Suppression of Feshbach Resonance Widths in Two-Dimensional Waveguides and Quantum Dots: A Lower Bound for the Number of Bound States in the Continuum

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The possibility of having bound states in the continuum was proposed by von Neumann and Wigner shortly after the birth of quantum mechanics. However, it is still considered a rare special phenomenon. Here we show how a lower bound to the number of bound states in the continuum can be calculated as a function of the open two-dimensional potential parameters of quantum dots and optical waveguides. The proof we present here holds for potentials that are symmetric in the perpendicular direction to the exits and entrances of the quantum dots or the waveguides.

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The possibility of having bound states in the continuum (BSCs) was proposed by von Neumann and Wigner shortly after the birth of quantum mechanics [1]. Bound states in the continuum have positive energies when the threshold energy for ionization or dissociation is set to be a zero reference energy. Because of the analogies between electronics and photonics [2,3], the reference threshold energy can be regarded as the index of refraction of the cladding in optical fibers or the asymptote of the effective index of refraction in waveguides [4]. The existence of bound states in the continuum has been regarded as a mathematical curiosity [5,6] for many years. About three decades ago (fifty years after the first indication that quantum mechanics permits the existence of bound states in continuum), Stillinger [7] and Herrick [8] proposed to use superlattices for constructing potentials which support bound states in the continuum. However, it was not until 1992 that Capasso and his co-workers from AT&T Bell Laboratories conducted an experiment where an electronic bound state embedded in the continuum was observed [9], in 2003 Cederbaum and his co-workers showed that conical intersections can induce bound molecular states embedded in the continuum [10], and in 2008 Marinica and his co-workers showed that bound states in the continuum in photonics should be feasible [11]. As has been pointed out in [11], the BSCs in superlattices, as used in the study of BSCs in electronics [9] and in photonics [11], result from the direct and via-the-continuum interaction between quasistationary (resonance) states [12–14] which gives birth to resonances with practically infinite lifetimes. However, it is known that it is possible to observe BSCs in much more simple two-dimensional (2D) structures. For example, Robnik showed a long time ago [15] that there are an infinite number of BSCs for a point particle in a plane region ($V = 0$) between two infinite parallel hard walls ($V = \infty$) and with a rectangular finite potential well ($V = -V_0$). These BSCs disappear with any infinite small perturbation that couples that two degrees of freedom and breaks the separability of the original Hamiltonian. More recently Sadreev, Bulgakov, and Rotter have shown that a rectangular billiard that is opened by attaching single-channel leads to it supports BSCs which may be observed by varying the shape of the quantum billiard [16]. The appearance of BSCs in two-dimensional potentials $V(x, y) = V(x, -y)$ where the leads to the quantum dot (QD) or waveguide (WG) are obtained for $x \to \pm\infty$ is clear. The exact solutions are either odd or even parity functions. Therefore, the Hamiltonian can be introduced as two-diagonal (i.e., uncoupled) block Hamiltonian matrices. The even y-parity eigenstates of the Hamiltonian are associated with the eigenvectors of one block Hamiltonian matrix, whereas the odd y-parity eigenstates are associated with the eigenvectors of the second block of the Hamiltonian matrix. It is clear that the ground bound state of the second block Hamiltonian matrix (associated with the odd parity solutions) has higher energy than the ground bound state of the y-even-parity eigenstate. However, it is not clear at all that the ground y-odd-parity bound state is embedded in the continuum of the first block Hamiltonian matrix which is associated with the y-even-parity solutions. Only numerical calculations can show if indeed a BSC has been obtained. Indeed numerical simulations [16] have shown that a single BSC or more exist for specific potential parameters of open rectangular potential. As a limiting case of the same case studied in [16] see Ref. [17]. The purpose of our Letter is to give two types of algorithms. One algorithm provides the condition that guarantees the bound y-odd-parity states are embedded in the continuum of the y-even-parity states. The second algorithm provides a lower bound to the number of bound y-odd-parity states which are embedded in the continuum of the y-even-parity states.

