sum_{b_1} |\varepsilon_{b_1}\rangle\langle\varepsilon_{b_1}|, \qquad P_w = |1_w\rangle\langle 1_w|, \qquad P_2 = \sum_{b_2} |\varepsilon_{b_2}\rangle\langle\varepsilon_{b_2}| \tag{26}$$

where $b_1 = 1, 2, b_2 = 1, 2$, and $|1_w\rangle$ is the one-dimensional eigenstate of the waveguide. Let E_m and $|m\rangle$ with $m = 1, \ldots, 5$ denote the five eigenenergies and eigenstates of (23), $H_B|m\rangle = E_m|m\rangle$. Then the elements of the left coupling matrix are

$$\langle l, E|V|m\rangle = \sum_{b_1}\langle l, E|V|\varepsilon_{b_1}\rangle\langle\varepsilon_{b_1}|m\rangle = \sum_{j_1=1,2}\sum_{b_1}\langle l, E|V|j_1\rangle\langle j_1|\varepsilon_{b_1}\rangle\langle\varepsilon_{b_1}|m\rangle. \tag{27}$$

Similar expressions can be derived for the right coupling matrix. Here we used the assumption that the left reservoir is connected only to the left single QB and the right reservoir only to the right single QB. As previously, the reservoirs are assumed to be half-infinite one-dimensional waveguides. Next we have to specify which sites of the left (right) single QB are connected to the left (right) reservoir. There are two possibilities.

(i) Assume the left reservoir is connected only to the first site $j_1 = 1$ of the left single QB. Then (27) becomes using (25)

$$\langle l, E|V|m\rangle = v\sqrt{\frac{\sin k}{2\pi}}\sum_{b_l}\langle\varepsilon_{b_l}|m\rangle. \tag{28}$$

A corresponding expression can be written for the right coupling matrix if the right reservoir is connected to the first site of the right single QB.

(ii) We can assume that the reservoirs are connected to both sites of the single QBs with the same coupling constant v. Then the elements of the coupling matrices (27) are the following

$$\langle l, E|V|m\rangle = v\sqrt{\frac{\sin k}{2\pi}}\sum_{j=1,2}\langle j|m\rangle, \qquad \langle r, E|V|m\rangle = v\sqrt{\frac{\sin k}{2\pi}}\sum_{j=4,5}\langle j|m\rangle \tag{29}$$

in the basis in which the Hamiltonian (23) is given.

The most important difference between the previous $d = 1$ case and the present $d = 2$ one for the single QB is that the system is now no longer necessarily one-dimensional. Therefore, zeros in the transmission probability may appear.

It can be shown that two eigenvalues of the Hamiltonian H_B coincide with the energies ε_1 and ε_2 of the single QB. The other three eigenvalues of (23) can be found by solving a cubic equation. In the following, we consider the main features of the transmission through a system with two states of each single QB numerically.

In figure 6, the transmission probability versus energy E and length L of the internal waveguide of a double QB is shown for the case that both sites of the single QBs are connected to the reservoir with the coupling matrix elements (29). We see that figure 6(*a*) closely reproduces a fragment of the total picture shown in figure 2, including the appearance of transmission zeros. The difference between the two figures arises from the restriction to one state in the waveguide and two states in each QB in figure 6 while there is no such restriction in figure 2.

According to figure 6(*b*), the positions and decay widths of the eigenstates 2 and 4 of the effective Hamiltonian are independent of the length L of the waveguide, while those of the other states depend on L. The state 3, lying in the middle of the spectrum, crosses the transmission zero at $L = 3.47$ (figures 6(*a*), (*b*)). This value of L corresponds to

$$\varepsilon_b = \varepsilon_w(L) = \frac{\varepsilon_1 + \varepsilon_2}{2}. \tag{30}$$

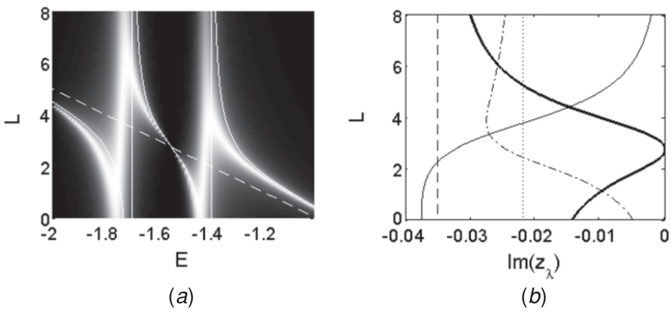

Figure 6. (*a*) The transmission through a double QB system with two identical single QBs that are connected by a waveguide according to figure 3, versus energy E and length L of the waveguide. The eigenenergies $\varepsilon_1 = -1.7$, $\varepsilon_2 = -1.4$ of the individual QBs are shown by solid thin lines. The eigenenergy of the waveguide $\varepsilon_w(L) = -1 - L/5$ is shown by a dashed line, the eigenvalues of H_B by full lines. $v = 0.3$, $u = 0.1$. (*b*) The imaginary part of the 5 eigenvalues z_k of the effective Hamiltonian as a function of L for $E = -1.5$. At ε_b and $L = 3.47$ the imaginary part of the third eigenvalue is equal to zero at all energies E.

