Comment on "Bound-state eigenenergy outside and inside the continuum for unstable multilevel systems", Phys. Rev. A 72, 063405 (2005)

E.N. Bulgakov[1,2], I. Rotter[1] and A.F. Sadreev[1,2,3]
[1] *Max-Planck-Institute für Physik komplexer Systeme, D-01187 Dresden, Germany*
[2] *Kirensky Institute of Physics, 660036, Krasnoyarsk, Russia and*
[3] *Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden*
(Dated: November 17, 2006)

We solve the basic equations of the N-level Friedrichs model by using the Feshbach projection operator technique and consider the relation between bound states in the continuum (BICs) and form factors. We give an answer to some questions left open in [1]. At the energy of the BIC, the sum of the individual form factors vanishes. The wave function of the BIC is localized inside the system. References to early papers on BICs (not cited in [1]) are given.

PACS numbers: 03.65.Nk, 42.50.Vk, 42.50.Md, 73.23.-b

In [1], the properties of bound states below and in the continuum are studied for unstable multilevel systems in the framework of the N-level Friedrichs model. The question whether or not bound states in the continuum (BICs) exist in real quantum systems is of principal interest and might be as well of interest for applications. The reason for this interest arises from the fact that the system is stabilized around the energy of a BIC and that the wave function is localized inside the system in spite of embedding it into the continuum of extended wave functions. The aim of the present Comment is (i) to point at the early papers on this topic published 20 and more years ago and not cited in [1], and (ii) to show that by solving the basic equations of the Friedrichs model using the Feshbach projection operator (FPO) technique [2], a definite answer to the relation between form factors and BICs in multilevel systems can be obtained.

The existence of BICs is shown already in 1929 by von Neumann and Wigner [3] (see also [4] for some improvement and [5]). In 1985 Friedrich and Wintgen [6] considered the problem by using the FPO technique. They demonstrated that the occurence of BICs is a natural feature of the common physical situation of two interfering resonances. They related the existence of BICs to avoided level crossings being another quantum mechanical phenomenon discussed by von Neumann and Wigner [7] in 1929. Since BICs are states that do not decay, the population probability of these states is constant in time (*population trapping*). Numerical calculations for concrete systems are performed for atoms in a laser field [8]. Similar results are obtained [9] in the time independent approach by using the FPO technique. According to these results, population trapping in a certain level can equivalently be described by the vanishing decay width of this level, i.e. by the existence of a BIC. These studies showed explicitely the relation between BICs and the avoided level crossing phenomenon as well as the role played by the interplay between different types of interaction. A similar study is performed for the transmission through a quantum billiard. Here, an BIC appears at that energy at which the resonant transmission crosses a transmission zero [10–12]. In these papers, the scattering problem is solved rigorously in the vicinity of the BICs. For further references on BICs in quantum dots see the references in [10–12].

The FPO formalism solves the basic equations of the N-level Friedrichs model after dividing the total function space into two subspaces with $Q + P = 1$ where Q projects onto the subspace of discrete states and P onto the supplementary subspace of scattering states. The advantage of this method consists, above all, in the fact that the solutions in the two subspaces can be found by standard methods: by diagonalizing the corresponding Hamiltonian H_B in the subspace of N discrete states and by coupled channel calculations in the subspace of scattering states described by the Hamiltonian H_C. Another ingredient of the method are the operators V_{BC} and V_{CB} that describe the coupling between the two subspaces. They contain the coupling matrix elements between the *eigenfunctions of* H_B and the scattering wave functions ξ_C^E of the P subspace. The Schrödinger equation in the total function space is $(H - E)\Psi_C^E = 0$ with the Hermitian Hamilton operator $H = H_B + H_C + V_{BC} + V_{CB}$ (see for comparison Eqs. (1), (2) and (3) of [1]). The solution reads [13]

$$\Psi_C^E = \xi_C^E + \sum_k \Omega_k \frac{\langle \Phi_k^* | V | \xi_C^E \rangle}{E - z_k} \tag{1}$$

where

$$\Omega_k = \left[1 + V_{BC}(E - H_C)^{-1} V_{CB}\right] \Phi_k \tag{2}$$

is the wave function of the resonance state k, Φ_k are the (biorthogonal) eigenfunctions and z_k the (complex) eigenvalues of the non-Hermitian Hamilton operator

$$H_{\rm eff} = H_B + V_{BC} \frac{1}{E - H_C} V_{CB} \ . \tag{3}$$

In contrast to H_B, the operator $H_{\rm eff}$ contains explicitely the coupling of the *closed system* (Q subspace) to the environment of decay channels. $H_{\rm eff}$ describes therefore

the properties of the *open* system. Eq. (1) is an exact expression for the solution Ψ_C^E. The calculated cross section is independent of the definition of the two subspaces. A careful definition of the two subspaces is however necessary in order to provide meaningful results for the positions and decay widths of the resonance states [13].

In the framework of this formalism, the positions and decay widths of the resonance states follow from the eigenvalues $z_k = E_k - \frac{i}{2}\Gamma_k$ of the non-Hermitian Hamilton operator (3) by solving the corresponding fixed-point equations. A BIC is a resonance state with a jump of the scattering phase by π although its decay width vanishes, $\Gamma_{k_0} \to 0$ [10].