The type of two-dimensional potentials that might support BSCs and can be constructed by well established available fabrication is shown in Fig. 1. The theoretical question which we answer here is how one can construct

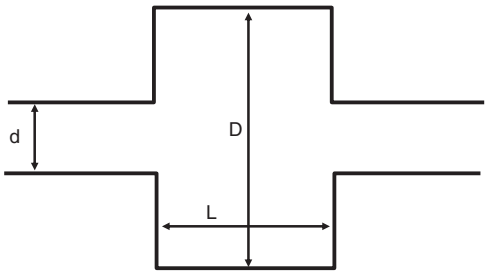

FIG. 1. A schematic diagram of the experimental setup for a two-dimensional QD, 0.4 μm wide and 0.5 μm long, which was produced at the Weizmann Institute of Science [18,19], and for a tunable microwave scattering device constructed of a rectangular cavity with leads attached symmetrically on opposite sides, which was produced at Philipps-University at Marburg (Fig. 1 in Ref. [20]). The entrances and exits to the 2D QD or WG are along the x axis, while y is perpendicular to x.

2D potentials that support at least N number of BSCs. The proof we give in this Letter is based on the use of adiabatic states of the 2D QD and WG potentials as a basis set in the construction of the exact nonadiabatic BSC solutions. This approach is very similar in its nature to the approach that has been taken by Cederbaum and his co-workers [10] where the Born-Oppenheimer states have been used as a basis set in order to prove that non-Born-Oppenheimer effects are responsible for the creation of molecular BSCs.

Figure 1 presents examples for 2D structures in a QD [18,19] and WG [20] that, respectively, can be constructed by using lithographic and planar silica over silicon technologies which have the symmetry structure which is required by our proof to support BSCs. As an example of a significant application of BSCs in optics we draw attention to the effort in fabrication semiconductor-based grating WG structures where the resonance spectral bandwidth is as low as possible, i.e., the resonance lifetime is as large as possible [21]. Such structures were placed inside a laser cavity and served as a back mirror to determine laser wavelength [21].

The exact 2D Hamiltonian for open systems in a basis set of the adiabatic states.—Mass weighted coordinates are used in order to emphasize the similarity between the solutions of the time-independent Schrödinger equation and the solutions of the scalar Maxwell equation (Helmholtz equation)

$$\hat{H} = -\partial_x^2 - \partial_y^2 + V(x, y), \tag{1}$$

where the entrance or exit channels are in the x direction and the potential is symmetric along the y and x directions, $V(x, y) = V(\pm x, -y)$. It is very important to mention that the threshold energies are the bound states of $V(|x| > L/2, y)$ (see the leads to the QD or WG in Fig. 1) since $V(x, y)$ is a separable potential in this region. This is a crucial point in our studies since inside the leads the adiabatic solutions are the exact solutions of Eq. (1). We will return to this point later. The exact eigenfunctions of the Hamiltonian which are given by

$$\hat{H}\Psi_j(x, y) = E_j\Psi_j(x, y); \qquad j = 0, 1, \ldots, \tag{2}$$

can be expanded in terms of the adiabatic states, $\varphi_n(y, x)$,

$$\Psi_j(x, y) = \sum_{n=0} \chi_{n,j}(x)\varphi_n(y, x). \tag{3}$$

The adiabatic states are obtained by ignoring the $-\partial_x^2$ term in $\hat{H}$ and by treating the x coordinate as a parameter,

$$[-\partial_y^2 + V(x, y)]\varphi_n(y, x) = \epsilon_n^{\mathrm{ad}}(x)\varphi_n(y, x), \tag{4}$$

where for any value of x the adiabatic states are orthonormal. Because of the symmetrical properties of the potential the eigenfunctions of the Hamiltonian $\hat{H}$ are either even or odd functions in y; i.e., $\Psi_j(x, y) = (-1)^j\Psi_j(x, -y)$. Similarly, the adiabatic functions are either even or odd parity functions $\varphi_n(y, x) = (-1)^n\varphi_n(-y, x)$; $n = 0, 1, \ldots$. Consequently, the Hamiltonian matrix which is constructed from the adiabatic functions that are served here as a basis set splits into two uncoupled block Hamiltonian matrices $\mathbf{H}^{(\mathrm{even})}$ and $\mathbf{H}^{(\mathrm{odd})}$.

