Phase rigidity and avoided level crossings in the complex energy plane

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We consider the effective Hamiltonian of an open quantum system, its biorthogonal eigenfunctions ϕ_λ, and define the value $r_\lambda=(\phi_\lambda|\phi_\lambda)/\langle\phi_\lambda|\phi_\lambda\rangle$ that characterizes the phase rigidity of the eigenfunctions ϕ_λ. In the scenario with avoided level crossings, r_λ varies between 1 and 0 due to the mutual influence of neighboring resonances. The variation of r_λ is an internal property of an *open* quantum system. In the literature, the phase rigidity ρ of the scattering wave function Ψ_C^E is considered. Since Ψ_C^E can be represented in the interior of the system by the ϕ_λ, the phase rigidity ρ of the Ψ_C^E is related to the r_λ and therefore also to the mutual influence of neighboring resonances. As a consequence, the reduction of the phase rigidity ρ to values smaller than 1 should be considered, at least partly, as an internal property of an open quantum system in the overlapping regime. The relation to measurable values such as the transmission through a quantum dot, follows from the fact that the transmission is, in any case, resonant at energies that are determined by the real part of the eigenvalues of the effective Hamiltonian. We illustrate the relation between phase rigidity ρ and transmission numerically for small open cavities.

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I. INTRODUCTION

The advances in nanotechnology make it possible to produce small quantum dots with desired controllable properties. The analogy between such a system and an atom has proved to be quite close [1]. Since, however, no natural restrictions for choosing the control parameters exist, the quantum dots may show new properties that we cannot obtain from studies on atoms. For example, Fano resonances have been observed experimentally in quantum dots [2], and the Fano parameters may be complex [3]. Theoretically, the Fano parameter expresses the interference between the resonant part of the transmission and a smooth (direct) nonresonant part. It is real when the resonance part is caused by the existence of an isolated resonance state [4] as it is the case usually in atoms. When, however, the resonant part itself results from the interference of, e.g., two neighboring resonance states, the Fano parameter becomes complex [5]. The same may appear in a cavity due to the absorption at the walls [6].

Further, it has been stated [7] that the line shape of a Fano resonance may be affected by some dephasing [8] that may be caused by intrinsic sources (e.g., from electron-electron interactions) as well as by extrinsic sources (e.g., radiation, magnetic impurities) [9]. For a quantitative study, the phase rigidity [10,11]

$$\rho = \frac{\int dr\Psi(r)^2}{\int dr|\Psi(r)|^2} = e^{2i\theta}\frac{\int dr[|\mathrm{Re}\,\tilde{\Psi}(r)|^2 - |\mathrm{Im}\,\tilde{\Psi}(r)|^2]}{\int dr[|\mathrm{Re}\,\tilde{\Psi}(r)|^2 + |\mathrm{Im}\,\tilde{\Psi}(r)|^2]} \quad (1)$$

has been introduced that characterizes the degree to which the wave function Ψ is really complex (the phase θ arises from a transformation so that $\mathrm{Re}\,\tilde{\Psi}$ and $\mathrm{Im}\,\tilde{\Psi}$ are orthogonal). An experimental and theoretical study [6] showed that the two different mechanisms, dephasing and dissipation, are equivalent in terms of their effect onto the evolution of Fano resonance line shapes.

Another interesting observation in the experimental results on quantum dots [2,7] is that, as a function of the gate voltage that controls the transparencies of the point contacts, the widths of the observed resonances behave nonmonotonic. The conductance peaks start as narrow Breit-Wigner resonances when the quantum dot is pinched off, then widen as the contacts are opened into resonances exhibiting the Kondo effect. As the contacts are opened further, the resonances become more narrow and have the Fano form with some background conductance. A similar result is obtained in a study on a tunable microwave scattering device [12]. The explanation given in Ref. [7] is that diffraction at the contacts to the quantum dots is strongest at intermediate point contact transparencies, leading to large sticking probabilities.

