Bound states in the continuum in open quantum billiards with a variable shape

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We show the existence of bound states in the continuum (BICs) in quantum billiards (QBs) that are opened by attaching single-channel leads to them. They may be observed by varying an external parameter continuously, e.g., the shape of the QB. At some values of the parameter, resonance states with vanishing decay width (the BICs) occur. They are localized almost completely in the interior of the closed system. The phenomenon is shown analytically to exist in the simplest case of a two level QB and is complemented by numerical calculations for a real QB.

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I. INTRODUCTION

In 1929, von Neumann and Wigner[1] claimed that the single-particle Schrödinger equation could possess solutions that correspond to isolated discrete eigenvalues embedded in the continuum of positive energy states. An extension and some correction of this work was done by Stillinger and Herrick[2] who presented a few examples of spherically symmetric attractive local potentials with bound states embedded in the continuum of scattering states (BICs). The results of von Neumann and Wigner have stimulated a considerable amount of theoretical and experimental work (see their recent paper[3]).

Friedrich and Wintgen[4] discussed the realization of BICs in a hydrogen atom in a magnetic field. In a follow-up paper,[5] they formulated a general method to find BICs in quantum systems. This method starts from Feshbach's unified theory of nuclear reactions and uses the fact that the appearance of BICs is directly related to the phenomenon of an avoided level crossing of neighbored resonance states. When two resonance states approach each other as a function of a certain continuous parameter, interferences cause an avoided crossing of the two states in their energy positions and, for a certain value of the parameter, the width of one of the resonance states may vanish exactly. Since it remains above threshold for decay into the continuum, this state becomes a BIC.

The phenomenon of avoided crossing of narrow resonance states and its relation to the redistribution of the spectroscopic values of quantum systems under the influence of their coupling to the continuum is considered in many papers (see the review[6]). The redistribution is caused by that part of the effective Hamiltonian H_{eff} which describes the coupling of the resonance states via the continuum of decay channels. Some years ago, many studies were performed using statistical assumptions for the resonance states. The coupling term via the continuum is purely imaginary in these studies, and states with vanishing widths may appear when this part of the Hamiltonian is large, e.g., Ref. 7. Recently, this method was applied to quantum dots.[8] In other studies, all the coupling matrix elements involved in the coupling term of the effective Hamiltonian via the continuum are calculated explicitly. In such a case, the coupling to the continuum causes not only the non-Hermitian part of the effective Hamiltonian but gives also an additional contribution to the Hermitian part.[6] While systems with a large number of states as well as channels are described well by using statistical assumptions, for small systems that are coupled to very few channels, it is necessary to perform the calculations without any statistical assumptions. Only in the last case, the appearance of BICs can be studied thoroughly. As the numerical results obtained for laser induced continuum structures in atoms[9] and for transmission zeros in quantum dots[10] show, the interplay between the Hermitian and the non-Hermitian parts of the effective Hamiltonian plays an important role for the question of whether or not BICs appear at small coupling strength between the system and the environment and may therefore be relevant to studies on realistic systems. These studies showed furthermore, that the conditions for the appearance of BICs and for states with almost vanishing decay width may be fulfilled in a broad parameter range and even for systems that are not fully symmetrical. These properties make the BICs interesting for experimental studies.

Recently, the existence of infinitely narrow resonances has been reported for the transmission through different specific systems.[10–16] We will show in the following that the phenomenon of infinitely narrow resonances appearing in the transmission is universal and occurs in single quantum billiards (QBs) by varying their shape continuously. We will study the existence of BICs in small open two-dimensional QBs that are coupled to a small number of channels. In a hard wall approximation the billiards are described by the Helmholtz equation $-\nabla^2\psi(x,y)=\epsilon\psi(x,y)$ with Dirichlet boundary conditions. Here $\epsilon=2md^2E/\hbar^2$ is the dimensionless energy related to the particle energy E and the width d of the leads. Below the well-defined threshold π^2 for the propagating states in the leads the energy eigenvalues are discrete and the corresponding eigenfunctions are square-integrable bound states. Above the threshold the eigenvalues are distributed continuously and the corresponding eigenfunctions are normalized via the delta function in energy. We show that square-integrable solutions of the Schrödinger equation with isolated discrete energy above the continuum threshold might appear for a sequence of shapes of QBs. These solutions are BICs having an infinitely long lifetime.