Consequently, $\mathbf{H}$ is constructed from two-diagonal block Hamiltonian matrices as has been indicated above,

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}^{(\mathrm{even})} & 0 \\ 0 & \mathbf{H}^{(\mathrm{odd})} \end{pmatrix}, \tag{5}$$

where $[\mathbf{H}^{(\mathrm{even})}]_{i,j} = \langle\varphi_{n'=2i}|\hat{H}|\varphi_{n=2j}\rangle_y$ and $[\mathbf{H}^{(\mathrm{odd})}]_{i,j} = \langle\varphi_{n'=2i+1}|\hat{H}|\varphi_{n=2j+1}\rangle_y$ where $\{i, j\} = 0, 1, \ldots$.

Conditions for bound states in the continuum.—As discussed above [below Eq. (1)] the threshold energies are the adiabatic energies at the leads. In Fig. 1 the Hamiltonian becomes separable when $|x| > L/2$. For smooth 2D potentials (see the illustrative numerical example given below) the 2D becomes separable as $|x| \to \infty$. The lowest threshold energy in $\mathbf{H}^{(\mathrm{even})}$ is given by $E_0^{\mathrm{th-even}} = \lim_{|x|\to\infty}\epsilon_0^{\mathrm{ad}}(x)$, and therefore all eigenvalues with energies below $E_0^{\mathrm{th-even}}$ are bound states that are even functions in y. Similarly, the lowest threshold energy in $\mathbf{H}^{(\mathrm{odd})}$ is given by $E_1^{\mathrm{th-odd}} = \lim_{|x|\to\infty}\epsilon_1^{\mathrm{ad}}(x)$, and therefore all eigenvalues with energies below $E_1^{\mathrm{th-odd}}$ are bound states that are odd functions in y. The bound states of $\mathbf{H}^{(\mathrm{odd})}$ which have energies within the interval of

$$E_0^{\mathrm{th-even}} < E_j^{\mathrm{odd}} < E_1^{\mathrm{th-odd}} \tag{6}$$

are by definition BSCs of the exact Hamiltonian as defined by Eq. (1). Equation (6) implies that the BSCs are obtained provided that (1) E_j^{odd} are bound states (i.e., $E_j^{\mathrm{odd}} < E_1^{\mathrm{th-odd}}$) and (2) E_j^{odd} are embedded in the continuum of the lowest open channel for decay which is by definition $E_0^{\mathrm{th-even}}$.

Condition (1) is satisfied by the requirement that the jth eigenvalue of $h_1(x) = \langle\varphi_1|\hat{H}|\varphi_1\rangle_y$ are bound states. A

proof will be provided below that if $\langle\varphi_1|\hat{H}|\varphi_1\rangle$ has N bound states, then the exact $\mathbf{H}^{(\mathrm{odd})}$ Hamiltonian matrix has at least N bound states.

Condition (2) is satisfied by the requirement that the lowest eigenvalue of the adiabatic Hamiltonian,

$$h_1^{\mathrm{ad}}(x) = -\partial_x^2 + \epsilon_1^{\mathrm{ad}}(x), \tag{7}$$

is larger than the lowest threshold energy $E_0^{\mathrm{th-even}}$. This condition is based on Epstein proof from 1966 that the ground state of a 2D system in the adiabatic approximation is a lower bound to the exact ground-state energy of the system ($E_0^{(\mathrm{odd})}$ in our case) [22].

A proof that if $\langle\varphi_1|\hat{H}|\varphi_1\rangle_y$ has N bound states the exact $\mathbf{H}^{(\mathrm{odd})}$ Hamiltonian matrix has at least N bound states as well.—The Hamiltonian matrix, $\mathbf{H}^{(\mathrm{odd})}$, which is associated with the y-odd parity eigenfunctions of the exact Hamiltonian given in Eq. (1), can be written as

$$\mathbf{H}^{(\mathrm{odd})} = \begin{pmatrix} h_1 & \mathbf{v} \\ \mathbf{v}^\dagger & \mathbf{h}_2 \end{pmatrix}, \tag{8}$$