The nonmonotonic increase of resonance widths as a function of the degree of opening the system, is however, a typical feature of open quantum systems [13]. It was found first in theoretical nuclear reaction studies by using the formalism of the effective non-Hermitian Hamiltonian H_{eff} [14], then in atoms [15] and in microwave cavities [16] where it is proven experimentally [6,12,17]. Also the transmission through a double quantum dot is studied as a function of the coupling strength between dot and attached leads [18]. In the theoretical studies, the nonmonotonic behavior of the resonance widths is caused by the width bifurcation that may appear at the avoided crossings of resonance states in the complex energy plane. Further studies of open quantum systems showed that the real and imaginary parts of the eigenfunctions of H_{eff} evolve more or less independently from one another in the avoided level crossing scenario [19] and that

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long-range correlations occur between the different states of the system [20].

The effective Hamiltonian used in the random matrix interpolation between the standard ensembles with real and complex matrix elements is $H(\alpha)=H_0+\alpha H_1$ where H_0 and H_1 are real and complex random Hermitian matrices, respectively, and α is a crossover parameter [21]. For such an ensemble, the eigenvector elements acquire correlations between the elements of the same eigenvector [10,22] and between different eigenvectors [23]. For individual systems, such a crossover may be observed already in a billiard with only two attached waveguides [24]. The wave functions in the crossover regime show long-range correlations [11] like the eigenvectors of the Hamiltonian $H(\alpha)$. These long-range correlations of the wave functions in the real-to-complex crossover have recently been measured in an open microwave billiard [25].

Thus the results obtained experimentally and theoretically for the profile of the transmission peaks, for the intensity fluctuations, and also for the long-range correlations of the wave functions point to the fact that the system through which the transmission occurs may be essentially different from the original closed quantum system without attached leads. The differences arise from the interaction of neighboring resonance states via the continuum of scattering states. In quantum dots, these differences can be traced experimentally by varying the gate voltage that controls the transparencies of the point contacts.

In the following, we will study the phases of the eigenfunctions of the effective Hamiltonian in the avoided level crossing scenario in detail. We will show that they are not fixed but vary due to the mutual influence of neighboring resonance states. In this spirit, a neighboring resonance state causes some "perturbation" for the considered state which is similar to that caused by an impurity. There is, however, an important difference between these two cases. In contrast to the perturbation by an impurity, the mutual interaction between neighboring states cannot be avoided. It is an internal property of an open quantum system in the regime of overlapping resonances.

In Sec. II, we repeat some general properties of the interplay between the internal and external interaction in an open quantum system. While the internal interaction is of standard type, the external interaction occurs additionally via the common continuum of scattering wave functions. The amplitude for the transmission through a quantum dot will also be given. It is resonant at energies that are determined by the real part of the eigenvalues of the effective Hamiltonian $H_{\rm eff}$ of the open quantum system. Then we define the phase rigidity r_λ of the eigenfunctions ϕ_λ of $H_{\rm eff}$. Further, we consider the scattering wave functions Ψ_C^E being solutions of $(H-E)\Psi_C^E=0$ in the total function space. In the interior of the system, the Ψ_C^E can be represented by the ϕ_λ and, as a consequence, the phase rigidity ρ of the scattering wave functions Ψ_C^E is related to that of the eigenfunctions ϕ_λ. In Sec. III, we provide numerical results for the relation between transmission and phase rigidity ρ of the scattering wave functions for three special cases. The results are summarized and some conclusions are drawn in the last section.

II. PHASE RIGIDITY OF THE EIGENFUNCTIONS AND OF THE SCATTERING WAVE FUNCTION IN AN OPEN QUANTUM SYSTEM

The relation between a closed and the corresponding open quantum system is as follows. A closed quantum system is described by a Hermitian Hamilton operator H_B the eigenvalues and eigenfunctions of which contain the interaction u of the discrete states (nondiagonal matrix elements of H_B; for details see [13]). The value u may be called *internal* interaction since H_B describes a closed system. For example, for a quantum system consisting of two (closed) subsystems, H_B reads [18,26]

$$H_B=\begin{pmatrix} h_1 & u \\ u & h_2 \end{pmatrix}, \tag{2}$$

where h_1 and h_2 are the Hamiltonians of the two subsystems that interact via the nondiagonal matrix elements u. When embedded into the common continuum of scattering states, the discrete eigenstates of the closed system (described by H_B) turn over into resonance states with a finite lifetime. The effective Hamiltonian $H_{\rm eff}$ of the open quantum system contains H_B as well as an additional term [13] that describes the coupling of the resonance states to the common environment,

