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Bound states in the continuum in open Aharonov-Bohm rings

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Using formalism of effective Hamiltonian we consider bound states in continuum (BIC). They are those eigen states of non-hermitian effective Hamiltonian which have real eigen values. It is shown that BICs are orthogonal to open channels of the leads, i.e. disconnected from the continuum. As a result BICs can be superposed to transport solution with arbitrary coefficient and exist in propagation band. The one-dimensional Aharonov-Bohm rings that are opened by attaching single-channel leads to them allow exact consideration of BICs. BICs occur at discrete values of energy and magnetic flux however it's realization strongly depend on a way to the BIC's point.

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I. Introduction. In 1929, von Neumann and Wigner [1] firstly pointed to the existence of discrete solutions of the single-particle Schrödinger equation embedded in the continuum of positive energy states. Their analysis has been examined by Stillinger and Herrick [2] in the context of possible bound states (BICs) in atoms and molecules. It has been demonstrated by Newton [3] that strong coupling between scattering channels can give rise to BIC. BIC can be observed in the stationary transmission as resonant states with width which tends to zero as at least two physical parameters vary continuously as it was formulated by Friedrich and Wintgen [4], who have also given the example of the hydrogen atom in a magnetic field. Such a BIC is a very fragile structure. A small perturbation transforms it into narrow resonance. Nevertheless, Capasso et al. [5] have reported direct evidence for BIC's in a semiconductor superlattice.

For better understanding of the phenomenon of BIC's in transport through electronic devices it is useful to study as simple quantum system as possible. Robnik [6] has shown that a simple separable two-dimensional Hamiltonian can develop BIC under perturbation of open channels. An explicit proof of an existence of BIC's was presented recently by Cederbaum et al. [7] in the molecular system, if the electronic and the nuclear motions are coupled. In the present letter we consider the open Aharonov-Bohm (AB) rings which are good candidates to observe BICs for the external magnetic field and energy of incident electron can be easily varied experimentally. Moreover the one-dimensional AB rings allow to treat BICs wholly analytically. A phenomenon of zero resonance widths at discrete values of energy of incident particle and some relevant physical parameter was established in many works since the work by Shahbazyan and Raikh [8 – 16], among of them external magnetic flux was considered in [17, 18]. In this letter we focus on the scattering wave function in the vicinity and at BIC's point and how BIC participated in transport.

II. The one-dimensional ring. Following Xia [19] we write the wave functions in the segments of the structure shown in inset of Fig.1 as

$$\begin{aligned} \psi_1(x) &= \exp(ikx) + r\exp(-ikx), \\ \psi_2(x) &= a_1\exp(ik^-x) + a_2\exp(-ik^+x), \\ \psi_3(x) &= b_1\exp(ik^+x) + b_2\exp(-ik^-x), \\ \psi_4(x) &= t\exp(ikx), \end{aligned} \tag{1}$$

where $k^- = k-\gamma$, $k^+ = k+\gamma$, $\gamma = 2\pi\Phi/\Phi_0$, $\Phi = B\pi R^2$ is the magnetic flux, $\Phi_0 = 2\pi\hbar c/e$. The ring length $2\pi R$ is chosen as unit. The boundary conditions (the continuity of the wave functions and the conservation of the current density) allow to find all coefficients in (1). We write the corresponding equation in matrix form

$$\hat{F}\psi = \mathbf{g}, \tag{2}$$

where $\hat{F}(k,\gamma)$ is the following matrix

$$\begin{pmatrix} -1 & 0 & 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 1 \\ 0 & -1 & e^{ik^-/2} & e^{-ik^+/2} & 0 & 0 \\ 0 & -1 & 0 & 0 & e^{ik^+/2} & e^{-ik^-/2} \\ 1 & 0 & \frac{k^-}{k} & -\frac{k^+}{k} & \frac{k^+}{k} & -\frac{k^-}{k} \\ 0 & -1 & \frac{k^-}{k}e^{i\frac{k^-}{2}} & -\frac{k^+}{k}e^{-i\frac{k^+}{2}} & \frac{k^+}{k}e^{i\frac{k^+}{2}} & -\frac{k^-}{k}e^{-i\frac{k^-}{2}} \end{pmatrix}, \tag{3}$$