where the modified adiabatic Hamiltonian $h_1(x)$ is given by $h_1(x) = \langle\varphi_1|\hat{H}|\varphi_1\rangle_y = h_1^{\mathrm{ad}}(x) + V_1^{\mathrm{NA}}(x)$ where the nonadiabatic potential term is given by $V_1^{\mathrm{NA}}(x) = -\int_{+\infty}^{+\infty} dy \varphi_1^*(y,x)\partial_x^2\varphi_1(y,x)$. Similarly the matrix elements of $\mathbf{h}_2$ are given by $[\mathbf{h}_2]_{l',l}(x) = \delta_{l',l}\langle\varphi_{2l+1}|\hat{H}|\varphi_{2l+1}\rangle_y\{l',l\} = 1,2,3,\ldots$. The elements of the coupling off diagonal row vector $\mathbf{v}$ are given by $[\mathbf{v}]_l(x) = \langle\varphi_1|\hat{H}|\varphi_{2l+1}\rangle_y = -\langle\varphi_1|\partial_x^2|\varphi_{2l+1}\rangle_y - 2\langle\varphi_1|\partial_x|\varphi_{2l+1}\rangle_y\partial_x$. The eigenvalues of $\mathbf{H}^{(\mathrm{odd})}$, E_j [eigenvalues of the exact Hamiltonian given in Eq. (1) which are associated with y-odd parity eigenfunctions] are the eigenvalues of an effective Hamiltonian,

$$[h_1 + \mathbf{v}^\dagger\hat{G}(E_j)\mathbf{v}]\chi_{1,j} = E_j\chi_{1,j}, \tag{9}$$

where the Green operator is defined as $\hat{G}(E_j) = \lim_{\eta\to 0^+}[E_j\mathbf{I} - \mathbf{h}_2 + i\eta]^{-1}$.

Equation (9) can be iteratively solved. The zeroth iteration solution is obtained when in Eq. (9) the second term which contains the Green operator is ignored, such that $h_1(x)\chi_{1,j}^{(0)}(x) = E_j^{(0)}\chi_{1,j}^{(0)}(x)$ where $E_j^{(0)}$ is a bound state which is embedded below the threshold energy $E_1^{\mathrm{th-odd}}$ and by varying the potential parameters we guarantee that it is embedded above the threshold energy $E_0^{\mathrm{th-even}}$. The first iteration solution is obtained by solving the following eigenvalue problem: $[h_1 + \mathbf{v}^\dagger\hat{G}(E_j^{(0)})\mathbf{v}]\chi_{1,j}^{(1)} = E_j^{(1)}\chi_{1,j}^{(1)}$. Under the condition that all eigenvalues of $\mathbf{h}_2$ are larger than the bound states $E_j^{(0)}$, then $[\mathbf{v}^\dagger\hat{G}(E_j^{(0)})\mathbf{v}]$ is an attractive potential operator (one can verify it by calculating the trace of this operator while using the spectral representation of the Green operator), and therefore $E_j^{(1)} < E_j^{(0)}$. This inequality holds for any step of the iteration procedure. Therefore, the iterative converged result provides the exact jth eigenvalue E_j which is lower than the jth bound state of the modified adiabatic Hamiltonian $\hat{h}_1$. This proof can be generalized by applying the Hylleraas-Undheim-MacDonald theorem [23] which proves that the eigenvalues obtained from linearly variational calculations are upper bounds to the same symmetry exact bound-state eigenvalues. The variational calculations are carried out by using the adiabatic eigenfunctions $\varphi_n(y,x)\chi_{n,j}(x)$ as basis functions. $\{\varphi_n(y,x)\}$ are defined in Eq. (4), whereas $\chi_{n,j}(x)$ are eigenfunctions of $\langle\varphi_n|\hat{H}|\varphi_n\rangle_y$. The above results show that by varying the potential parameters one can always get bound states in the continuum for potentials that are symmetric to an inverse operation of an axis which is perpendicular to the directional axis of the entrances and exits to the QDs or WGs. The number of bound states in the continuum depends on the shape of the y-symmetric 2D potential. The number of the bound states in the continuum can be controlled by varying the potential parameters since while the threshold energies depend only on the width of the leads (see Fig. 1) and are unaffected by the variation of the size of the 2D QD or WG, the number of the adiabatic bound states which are localized inside the QD or WG is varied with the variation of the QD or WG parameters. For the proof that a symmetric 1D potential well has always at least one bound state, see, for example, Ref. [24]. It might happen, however, that the nonadiabatic potential term introduces potential barriers such that the lower bound to the number of BSCs is zero. It should be emphasized here that the conditions that guarantee that there are bound states embedded in the continuum (BSCs) and the lower bound to the number of BSCs can be calculated not only for 2D potentials but also for 3D problems. The conditions derived here are applicable not only to the cases where the potentials have closed form analytical expressions (see, for example, the numerical case studied in Ref. [16]) but also for nonanalytical piecewise potentials as is shown, for example, in Fig. 1 (see also Ref. [16]). For the application of the adiabatic approximation to piecewise 2D potentials as presented in Fig. 1 and for the calculations of the nonadiabatic correction terms, see Ref. [25].