At ε_b, one gets for the eigenenergies of (23)

$$E_{1,5} = \varepsilon_b \pm \eta, \qquad E_2 = \varepsilon_1, \qquad E_3 = \varepsilon_b, \qquad E_4 = \varepsilon_2 \tag{31}$$

and for the eigenvectors

$$\begin{aligned}
\langle 1| &= \frac{\sqrt{2}u}{\eta}\left(\frac{u}{\eta-\Delta\varepsilon}, \frac{u}{\eta+\Delta\varepsilon}, -1, \frac{u}{\eta+\Delta\varepsilon}, \frac{u}{\eta-\Delta\varepsilon}\right) \\
\langle 2| &= \frac{1}{\sqrt{2}}(1, 0, 0, 0, -1) \\
\langle 3| &= \frac{u}{\eta}\left(1, -1, \frac{\Delta\varepsilon}{u}, -1, 1\right) \\
\langle 4| &= \frac{1}{\sqrt{2}}(0, 1, 0, -1, 0) \\
\langle 5| &= \frac{\sqrt{2}u}{\eta}\left(\frac{u}{\eta+\Delta\varepsilon}, \frac{u}{\eta-\Delta\varepsilon}, 1, \frac{u}{\eta-\Delta\varepsilon}, \frac{u}{\eta+\Delta\varepsilon}\right),
\end{aligned} \tag{32}$$

where $\eta^2 = \Delta\varepsilon^2 + 4u^2$, $\Delta\varepsilon = (\varepsilon_2 - \varepsilon_1)/2$. Substituting (32) into (29) we obtain

$$\langle m|V|E, C = L, R\rangle = v\sqrt{\frac{\sin k}{8\pi}}(1 \pm 10 \pm 11) \tag{33}$$

for the elements of the coupling matrix. One can see that, under the condition (30), the wire decouples from the rest of the system. The substitution of (33) into (14) shows that at $\varepsilon_w = \varepsilon_b$ the effective Hamiltonian matrix 5×5 decomposes as $H_{\text{eff}} = H_1 \bigoplus E_3 \bigoplus H_2$ where

$$H_1 = \begin{pmatrix} E_1 + \Gamma & \Gamma \\ \Gamma & E_5 + \Gamma \end{pmatrix}, \qquad H_2 = \begin{pmatrix} E_2 + \Gamma & \Gamma \\ \Gamma & E_4 + \Gamma \end{pmatrix} \tag{34}$$

and $\Gamma = -v^2 \exp(\mathrm{i}k)/2$. Obviously, the imaginary part of the third eigenvalue of the equation $H_{\text{eff}}|\lambda\rangle = z_\lambda|\lambda\rangle$ is zero, i.e. the width of the third eigenvalue vanishes. According to formula (105) of [17], the scattering wavefunction can be decomposed in the set of eigenfunctions of H_{eff},

$$\psi = \sum_{\lambda, C=l,r} \frac{V_\lambda(E, C)}{E^+ - z_\lambda}\psi_\lambda, \tag{35}$$

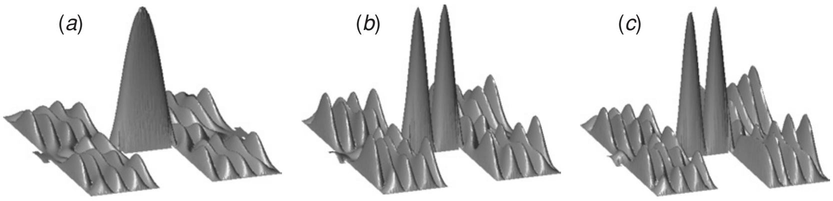

Figure 7. An amplitude of the scattering wavefunction for the transmission through the double billiard shown in figure 1: (a) at $E = 15.83$ and $W = 0.65$, (b) at $E = 15.83$ and $W = 0.75$. White corresponds to the maximum of the wavefunction and dark to the minimum one. These points are shown in figure 2 by bold open circles. (c) The case of the different billiards for $E = 15.6096$, $W = 0.7595$ at which the width of resonance reaches the minimum.