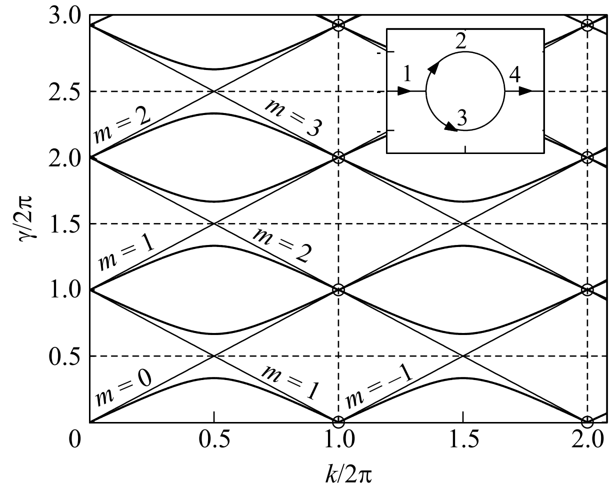

Fig.1. Transmission zeros $|t|^2 = 0$ and ones $|t|^2 = 1$ of the one-dimensional ring as function of the wave number k and flux γ. The zeros (ones) are shown by dashed (solid) lines. The thin solid lines represent the eigenenergies of the closed ring

$\mathbf{g}^T = (1\ 1\ 0\ 0\ 1\ 0)$. The vector $\boldsymbol{\psi}^T = (r\ t\ a_1\ a_2\ b_1\ b_2)$ is the solution for the scattering wave function:

$$\begin{aligned} r &= 2(3\cos k - 4\cos\gamma + 1)/Z, \\ t &= 16i(\sin\tfrac{k}{2}\cos\tfrac{\gamma}{2})/Z, \\ a_1 &= 2(2e^{i\gamma} - 3e^{-ik} + 1)/Z, \\ a_2 &= 2(e^{ik} + 1 - 2e^{i\gamma})/Z, \\ Z &= 8\cos\gamma - 9e^{-ik} - e^{ik} + 2, \end{aligned} \tag{4}$$

$b_{1,2}(k,\gamma) = a_{1,2}(k,-\gamma)$. In Fig.1 we show lines of the transmission zeros ($|t(k,\gamma)| = 0$, dashed lines) which cross the lines of the transmission ones ($|t(k,\gamma)| = 1$, solid lines) at points

$$\begin{aligned} k_m &= 2\pi m, m = \pm 1, \pm 2, \dots, \\ \gamma_n &= 2\pi n, n = 0, \pm 1, \pm 2, \dots . \end{aligned} \tag{5}$$

As can be seen from the expression for the denominator Z in Eqs. (1), the imaginary part of the poles vanishes at these points. Simultaneously at these points, there is a degeneracy of eigenenergies of closed ring $(k_m - \gamma)^2$. Here m is the magnetic quantum number that defines the eigen functions of the closed ring $\psi_m(x) = \exp(ik_m x)$. The point $k = 0$ is excluded from the consideration since it gives zero conductance. The peculiar points (5) were shown in [17] for the case of single lead attached to the 1d ring. To show that the bound states in continuum (BICs) appear at the points (5), let us consider one of the points, say, $\mathbf{s}_0 = (k_1, \gamma_1) = 2\pi(1,\ 1)$. All the other points are equivalent because of the periodical dependence of the system on k and γ. In the vicinity of the point $\mathbf{s}_0$ we write Eqs. (1) in the following approximated form

$$\begin{aligned} t &\approx \frac{\Delta k}{\Delta k + i(\Delta\gamma)^2/2},\ r \approx \frac{i(3\Delta k^2 - 4\Delta\gamma^2)}{4(2\Delta k + i\Delta\gamma^2)}, \\ a_1 &\approx \frac{3\Delta k + 2\Delta\gamma}{4\Delta k + 2i\Delta\gamma^2},\ a_2 \approx \frac{\Delta k - 2\Delta\gamma}{4\Delta k + 2i\Delta\gamma^2}, \end{aligned} \tag{6}$$