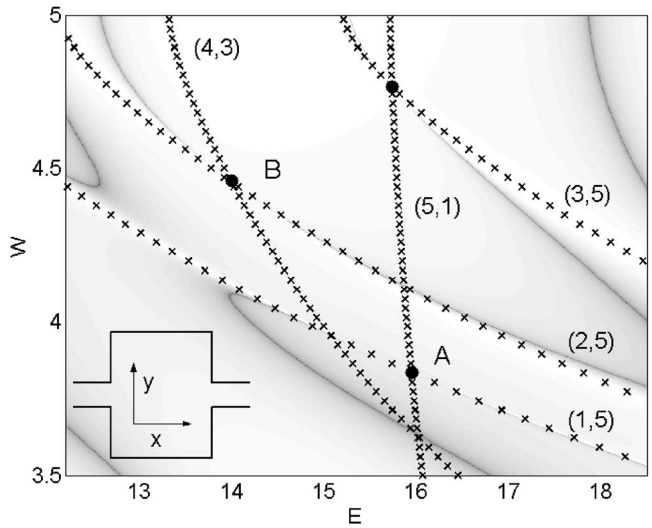

FIG. 1. The log scale probability for the transmission through the rectangular billiard shown in the inset, versus energy E and width W of the billiard (in terms of the width of the lead). The dark areas correspond to low transmission probability. The length of the QB along the x axis is four. The eigenenergies of the closed billiard are marked by crosses. The positions of the BICs are shown by bold circles. The patterns of the two BICs A and B are shown in Fig. 3.

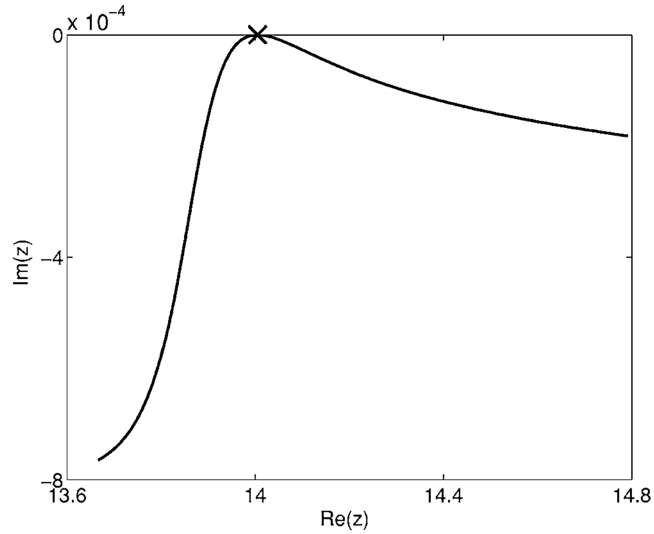

FIG. 2. The evolution of resonance width Im(z) and position Re(z) of one of the two resonance states in the vicinity of the BIC B in Fig. 1 for W=[4.3,4.6]. Im(z) vanishes at W=4.45 (marked by a cross). The widths of the other resonance states are much larger and are not shown here.

II. NUMERICAL RESULTS

We performed the numerical study for a QB of rectangular shape with a variable width W (see the inset in Fig. 1). In order to vary the width of the QB we apply an auxiliary potential (Ref. 17)

$$V(y) = V_0\{1 + 0.5[\tanh(C(y - W/2)) - \tanh(C(y + W/2))]\} \tag{1}$$

with V_0=100, C=17. The system is coupled to two continua represented by left and right single-channel leads that are attached to the QB as shown in the inset of Fig. 1. The eigenvalues and eigenstates of the closed rectangular QB are specified by the two quantum numbers (m,n). Further, the eigenstates have a definite parity relative to the x and y axes. Since only the even eigenstates relative to the y axis participate in the first-channel transmission, we have shown in Fig. 1 the eigenenergies of those states which are even relative to $y \to -y$ $(n=1,3,5,\ldots)$. We solve the problem of particle transmission through the billiard with incident particles from the left lead numerically using the tight-binding lattice model[18,22] for sufficiently large grids.