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

Here V_{BC}, V_{CB} stand for the coupling matrix elements between the *eigenstates* of H_B and the environment that may consist of different continua C, e.g., the scattering waves propagating in the left $(C=L)$ and right $(C=R)$ leads attached to a quantum dot [27]. They are described by the Hamiltonian H_C. We use v as the abbreviation for the concrete nondiagonal matrix elements

$$v=\sum_C{}' V_{BC}(E^+-H_C)^{-1}V_{CB}. \tag{4}$$

The value v may be called an *external* interaction since it describes the interaction of two eigenstates of H_B via the continuum. $H_{\rm eff}$ is non-Hermitian, its eigenvalues z_λ and eigenfunctions ϕ_λ contain (additionally to u) the interaction v of the resonance states via the continuum. While u and $\mathrm{Re}(v)$ cause level repulsion in energy, $\mathrm{Im}(v)$ is responsible for the bifurcation of the widths of the resonance states.

As long as $|u/v|\gg 1$, the spectroscopic properties of the open system are similar to those of the corresponding closed system. The lifetimes (widths) of the resonance states are, as a rule, comparable in value, i.e., the states exist at the same time and can influence one another. Usually, the states avoid crossing in the complex energy plane in a similar manner as it is well-known from the avoided crossings of the discrete states of a closed system. When, however, $|u/v|\ll 1$, the resonance states do no longer exist at the same time due to their different lifetimes owing to widths bifurcation [13,19]. They do not cross therefore in the complex energy plane. Most interesting is the situation $|u|\approx|v|$. The interplay between u and v may cause unexpected and even counterintui-

tive results such as the nonmonotonic dependence of the resonance widths on the degree of opening the system [13,15–18].

Since the effective Hamiltonian H_{eff} depends explicitly on the energy E, so do its eigenvalues z_λ. The energy dependence is weak, as a rule, in an energy interval that is determined by the width of the resonance state. The solutions of the fixed-point equations $E_\lambda = \text{Re}(z_\lambda)_{|E=E_\lambda}$ and of $\Gamma_\lambda = -2\,\text{Im}(z_\lambda)_{|E=E_\lambda}$ are numbers that coincide approximately with the poles of the S matrix. The width Γ_λ determines the time scale characteristic of the resonance state λ. The amplitude for the transmission through a quantum dot is [27]

$$t = -2\pi i \sum_\lambda \langle \xi_L^E | V | \phi_\lambda \rangle \frac{(\phi_\lambda | V | \xi_R^E \rangle}{E - z_\lambda}, \tag{5}$$

where the scattering wave functions in the leads are denoted by ξ_C^E. According to Eq. (6), the transmission is *resonant* at the energies E_λ, i.e., at energies that are determined by the real part $\text{Re}(z_\lambda)$ of the eigenvalues z_λ of the effective Hamiltonian H_{eff}. In Eq. (5), the eigenvalues z_λ with their full energy dependence are involved.

The eigenfunctions ϕ_λ of H_{eff} are complex and biorthogonal,

$$(\phi_\lambda | \phi_{\lambda'}) \equiv \langle \phi_\lambda^* | \phi_{\lambda'} \rangle = \delta_{\lambda,\lambda'}, \tag{6}$$

$$\langle \phi_\lambda | \phi_\lambda \rangle \equiv A_\lambda \geqslant 1; \quad |\langle \phi_\lambda | \phi_{\lambda'} \rangle| \equiv B_\lambda^{\lambda'} \geqslant 0. \tag{7}$$

The value

$$r_\lambda = \frac{\int dr \phi_\lambda^2}{\int dr |\phi_\lambda|^2} = \frac{1}{A_\lambda} = \frac{\int dr [|\text{Re}\ \phi_\lambda(r)|^2 - |\text{Im}\ \phi_\lambda(r)|^2]}{\int dr [|\text{Re}\ \phi_\lambda(r)|^2 + |\text{Im}\ \phi_\lambda(r)|^2]} \tag{8}$$

is a measure for the biorthogonality of the eigenfunctions ϕ_λ of H_{eff} and for their phase rigidity, $0 \leqslant r_\lambda \leqslant 1$. Note that Re ϕ_λ and Im ϕ_λ are orthogonal to one another because of the biorthogonality relation (6). The value r_λ is large, $r_\lambda = 1$, for an isolated resonance state at the energy $E = E_\lambda$, where the transmission probability has a peak. In the regime of overlapping resonance states, however, where avoided level crossings appear [19], r_λ is usually small. Approaching a branch point in the complex energy plane where two eigenvalues z_λ and $z_{\lambda'}$ coalesce, we have [15,19,28] $A_{\lambda(\lambda')} \to \infty$ and $r_{\lambda(\lambda')} \to 0$, and further