where $\Delta k = k - k_1,\ \Delta\gamma = \gamma - \gamma_1$. The transmission amplitude in the vicinity of the point $\mathbf{s}_0$ in (6) is similar to the expressions obtained for a shifted von Neumann-Wigner potential [20]. One can see that all amplitudes $a_{1,2},\ b_{1,2}$ of the inner wave functions are singular at the point $\mathbf{s}_0$. Such a result for the BIC points was firstly found by Pursey and Weber [20].

Eqs. (2) and (3) allow to show that the point $\mathbf{s}_0$ corresponds to the BIC one in an open one-dimensional ring. At this point the matrix (3) takes the following form

$$\hat{F}(\mathbf{s}_0) = \begin{pmatrix} -1 & 0 & 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 1 & 1 \\ 0 & -1 & 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & -2 & 2 & 0 \\ 0 & -1 & 0 & -2 & 2 & 0 \end{pmatrix}. \tag{7}$$

The determinant of the matrix $\hat{F}(\mathbf{s}_0)$ equals zero. Therefore, $\hat{F}\mathbf{f}_0 = 0$. By direct substitution of the vector $\mathbf{f}_0^T = \frac{1}{2}(0\ 0\ 1\ -1\ -1\ 1)$ one can verify that $\mathbf{f}_0$ is the right eigenvector which is the null vector. The corresponding left null eigenvector is $\tilde{\mathbf{f}}_0 = \frac{1}{2}(-1\ 1\ 1\ \ -1\ 0\ 0)$. It is well known from linear algebra, that if the determinant of matrix $\hat{F}$ is equaled to zero, then the necessary and sufficient condition for existence of solution of the equation (2) is that the vector $\tilde{\mathbf{f}}_0$ is orthogonal to vector $\mathbf{g}$ [21]. In holds, indeed, $\tilde{\mathbf{f}}_0 \cdot \overrightarrow{g} = 0$. The solution of Eq. (2) at the point $\mathbf{s}_0$ can therefore be presented as

$$\boldsymbol{\psi}(\mathbf{s}_0) = \alpha\mathbf{f}_0 + \boldsymbol{\psi}_p, \tag{8}$$

where α is an *arbitrary* coefficient and $\boldsymbol{\psi}_p$ is particular transport solution of Eq. (2). By direct substitution one can verify that $\boldsymbol{\psi}_p^T = \left(0\ 1\ \frac{3}{4}\ \frac{1}{4}\ \frac{3}{4}\ \frac{1}{4}\right)$ is the particular solution of Eq. (2). It is worthwhile to note that this result completely agrees with the scattering theory on graphs [22, 23]. Texier [22] has shown that for certain graphs the stationary scattering state gives the solution of the Schrödinger equation for the continuum spectrum apart for discrete set of energies where some additional states are localized in the graph and thus are not probing by scattering, leading to the failure of the state counting method from the scattering.