In order to find the positions and widths of the resonance states, we explore the non-Hermitian effective Hamiltonian, which can be obtained by projection of the function space of the whole system onto the Hilbert space of the closed system.[6,7,20,22] The effective Hamiltonian is energy dependent and can be written, on the basis of the closed billiard's eigenvectors, as follows (Refs. 18 and 22):

$$\langle b|H_{\text{eff}}|b'\rangle = E_b\delta_{bb'} - \sum_{C=L,R} V_b(C)V_{b'}(C)e^{ik_C}. \tag{2}$$

Here E_b and $|b\rangle$ are the eigenvalues and eigenfunctions of the closed $2d$ ring with the quantum numbers b, and C enumerates the left and right leads. Both leads have the same wave number $k_C = \sqrt{\pi^2 - E}$ for the first channel transmission where E is the energy of the incident particle. A recipe to calculate the matrix elements $V_b(C)$ for the billiard's case is given in.[20,22] For the particular case of the rectangular billiard the matrix elements are calculated below. The positions and widths of the resonance states are defined by the following nonlinear fixed-point equations (Ref. 6)

$$E_\lambda = \text{Re}(z_\lambda(\gamma, E_\lambda)), \quad 2\Gamma_\lambda = -\text{Im}(z_\lambda(\gamma, E_\lambda)). \tag{3}$$

Here z_λ are the complex eigenvalues of the effective Hamiltonian (2), $H_{\text{eff}}|\lambda) = z_\lambda|\lambda)$, with the right eigenstates $|\lambda)$.

In Fig. 1 we present the transmission probability in logarithm scale in order to show clearly the transmission zeros. They appear between the energies of the eigenstates with the same parity relative to the transmission axis, as shown by Lee.[19] The most interesting features appear at the points at which the degenerated states of the closed QB touch the transmission zeros (three such points are marked by bold circles in Fig. 1). At such a point, the width of the narrower resonance state vanishes for a certain value of W as shown in Fig. 2. Approaching this point, the scattering wave function (solution of the Schrödinger equation $H\psi = E\psi$ in the whole function space) diverges in the interior of the billiard. A similar behavior of the scattering wave function has been observed in a system consisting of two double dots that are connected by a wire of variable length[14] and in the scattering by cage potentials.[16] The divergence of the scattering wave function in the interior of the QB shows that the probability to find a quantum particle in the interior of the QB becomes prevailing. In fact, the incident quantum particle is localized inside the QB at the BIC's point with a corresponding square-integrable wave function as two examples show in Fig. 3.

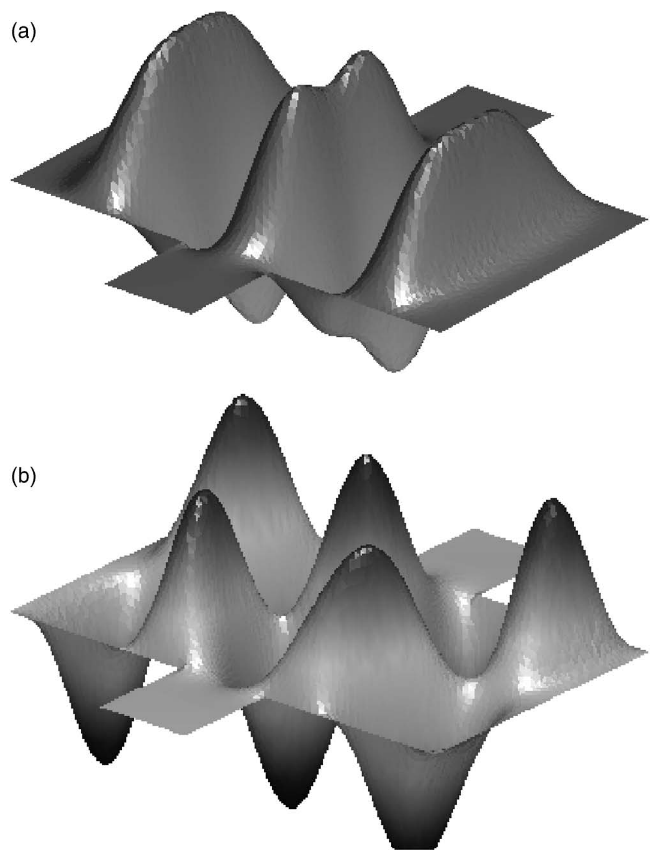

FIG. 3. The patterns of the two BICs A and B marked in Fig. 1 by bold circles.