where the $V_\lambda(E, C) \equiv (\lambda|V|C, E\rangle$ are the coupling matrix elements between the leads C and the *open* double QB described by the eigenstates λ of H_{eff}. Since the eigenvalue z_3 is real, $V_3(E, c) \to 0$ if $E \to z_3 = E_3 = \varepsilon_b$. Therefore, a particle moving from the left lead to the left QB or from the right lead to the right QB is fully reflected. That means, the wire is decoupled from the reservoirs and the electrons are trapped inside the wire. According to (21), the contributions from $\lambda = 1$ and 5 as well as those from $\lambda = 2$ and 4 to the transmission cancel each other at $E = \varepsilon_b$ due to the symmetry in relation to ε_b while the contribution from $\lambda = 3$ vanishes. As a consequence, an electron will not be transmitted at the energy $E = \varepsilon_b$. According to (34), the existence of the locked state does depend neither on the value u of the coupling of the internal wire to the QBs nor on the value v of the coupling of the billiards to the reservoirs.

In the realistic double QB system with many states, there are many transmission zeros in the E, W plane (figure 2(a)) or in the E, L plane (figure 2(b)) which are of second order and independent of the size of the waveguide [12]. At the two points in figure 2 which are marked by open circles, the eigenenergies of the closed system cross the transmission zeros. Here the corresponding eigenenergies of the effective Hamiltonian are real and the particle is trapped in the internal waveguide indeed: figures 7(a) and (b) show the scattering wavefunction at these points. It can immediately be seen that the width of the corresponding resonance state is zero. When the two single QBs are slightly different from one another, the transmission zeros are of first order and the width of the crossing state is small but different from zero [12]. The scattering wavefunction of such a case shows slight excess of amplitude in those billiards which are larger, as can be seen from figure 7(c).

We remark that resonance states with vanishing decay widths are considered also by other authors. In [31], they appear in a double well potential under the influence of a time-periodic perturbation. In [27], they are called ghost Fano resonances that appear in a double quantum dot when attached to leads. In atomic physics, the phenomena related to resonance states with vanishing decay widths are known as population trapping [11]. They result from the interplay of the direct coupling of the states and their coupling via the continuum under the influence of, e.g., a strong laser field. Physically, population trapping in atoms is a phenomenon similar to that considered by us in the present paper, i.e. trapping of electrons in the waveguide that connects the two single QBs of a double QB.

6. Concluding remarks

From the present study, we can conclude that the simple model used by us for the description of a double QB system consisting of two single QBs coupled by a waveguide describes qualitatively the features of the transmission through a realistic double QB of the same structure. The difference between the transmission through the double QB system shown in figure 2 and the model cases shown in figures 4 and 6 consists, above all, in the fact that all features of the simple model are multiply repeating in figure 2. These multiple effects are related, obviously, to the large dimension of the single QBs and to the large number of eigenmodes of the waveguide inside the double QB system.

Summarizing the results of the present paper, we state the following. Firstly, we derived the equations for the transmission through a QB that consists of two single QBs connected by a waveguide, by taking into account the coupling of the resonance states via the waves propagating in the attached leads. This coupling is simulated by the parameter v. It appears additionally to all the other possible mechanisms by which the resonance states of the system could be coupled. It is seldom considered in the literature. As a result of our analytical studies, we state

(i) the transmission through the system is always resonant according to (21) and
(ii) the eigenvalues z_λ of the effective Hamiltonian depend strongly on the ratio v/u between the external and internal couplings according to (16).

According to (ii) (equation (16)), the eigenvalues are completely different from one another in the two limiting cases $v \to 0$ and $u \to 0$. That means that, according to (i) (equation (21)), also the transmission through the system at small v/u is completely different from that at large v/u. From this result we conclude that the coupling mechanism of the resonance states via the continuum cannot be neglected in calculating the transmission when the QB as a whole is fully opened.

Secondly, we applied the equations to a double QB for fixed values u and v by varying the geometrical size of the waveguide that connects the two single QBs in the double QB system. The most interesting result is that the electrons may be *trapped* in the waveguide if the two single QBs are identical and have at least two levels each. In such a case, the decay width of one of the resonance states approaches zero (as a function of a certain parameter) when crossing the transmission zero. That means, the waveguide is completely decoupled from the leads attached to the double QB at this parameter value and the transmission approaches zero. The trapping of electrons inside the waveguide appears at all values of u and v.

The results obtained for the transmission through double QBs are of relevance also for the transmission through double quantum dots. The point is that all the characteristic features of the interplay between external and internal couplings, which are discussed here, are the same in both cases. Differences appear due to the different absolute values of the internal and external coupling strengths in the two cases, especially due to the Coulomb interaction.

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