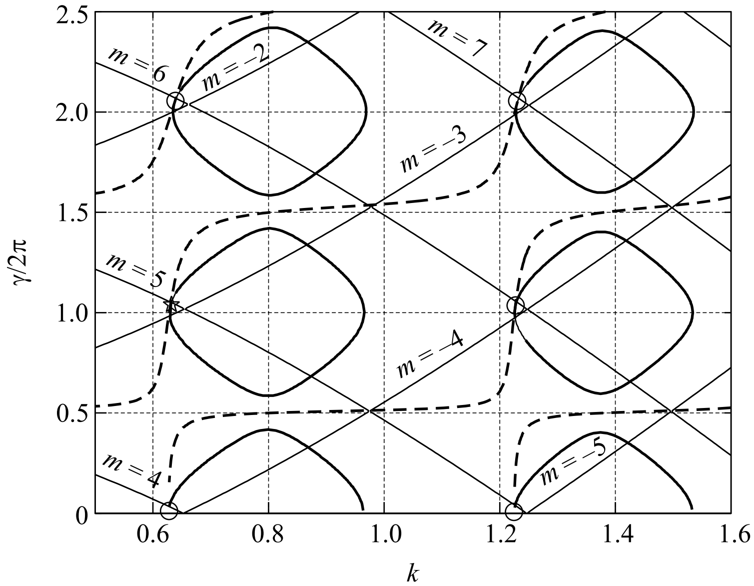

Fig.2. Zeros (dashed lines) and ones (solid lines) of the transmission probability of the two-dimensional ring as function of wave number $k = \sqrt{E - \pi^2}$ and flux $\gamma = B\pi R^2/\Phi_0$, $\Phi_0 = 2\pi\hbar c/e$. $R = 2.5$ is mean radius of the ring. The width of the ring and those of the leads are equaled to unit. The eigenenergies of the closed two-dimensional ring are shown by thin lines. The BIC points are marked by open circles and star

In the vicinity of the BIC point $\mathbf{s}_0$ the scattering state using (6) becomes, to leading order of Δk, $\Delta\gamma$,

$$\boldsymbol{\psi}(\mathbf{s}) \approx \frac{\Delta\gamma \mathbf{f}_0 + \Delta k \boldsymbol{\psi}_p}{\Delta k + i\Delta\gamma^2/2}, \tag{9}$$

where $\mathbf{s} = (k, \gamma)$. Thus, the scattering state in the nearest vicinity of the BIC point also is superposed of the BIC vector $\mathbf{f}_0$ and of the particular solution $\boldsymbol{\psi}_p$. Eq. (9) shows that the limiting scattering wave state $\boldsymbol{\psi}$ depends on a way $\mathbf{s} \to \mathbf{s}_0$. If we at first take $\Delta\gamma = 0$, then obtain $\boldsymbol{\psi} = \boldsymbol{\psi}_p$ which is a transport solution. If we, however, choose at first $\Delta k = 0$, then have $\boldsymbol{\psi} = \frac{2}{i\Delta\gamma}\mathbf{f}_0$, i.e. the scattering state is diverging interior the ring. This formula shows that the BIC state $\mathbf{f}_0$ can be extracted from the scattering state by a special limit in (9).

III. Two-dimensional devices. Typical open two-dimensional structures are dots or rings with attached leads. Numerically the transmission through them are solving by finite-difference equations which are equivalent to the tight-binding lattice model [24, 25]. The case of the quantum dots was considered in [16]. Here we present results of computation for the two-dimensional ring with symmetrically attached identical leads. In Fig.2 we show the transmission zeros (dashed lines) and the transmission ones (solid lines) for the single-channel transmission.

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 whole system onto Hilbert space of closed system [25–27]. The effective Hamiltonian in the basis of closed system's eigenvectors can be written as [24, 25]

$$\langle b|H_{\text{eff}}|b'\rangle = E_b\delta_{bb'} - \sum_p \sum_{C=L,R} V^C_{b,p}V^C_{b',p}e^{ik^C_p}. \tag{10}$$

Here E_b and $|b\rangle$ are the eigenvalues and the eigenfunctions of closed system are given by quantum numbers b, C enumerates left and right leads and p does the open channels of leads. A recipe to calculate the matrix elements $V^C_{b,p}$ is given in [26, 25]. Because of energy dependence of the effective Hamiltonian the positions and widths of the resonance states are defined by the following nonlinear fixed point equations [27]

$$E_\lambda = \mathrm{Re}(z_\lambda(\gamma, E_\lambda)), \quad 2\Gamma_\lambda = -\mathrm{Im}(z_\lambda(\gamma, E_\lambda)). \tag{11}$$

Here z_λ are the complex eigenvalues of the effective Hamiltonian (10) $H_{\text{eff}}|\lambda) = z_\lambda|\lambda)$ with right eigenstates $|\lambda)$. All the points at which $\Gamma_\lambda = 0$, i.e. the width of the resonant transmission vanishes are marked in Fig.2 by open circles and star.