Although the BICs are mostly localized inside the QB, exponentially small tails remain in the leads. They originate from evanescent modes. The numerical study shows that the magnitude of the tails is of the order of magnitude 10^{-3}. Without evanescent modes in the leads, the BIC would be localized completely in the interior of the QB. As can be seen further from Fig. 1, the BIC A consists mainly of the two QB eigenstates (1,5) and (5,1). The moduli of the superposition coefficients are 0.991 and 0.131. The BIC B consists of the states (4,3) and (2,5) with the superposition coefficients 0.374 and 0.927, respectively. The contributions of the other eigenstates of the QB with eigenenergies above π^2 are of the order of magnitude of 10^{-5}. The wave functions of the BICs are orthogonal to all bound states lying below π^2.

Figure 4 shows the transmission probability through the same rectangular billiard but weakly connected to the leads via diaphragms. They make the closed billiard nonintegrable. Correspondingly, the eigenstates of the billiard repel each other in energy provided that they have the same parity relative to the y axis being perpendicular to the transport axis. In this case, BICs appear at those places at which the lines of the resonant transmission (which almost coincide with eigenenergies of the closed QB in the vicinity of BICs) touch the transmission zeros (shown by bold circles in Fig. 4).

III. TWO-STATE APPROXIMATION

BICs in an open billiard can be considererd analytically if we truncate the effective Hamiltonian $H_{\mathrm{eff}}=E_b\delta_{bb'}-i\pi VV^{+}$

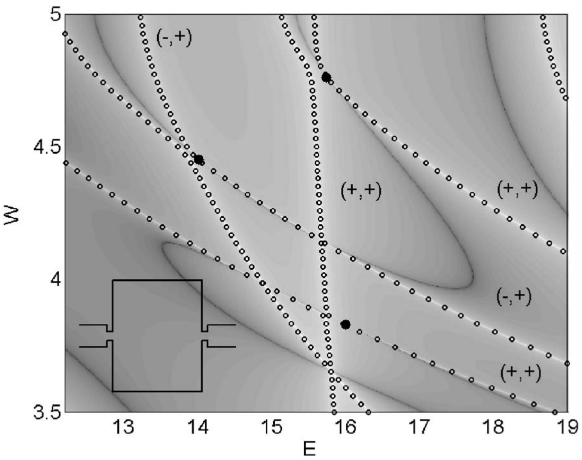

FIG. 4. The same as in Fig. 1 but the QB is weakly connected to the leads by diaphragms. Due to the diaphragms the billiard becomes nonintegrable. As a result the eigenenergies of the closed QB slightly repel each other. They are marked by a line of small open circles, and the parity relative to the y axis is indicated by a plus or minus.

where the matrix V of rank $N\times K$ describes the coupling of the N-state quantum billiard to the K channels of the leads. For the single-channel transmission, $K=L,R$ enumerates only the left and right leads. Then the coupling matrix elements of the left/right lead with the rectangular billiard are (Refs. 20–22)

$$V_{mn}(L,R) = \pm \left.\frac{\partial\psi_m}{\partial x}\right|_{x_L,x_R} \int_{-d/2}^{d/2} dy\,\phi(y)\psi_n(y), \qquad (4)$$

where $x_L,\ x_R$ are the positions of the boundaries at which the leads are connected to the billiard with the eigenfunctions $\psi_m(x)\psi_n(y)$ and sizes $L_x,\ L_y$. The transverse solution in the straight leads is $\phi(y)$. According to Figs. 1 and 4, mainly two states of the billiard participate in the vicinity of a BIC. These are, e.g., at the point A the states ψ_1 with quantum numbers $m=1$, $n=5$, and ψ_2 with $m=5$, $n=1$. It is reasonable therefore to truncate the effective Hamiltonian to a 2×2 matrix, similar to the two-level approximation in closed quantum systems. For any pair of eigenfunctions of the rectangular billiard, which defines the BIC, the coupling matrix elements (4) are the same for both leads ($K=L,R$). We denote them by $V_1=\sqrt{\Gamma_1/2\pi}$, $V_2=\sqrt{\Gamma_2/2\pi}$. Then the truncated effective Hamiltonian takes the following form:

$$H_{\mathrm{eff}} = H_B - i\pi V^{+}V = \begin{pmatrix} \epsilon - i\Gamma_1 & u - i\sqrt{\Gamma_1\Gamma_2} \\ u - i\sqrt{\Gamma_1\Gamma_2} & -\epsilon - i\Gamma_2, \end{pmatrix}, \qquad (5)$$

where

$$V = \begin{pmatrix} V_1 & V_1 \\ V_2 & V_2 \end{pmatrix}. \qquad (6)$$

Such a model is explored in the description of different scattering phenomena.[6,11,20,23] One can see that rank of matrix $V^{+}V$ equals 1. Therefore, we can apply here the single-channel model (5) for our case of two continua. We choose the

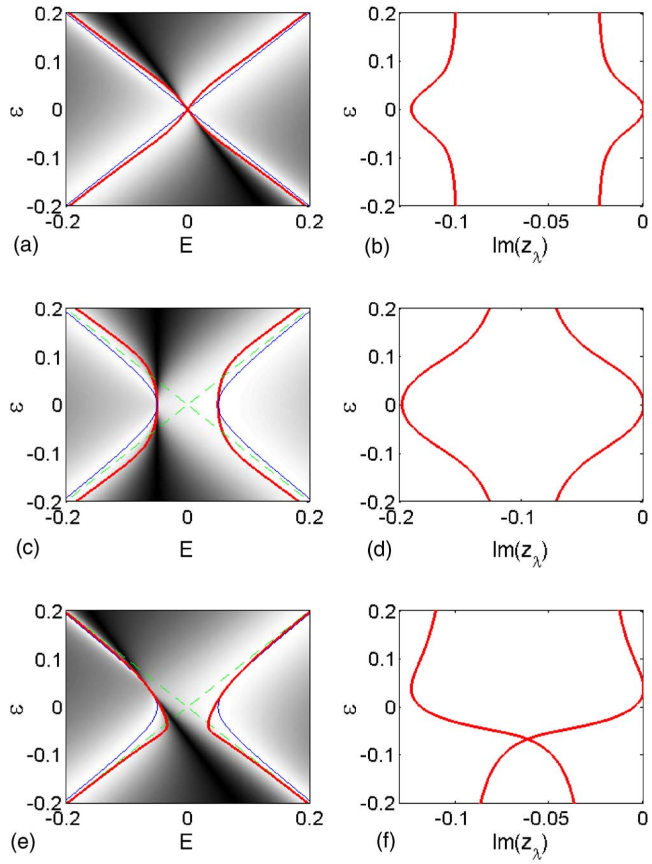

FIG. 5. (Color online) Left panel: The transmission probability $|T|$ through the two-state QB versus incident energy E and ϵ, and $\mathrm{Re}(z_\lambda)$ (solid lines). The dark areas correspond to low transmission probability. T and z_λ are defined by (7) and (8), respectively. The eigenenergies $\pm\epsilon$ of the QB are shown by thin solid lines. Right panel: the resonant widths $\mathrm{Im}(z_\lambda)$ as a function of ϵ (solid lines). (a) and (b) $u=0$, $\Gamma_1=0.1$, $\Gamma_2=0.05$. (c) and (d) $u=0.05$, $\Gamma_1=\Gamma_2=0.1$. (e) and (f) $u=0.05$, $\Gamma_1=0.1$, $\Gamma_2=0.05$.

levels as $\varepsilon_1=\epsilon$, $\varepsilon_2=-\epsilon$ (dashed lines in Fig. 5). The off-diagonal terms u in (5) transform the integrable closed QB into a nonintegrable one.