The relation between Γ_k and the coupling matrix elements is [13]

$$\Gamma_k = -2\,\mathrm{Im}(z_k) \le 2\pi \sum_C |\langle \Phi_k^* | V | \xi_C^E \rangle|^2 \qquad (4)$$

at all energies (C denotes the channels). The nonequality in (4) is caused by the biorthogonality of the functions Φ_k. As a consequence, a state being decoupled from all channels of the continuum of scattering states according to

$$\langle \xi_C^E | V | \Phi_{k_0} \rangle \to 0\,; \quad \langle \Phi_{k_0}^* | V | \xi_C^E \rangle \to 0 \qquad (5)$$

is a BIC with $\Gamma_{k_0} \equiv 2\,\mathrm{Im}(z_{k_0}) \to 0$. The opposite case follows by considering the S matrix

$$\begin{aligned} S_{CC'} &= e^{2i\delta_C}\delta_{CC'} - 2i\pi \langle \chi_{C'}^E | V | \xi_C^E \rangle \\ &\quad -2i\pi \sum_{k=1}^{N} \frac{\langle \xi_{C'}^E | V | \Phi_k \rangle \langle \Phi_k^* | V | \xi_C^E \rangle}{E - z_k}\,. \end{aligned} \qquad (6)$$

At the position of a BIC, we have $E - z_{k_0} \to 0$ and, due to the unitarity of the S matrix, it follows (5). That means: the decoupling from all channels of the continuum described by (5) is a necessary and sufficient condition for a resonance state to be a BIC, i.e. a state with vanishing decay width $\Gamma_{k_0} = 0$. Hence the wave function of a BIC is, according to (2), eigenfunction of $H_{\rm eff}$ and, consequently, localized. This result is independently of the strength of the coupling between the two subsystems. Analytical studies and numerical examples are given for the transmission through quantum billiards [10–12].

In contrast to the coupling matrix elements (5), the form factors $\langle \xi_C^E | V | \Phi_{k_0}^B \rangle$ and $\langle \Phi_{k_0}^B | V | \xi_C^E \rangle$ considered in [1] contain the eigenfunctions Φ_k^B of the Hamiltonian H_B of the closed system. Since the eigenfunctions Φ_k of $H_{\rm eff}$ can be represented as $\Phi_k = \sum a_{k,k'} \Phi_{k'}^B$ with complex coefficients $a_{k,k'}$, a sum of individual form factors vanishes at the position of a BIC according to (5),

$$\sum_{k'} a_{k_0,k'} \langle \xi_C^E | V | \Phi_{k'}^B \rangle \to 0\,; \;\; \sum_{k'} a_{k_0,k'}^* \langle \Phi_{k'}^B | V | \xi_C^E \rangle \to 0\,. \qquad (7)$$

Only if, in a particular case, all $a_{k_0,k' \ne k_0}$ are (almost) zero, the sum in (7) reduces to one term. In such a case it holds, as a rule, $E_{k_0} \approx E_{k_0}^B$ (here $E_{k_0}^B$ is eigenvalue of H_B and E_{k_0} is the real part of the corresponding eigenvalue of $H_{\rm eff}$). The "multilevel effect" allows a presence of a BIC without zeros of the individual form factors due to the interferences involved in (7). Generally, the position E_{k_0} of the BIC differs from the position E_k^B of any eigenstate of H_B, i.e. it is "misplaced" (although a BIC is a bound state). This result is true in all coupling regimes.

Thus, by using the FPO technique in solving the basic equations of the Friedrichs model it is possible to receive a definite answer to the question left open in [1]. Multilevel effects are contained in the non-diagonal matrix elements of the non-Hermitian coupling term $V_{BC}(E - H_C)^{-1} V_{CB}$ in the Hamilton operator $H_{\rm eff}$, Eq. (3), and can be studied easily. Invaluable for applications is the possibility to study the stabilization of the system not only at the single point of the BIC but also in its neighborhood (where $\Gamma_\lambda \gtrsim 0$) when the FPO technique is used, see e.g. [9, 10].

Acknowledgments: We thank the MPIPKS for hospitality. This work has been supported by RFBR Grant No. 05-02-97713 "Enisey".

[1] M. Miyamoto, Phys. Rev. A **72**, 063405 (2005).
[2] H. Feshbach, Ann. Phys. (NY) **5**, 357 (1958) and **19**, 287 (1962).
[3] J. von Neumann and E. Wigner, Phys. Z. **30**, 465 (1929).
[4] F.H. Stillinger and D.R. Herrick, Phys. Rev. A **11**, 446 (1975).
[5] L. Fonda and R.G. Newton, Ann. Phys. (N.Y.) **10**, 490 (1960); R.G. Newton, *Scattering Theory of Waves and Particles*, Springer, Berlin, 1982.
[6] H. Friedrich and D. Wintgen, Phys. Rev. A **31**, 3964 (1985) and **32**, 3231 (1985); H. Friedrich, *Theoretical Atomic Physics*, Springer, Berlin Heidelberg, 1990.
[7] J. von Neumann and E. Wigner, Phys. Z. **30**, 467 (1929).
[8] P.L. Knight, M.A. Lauder and B.J. Dalton, Phys. Rep. **190**, 1 (1990); N.J. Kylstra and C.J. Joachain, Phys. Rev. A **57**, 412 (1998).
[9] A.I. Magunov, I. Rotter, and S.I. Strakhova, J. Phys. B **32**, 1669 (1999) and **34**, 29 (2001).
[10] I. Rotter and A.F. Sadreev, Phys. Rev. E **71**, 046204 (2005).
[11] A.F. Sadreev, E.N. Bulgakov, and I. Rotter, J. Phys. A **38**, 10647 (2005); JETP Letters **82**, 498 (2005); Phys. Rev. B **73**, 235342 (2006).
[12] E.N. Bulgakov, K.N. Pichugin, A.F. Sadreev, and I. Rotter, JETP Letters **84**, 430 (2006).
[13] I. Rotter, Rep. Prog. Phys. **54**, 635 (1991), J. Okolowicz, M. Ploszajczak, and I. Rotter, Phys. Rep. **374**, 271 (2003).