The equation for the scattering wave function mapped interior the ring $|\psi_R\rangle$ can be derived from the Lippmann-Schwinger equation [25–27] and takes the following form

$$(H_{\text{eff}} - E)|\psi_R\rangle = V^L|E, L, p = 1\rangle. \tag{12}$$

Here V^L is the coupling matrix between the left lead and the ring provided that a particle incidents from the

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Fig.3. The BIC function $|\psi_{\lambda_0}|$ which is the eigen function of the effective Hamiltonian (10) (a) and the transport solution $|\psi_p|$ (b) at BIC point marked in Fig.2 by star

left lead in the first channel. This formula is similar to (2) for the 1d ring. If $\mathrm{Det}(H_{\mathrm{eff}} - E) \neq 0$, then in the biorthogonal basis $|\lambda)$ the scattering wave function takes a simple form [25, 27]

$$|\psi_R\rangle = \sum_{\lambda} \frac{V_\lambda(\gamma, E)}{E - z_\lambda(\gamma, E)} |\lambda), \tag{13}$$

where

$$V_\lambda = (\lambda|V|E, L, p = 1\rangle = \int dy_B \widetilde{\psi}_\lambda(y_B) \sin(\pi y_B), \tag{14}$$

$\widetilde{\psi}_\lambda$ are the left eigen functions of H_{eff}, y_B runs over the boundary that connects the closed ring and the left lead with the first channel excited ($p = 1$). We assume that magnetic field subjects only the ring.

Let us denote a set of physical parameters of the system as $\mathbf{s}$. For example, for present case of the ring $\mathbf{s} = (E, \gamma)$, although for the quantum dot $\mathbf{s}$ might be energy and confined potential [16]. Let us consider the point $\mathbf{s}_0 = (E_0, \gamma_0)$ at which Eq. (11) is fulfilled $E_0 = z_{\lambda_0}(E_0, \gamma_0)$ and $\Gamma_{\lambda_0} = 0$, i.e. one of the complex eigenvalues of H_{eff} is real at this point. For $E = E_0$ one have equality $(H_{\mathrm{eff}} - E)|\lambda_0) = 0$. Comparing this equation to (12) we see that the eigen state $|\lambda_0)$ corresponds to the solution of the Lippmann-Schwinger equation if there were no ingoing current in the left lead. Respectively, the state $|\lambda_0)$ can not give rise to outgoing currents because of the continuity equation for the current density. In order to fulfill that we have to consider that the eigen function ψ_{λ_0} does not overlap with the first channel of the left lead, i.e. $V_{\lambda_0}^L(\mathbf{s}_0) = 0$. This may be also established by consideration of the transmission amplitude [25]

$$t = -2\pi i \sum_{\lambda} \frac{\langle E, L|V^L|\lambda)(\lambda|V^R|E, R\rangle}{E - z_\lambda}. \tag{15}$$

Because of symmetry of the system relative to the left and right leads $|V_{\lambda_0}^L| = |V_{\lambda_0}^R|$. In approaching the point $\mathbf{s} \to \mathbf{s}_0$ the denominator $E - z_{\lambda_0}(\mathbf{s}) \to 0$. Therefore, in order the ratio $|V_{\lambda_0}^L(\mathbf{s})|^2/(E - z_{\lambda_0}(\mathbf{s}))$ remained finite in (15) it is necessary $|V_{\lambda_0}^L(\mathbf{s})| \to 0$ for $\mathbf{s} \to \mathbf{s}_0$. Thus, at the BIC point we have orthogonality of the righthand state $(V|E, L, p = 1\rangle)$ in Eq. (12) to the left eigen state $(\lambda_0|$. Then, in full correspondence to the consideration of the 1d ring (Eq. (8)), we have the following solution for the scattering state interior the ring

$$|\psi_R(\mathbf{s}_0)\rangle = \alpha|\lambda_0(\mathbf{s}_0)) + |\psi_p(\mathbf{s}_0)\rangle, \tag{16}$$