The transmission amplitude is (Ref. 23)

$$T=2\frac{E\Gamma+\epsilon\Delta\Gamma+u\sqrt{\Gamma_1\Gamma_2}}{(E-z_1)(E-z_2)}, \qquad (7)$$

where $z_{1,2}$ are the eigenvalues of the effective Hamiltonian (5)

$$z_{1,2}=-i\Gamma\pm R, \quad R^2=(\epsilon-i\Delta\Gamma)^2+(u-i\sqrt{\Gamma_1\Gamma_2})^2,$$

$$\Gamma=\frac{\Gamma_1+\Gamma_2}{2}, \quad \Delta\Gamma=\frac{\Gamma_1-\Gamma_2}{2}. \qquad (8)$$

With $\mathrm{Im}(z_\lambda)=0$ characteristic of a BIC, from (8) follows directly the condition $\Gamma=\mathrm{Im}(R)$ for its existence. The solution of this equation in general form was found by Volya and Zelevinsky:[23] $u=\sqrt{\Gamma_1\Gamma_2}\epsilon/\Delta\Gamma$. In particular, when $u=0$, then a BIC occurs for $\epsilon=0$ that corresponds to Fig. 1. When however, $\Gamma_1=\Gamma_2(\Delta\Gamma=0)$ but $u\neq 0$ then a BIC realizes under the same condition $\varepsilon=0$.

In the vicinity of the BIC's point $\epsilon=0$, $E=0$ for the particular case $u=0$, $\Delta\Gamma=0$ the eigenvalues of H_{eff} can be approximated as $z_1\approx -i\epsilon^2/2\Gamma$, $z_2\approx -2i\Gamma$. Correspondingly the transmission amplitude (7) takes the simple form

$$T(E,\epsilon)\approx -\frac{2iE\Gamma}{2E\Gamma+i\epsilon^2}. \qquad (9)$$

It follows $|T|=0$ for $E=0$, $\epsilon\neq 0$, and $|T|=1$ for $\epsilon=0$, $E\neq 0$. Therefore, the BIC is a singular point in the sense that the value of the transmission amplitude depends on the way to approach this point. If $\Delta\Gamma\neq 0$ the transmission zero follows $E=\epsilon\Delta\Gamma/\Gamma$.

The behavior of the transmission $|T(E,\epsilon)|$ is shown in Fig. 5 (left panel) and that of the resonance widths in Fig. 5 (right panel) for different cases. Figures 5(a), 5(c), and 5(e) completely reproduce fragments of the transmission probability shown in Figs. 1 and 4. According to Fig. 5(a), not only the eigenenergies of the closed integrable QB are crossing for $u=0$ but also the $\mathrm{Re}(z_\lambda)$ that define the positions of the resonant states of the open QB.

Next, we consider the scattering wave function ψ which is a solution of the Schrödinger equation in the total function space (involving leads and QB) (Refs. 6 and 22)

$$|\psi\rangle=|C,E\rangle+\sum_\lambda (1+G_C^{(+)}V)\frac{|\lambda)(\lambda|V|C,E\rangle}{E-z_\lambda}, \qquad (10)$$

where $|C,E\rangle$ are the states in the leads with $C=L,R$ (left and right), $G_C^{(+)}$ is the Green's function in the function space of the lead states. $H_{\mathrm{eff}}|\lambda)=z_\lambda|\lambda)$, $(\lambda|\lambda')=\delta_{\lambda\lambda}$, $(\lambda|=|\lambda)^T$. The left eigenstates are equal to

$$(1|=(\alpha\beta), \quad (2|=(-\beta\alpha)$$

$$\alpha=\frac{1}{A}(u-i\sqrt{\Gamma_1\Gamma_2}), \quad \beta=\frac{1}{A}(-\epsilon+i\Delta\Gamma+R),$$

$$A^2=(-\epsilon+i\Delta\Gamma+R)^2+(u-i\sqrt{\Gamma_1\Gamma_2})^2. \qquad (11)$$

Substituting (11) and (6) into $V_\lambda=\Sigma_m V_m\langle m|\lambda)$ and taking for simplicity $\Gamma_1=\Gamma_2$ we obtain

$$V_\lambda=(\lambda|V|C,E\rangle=\sqrt{\Gamma/\pi}(\alpha+\beta,\alpha-\beta). \qquad (12)$$

In the vicinity of the BIC's point $\epsilon=0$, $E=0$, the eigenstates (11) can, for $u=0$, $\Delta\Gamma=0$, be approximated as

$$\alpha\approx -\frac{1}{\sqrt{2}}\left(1+\frac{i\mu}{2}\right), \quad \beta\approx\frac{1}{\sqrt{2}}\left(1-\frac{i\mu}{2}\right), \qquad (13)$$

where $\mu=\epsilon/\Gamma$. Formulas (11)–(13) allow one to write the scattering wave function (10) in the vicinity of the BIC. It is of the order 1 inside the leads. In the interior of the QB it takes the following form:

$$\psi \approx \sqrt{\frac{\Gamma}{4\pi}}(a+b, \ -a+b), \tag{14}$$

where $a=\frac{i\mu}{E+i\Gamma\mu^2/2}$, $b=\frac{2}{E+2i\Gamma}$. Equation (14) shows that the scattering wave function diverges when approaching the BIC's point, meaning localization of the incident particle inside the QB.