Illustrative numerical example.—For the sake of simplicity we will demonstrate here the use of the conditions that guarantee BSCs and the calculations of the lower bound of the number of the BSCs for a simple 2D problem $-0.5(\partial_x^2 + \partial_y^2) + V(x,y)$ where the analytical potential is equal to zero, $V(x,y) = 0$, when $-L(x)/2 < y < +L(x)/2$ and $V(x,y) = \infty$ elsewhere [i.e., $|y| \geq +L(x)/2$]. We have chosen

$$L(x) = (d/2)^{1/2}/[1 - d/(2\pi^2\cosh^2 x)]^{1/2}, \tag{10}$$

where $d^{1/2}$ is the width of the leads (see, for example, Fig. 1). This expression for $L(x)$ has been chosen to have a solvable adiabatic Hamiltonian,

$$\hat{H}^{\mathrm{ad}}_{n_y} = -0.5\partial_x^2 - 0.5n_y^2/\cosh^2 x + (n_y\pi)^2/d. \quad (11)$$

The adiabatic bound states' energies are as for the Rosen-Morse potential [26], $E^{\mathrm{ad}}_{n_y,n_x} = (n_y\pi)^2/d - [2n_x - 1 - (1 + 4n_y^2)^{1/2}]^2$ where $n_x = 1, 2, \ldots, N_b$ and $n_y = 1, 2, \ldots$. The number of BSCs are obtained for $n_y = 2$, and it is the maximal value of N_b for which $2N_b - 1 - \sqrt{17} > 0$ provided that $E^{\mathrm{ad}}_{n_y=2,n_x} > \pi^2/d$. It is important to emphasize that only the number of bound states of

$$\hat{H}^{\mathrm{ad}}_{n_y=2} + \hat{V}^{\mathrm{NA}} + (2\pi)^2/d \quad (12)$$

where the nonadiabatic potential term $V^{\mathrm{NA}}(x)$ is included provides a lower bound to the number of BSCs (provided they are larger than π^2/d, the threshold of the uncoupled even y-symmetry channel). The nonadiabatic potential term is defined as

$$V^{\mathrm{NA}}(x) = -0.5\int_0^{L(x)} dy\,\varphi^{\mathrm{ad}}_{n_y}(y,x)\partial_x^2\varphi^{\mathrm{ad}}_{n_y}(y,x), \quad (13)$$

where $\varphi^{\mathrm{ad}}_{n_y}(y,x) = [2/L(x)]^{1/2}\sin[n_y\pi/L(x)]$. In our illustrative numerical example, $V^{\mathrm{NA}}(x) = [d^2\sinh^2 x(3 + 4n_y^2\pi^2)]/[24\cosh^2 x(4\pi^2\cosh^4 x - 4d\pi^2\cosh^2 x + d^2)]$. Our calculations show that for $d = 12$ the lower bound to the number of BSCs is two but for $d = 12.4$ it is one, although the number of adiabatic bound states is still two. For $d = 14.9$ our calculations show that the lower bound to the number of bound states is equal to zero in spite of the fact that on the basis of simple (''trivial'') parity arguments one may expect to have at least one BSC. In reality, due to external uncontrolled perturbations the bound states in the continuum are turned to be metastable (resonance) states with a finite lifetime [27]. By adding nonuniform potential inside the WG or QD (e.g., by using a gate bias for electrons or by adding some nonuniform dielectric material for light), the symmetry of the 2D potentials is deformed in such a way that one can control the widths of the BSCs. The ability to control the finite width (inverse lifetime) of a resonance state enables the construction of a device with an almost complete transmission of electrons through QDs or an almost complete transmission of waves through an open WG. Also by using suitable potential parameters one is able to construct devices that have a complete reflection of the electrons from a 2D QD or a complete reflection of waves from a 2D WG. The fact that the width of a selected resonance state can be reduced almost to zero (an almost bound state in the continuum is produced) opens a door for the construction of diodes and optical switches that operate with a very narrow band width, or reflectors or mirrors for a selected frequency electromagnetic radiation.

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