where coefficient α is arbitrary. Right eigen function $\psi_{\lambda_0(\mathbf{s}_0)}$ of the effective Hamiltonian is squared integrable and therefore is the BIC function shown in Fig.a. Although the BIC function is disconnected from the first channel of the left lead, it couples with the next channels $p > 1$ of the leads which are evanescent modes. As a result the BIC function has exponentially small tails in the leads as might be seen from Fig.3a. Moreover the coupling of the 2d ring with the evanescent modes gives rise to that as Fig.2 shows the BIC points are close to but different from points at which two eigen functions of closed 2d ring classified by magnetic quantum numbers m have the same energy. The evanescent modes have imaginary wave numbers k_p which change effectively the Hamiltonian of closed ring by matrix

$$\sum_{p \neq 1} \sum_{C = L, R} V_{b,p}^C V_{b',p}^C e^{-|k_p|} \sim (d/R)^2$$

via Eq. (10). Therefore only for limiting case of the 1d ring $d/R \to 0$ the BIC state will consists of a pair of eigen states of closed ring as seen from Fig.1 and as was confirmed by computations.

In the vicinity of $\mathbf{s}_0$ a value $E - z_{\lambda_0}(E, \gamma)$ is small. Then we can split the summation over λ in (13) by two parts, $\lambda = \lambda_0$ and $\lambda \neq \lambda_0$ and similar to (8) write the scattering state as

$$|\psi_R(\mathbf{s})\rangle = \alpha(\mathbf{s})|\lambda_0(\mathbf{s})) + |\psi_p(\mathbf{s})\rangle, \quad (17)$$

where

$$\alpha(\mathbf{s}) = \frac{V_{\lambda_0}(\mathbf{s})}{E - z_{\lambda_0}(\mathbf{s})}, \quad (18)$$

and $|\psi_p\rangle$ is contribution of all other resonances.

As different from the 1d ring, we can study behavior of singular coefficient (18) only numerically. Let us encircle the BIC point $k_0 = \sqrt{E_0 - \pi^2}, \gamma_0$ as $\Delta k = r\cos\phi$, $\Delta\gamma = r\sin\phi$ as shown in Fig.4a where r is the radius of encircling. Angular behaviors of quantities defining the parameter α are shown in Fig.4b,c. In particular the numeric shows that $|V_0(\mathbf{s})| \sim |\mathbf{s} - \mathbf{s}_0|^{1/2}$. The behavior of α in Fig.4d is very similar to the behavior of the parameter $\alpha = \Delta\gamma/(\Delta k + i\Delta\gamma^2/2)$ for the 1d ring (see (9)) except that in the 2d ring we observe phase difference. As one can see from Fig.4d at $\phi = 0, \pi$ $(\Delta\gamma = 0)$ the parameter $\alpha = 0$, and at $\phi = \phi_0 < \pi/2$, $\alpha \to \infty$. The angle ϕ_0 exactly corresponds to the direction of tangential line of transmission zero shown by dashed line in Fig.2. Therefore in order to extract the $|\psi_p\rangle$ from the scattering wave function (13) we should put at first $\Delta\gamma = 0$ and then limit $\Delta k \to 0$. If take limit to the BIC point along $\Delta\gamma = tan(\phi_0)\Delta k$, the scattering state transforms to the BIC state $|\lambda_0)$ shown in Fig.3a. The particular solution for the scattering wave function $|\psi_p\rangle$ is shown in Fig.3b.