IV. CONCLUDING REMARKS

A BIC arises at those points at which the line of resonant transmission crosses or touches the transmission zero. For integrable QBs (or for QBs close to integrable ones), the BICs are close to the points of degeneracy (or quasidegeneracy) of eigenenergies of the closed quantum system provided that the eigenenergies are in the continuous part of the spectrum and the interaction u is small. The model consideration shows the existence of BICs also at strong repulsion $u \sim 1$. In such a case, the position of the BIC may be rather far from that in the integrable QB as can be seen from Figs. 5(e) and 5(f). Nevertheless the BIC is related to the avoiding crossing of eigenstates of the closed nonintegrable QB also in this case. We conclude therefore that the existence of BICs does not depend on the type of the QB. Furthermore, according to formula (8), it does also not depend on the coupling strength to the continuum. However, the wave function and the energy of the BIC can depend on the propagating mode in the leads and on the manner the leads are attached to the QB. For example, if we attach the leads nonsymmetrically, one could find more BICs than in the symmetrical case considered here. Summarizing we state that the appearance of BICs is a general phenomenon in open QBs with continuously varying parameters such as energy and shape of the billiard.

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[1] J. von Neumann and E. Wigner, Phys. Z. **30**, 465 (1929).
[2] F. H. Stillinger and D. R. Herrick, Phys. Rev. A **11**, 446 (1975).
[3] L. S. Cederbaum, R. S. Friedman, V. M. Ryaboy, and N. Moiseyev, Phys. Rev. Lett. **90**, 013001 (2003).
[4] H. Friedrich and D. Wintgen, Phys. Rev. A **31**, 3964 (1985).
[5] H. Friedrich and D. Wintgen, Phys. Rev. A **32**, 3231 (1985).
[6] I. Rotter, Rep. Prog. Phys. **54**, 635 (1991); J. Okołowicz, M. Płoszajczak, and I. Rotter, Phys. Rep. **374**, 271 (2003).
[7] V. V. Sokolov and V. G. Zelevinsky, Ann. Phys. (N.Y.) **216**, 323 (1992).
[8] R. Berkovits, F. von Oppen, and J. W. Kantelhardt, Europhys. Lett. **68**, 699 (2004).
[9] A. I. Magunov, I. Rotter, and S. I. Strakhova, J. Phys. B **32**, 1669 (1999).
[10] I. Rotter and A. F. Sadreev, Phys. Rev. E **71**, 046204 (2005).
[11] T. V. Shahbazyan and M. E. Raikh, Phys. Rev. B **49**, 17 123 (1994).
[12] O. Olendski and L. Mikhailovska, Phys. Rev. B **66**, 035331 (2002).
[13] M. L. Ladron de Guevara, F. Claro, and P. A. Orellana, Phys. Rev. B **67**, 195335 (2003).
[14] A. F. Sadreev, E. N. Bulgakov, and I. Rotter, JETP Lett. **82**, 498 (2005).
[15] G. Ordonez, K. Na, and S. Kim, Phys. Rev. A **73**, 022113 (2006).
[16] K. D. Rowe and P. J. Siemens, J. Phys. A **38**, 9821 (2005).
[17] J. H. Davies, I. A. Larkin, and E. V. Sukhorukov, J. Appl. Phys. **77**, 4504 (1995).
[18] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, 1995).
[19] H.-W. Lee, Phys. Rev. Lett. **82**, 2358 (1999).
[20] F. M. Dittes, Phys. Rep. **339**, 215 (2000).
[21] K. Pichugin, H. Schanz, and P. Šeba, Phys. Rev. E **64**, 056227 (2002).
[22] A. F. Sadreev and I. Rotter, J. Phys. A **36**, 11413 (2003).
[23] A. Volya and V. Zelevinsky, Phys. Rev. C **67**, 054322 (2003).