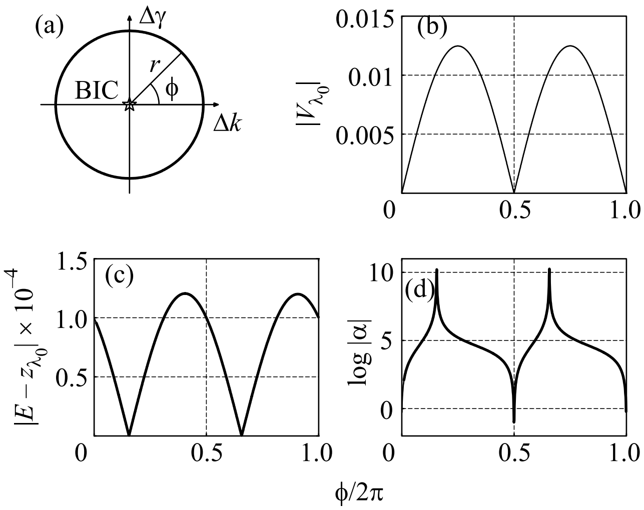

Fig.4. Angular behavior of quantities defining the parameter (18) around the BIC point marked by star in Fig.2

IV. Conclusion. Formulas (8) and (17) are the key ones which show that scattering wave function ψ is not unique since BIC can be superposed with arbitrary coefficient α to ψ. Such kind of decomposition was established recently for the scattering theory on graphs [22, 23]. Thus, at the point the $\mathbf{s}_0$, the system becomes degenerate. Usual transport solution with energy $E = E_0$ is complemented by the squared integrable (localized interior the ring) state $|\lambda_0(\mathbf{s}_0))$ with the same energy E_0 orthogonal to the former. The last state is therefore BIC. Our consideration shows exactly that BIC is the eigen vector of the non-hermitian effective Hamiltonian H_{eff} at those point at which the complex eigenvalue of H_{eff} becomes real and coincides with the energy of incident particle. The scattering matrix is unique but not analytical at the BIC points as could be seen from formula (6). As seen from there, the transmission zeros cross the transmission ones at the BIC point. Note that these results are not restricted by only AB rings but applicable for any open quantum system which allow to vary at least two physical relevant parameters, for example, energy of incident particles and shape of billiard [16].

BIC is disconnected from both single channel continua. In order to achieve that BIC is to be a such superposition of eigen states of closed system that overlapping (14) vanishes at BIC points. Specifically in the present case of the AB ring attached to the single channel leads this superposition becomes odd function relative to the even function of the leads as seen from Fig.3a. For the 1d ring nodes of BIC are to be at points of connection of the ring to leads, thereby at those points where the ratio of lengths of the arms is rational [22]. However for the 2d ring the leads are to be attached exactly symmetrically as shown in Fig.3. It follows then that a violation of symmetry of the system relative to transport axis x leads to breakdown of BIC. In particular it occurs for system disordered by impurities. In order BIC could survive under this violation of symmetry one can use geometry given in [28] in which infinite strip attached to the ring. Moreover impurities lift a degeneracy of closed ring [29]. However as shown in [16] a condition for BIC to survive is still remaining. From above it follows that for the system symmetrical relative the y-axis (axis perpendicular to the transport axis) all odd eigen states of closed system are BIC's provided that the leads are excited in the first even channel. Then a perturbation which lifts this symmetry transforms BIC's into resonance states widths of which are proportional to the perturbation. The external magnetic field which subjects only the ring is an example of such a perturbation.

The electron-electron interactions preserve degeneracy of closed ring [29]. They modify the energy spectrum and the coupling between leads and closed ring.

As shown in [13] variation of the coupling changes a position of BIC $\mathbf{s}_0$ however is not important to achieve real value of the complex eigen value of the effective Hamiltonian. However the Coulomb interactions might be important in respect that BIC's can exhibit discrete charging similar to that predicted for resonance trapping in quantum dots strongly connected to the leads [30]. The strong coupling of closed quantum system with leads ($|V^C_{b,p}| \gg |E_b - E_{b'}|$ in terms of (10)) is hardly achievable while an existence of BICs is free of a value of the coupling between the closed system and continua.

Processes of inelastic scattering give rise to finite resonance width. In that sense BIC is very subtle phenomenon for electron transmission. However as formulas (9) and (17) show, BIC state participates in the scattering wave function. If above mentioned processes are efficiently small BIC state can dominate in the vicinity of the BIC point for proper choice of physical parameters, energy and flux, as shown in Fig.4d.

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