$$|\phi_\lambda) \to \pm i |\phi_{\lambda' \neq \lambda}). \tag{9}$$

Here, the widths bifurcate: with further increasing v, one of the states aligns with a scattering state (channel wave function $\xi_{C=R}^E$ or $\xi_{C=L}^E$ in the one-channel transmission) and becomes short-lived while the other one becomes long-lived. For large v, we have therefore only one long-lived resonance state and, as for nonoverlapping resonance states, $r_\lambda \to 1$ at the energy $E = E_\lambda$ of the long-lived state.

The scattering wave function Ψ_C^E is the solution of the Schrödinger equation $(H - E)\Psi_C^E = 0$ in the total function space that consists of the discrete states of the quantum dot and of the scattering states ξ_C^E in the attached leads, $H \equiv H_B + H_C + H_{BC} + H_{CB} = H_B + H_C + V_{BC} + V_{CB}$. The Hamiltonian H is Hermitian. The solution reads [13]

$$\Psi_C^E(r) = \xi_C^E(r) + \sum_\lambda \Omega_\lambda^C(r) \frac{(\phi_\lambda | V | \xi_C^E \rangle}{E - z_\lambda}, \tag{10}$$

where $\Omega_\lambda^C(r) = [1 + (E^+ - H_C)^{-1} V]\phi_\lambda(r)$ is the wave function of the resonance state λ. According to Eq. (10), the eigenfunctions $\phi_\lambda(r)$ of the effective Hamiltonian H_{eff} give the main contribution to the scattering wave function $\Psi_C^E(r)$ in the interior of the cavity. Here,

$$\Psi_C^E(r) \to \sum_\lambda \phi_\lambda(r) \frac{(\phi_\lambda | V | \xi_C^E \rangle}{E - z_\lambda}. \tag{11}$$

According to the relation (11), the phase rigidity ρ of the scattering wave function, Eq. (1), is generally determined by the values of the phase rigidity r_λ of the individual resonance states λ. While r_λ characterizes the phase rigidity of the special resonance state λ, ρ contains the r_λ from the different states that contribute to the scattering wave function Ψ_C^E in the considered energy region. This difference between ρ and r_λ is illustrated best by the following example. Approaching a branch point in the complex energy plane, the contributions to Eq. (11) from the two states λ and λ' with the relation (9) of their wave functions to each other, (more or less) cancel each other. The phase rigidity ρ of the scattering wave function is determined therefore by the contributions of other states that, as a rule, are relatively far from one another. That means, in spite of $r_\lambda = r_{\lambda'} = 0$, $|\rho|$ might be large at the branch point.

We mention that the scattering wave function (11) has a similar structure as the transmission amplitude (5). Both expressions consist of a sum over overlapping resonance states with the weight factor $(\phi_\lambda | V | \xi_C^E \rangle / (E - z_\lambda)$. We expect therefore some correlation between both values. This relation, being trivial for isolated resonances, is of special interest in the regime of overlapping resonances. The transmission may be large not only at the positions $E = E_\lambda$ of the resonance states λ as in the case of isolated resonances. It may be enhanced in a larger energy region when $|\rho| < 1$, i.e., when some states λ are (partly) aligned with the scattering states ξ_C^E so that $r_\lambda < 1$ for them. In such a case, the matrix elements $\langle \xi_C^E | V | \phi_\lambda \rangle$ may be large not only at $E = E_\lambda$ but in a larger energy region. For illustration, we will provide in the following section some numerical results for $|t|$ and $|\rho|$ for two model quantum billiards with a small number of states the transmission through which is studied earlier, and for a realistic chaotic quantum billiard. The correlation between $|t|$ and $1 - |\rho|$ in the overlapping regime can clearly be seen in all cases.

III. NUMERICAL EXAMPLES

A. One-dimensional system

For illustration, let us first consider the relation between the degree of resonance overlapping and the phase rigidity in the transmission through a one-dimensional system. The de-

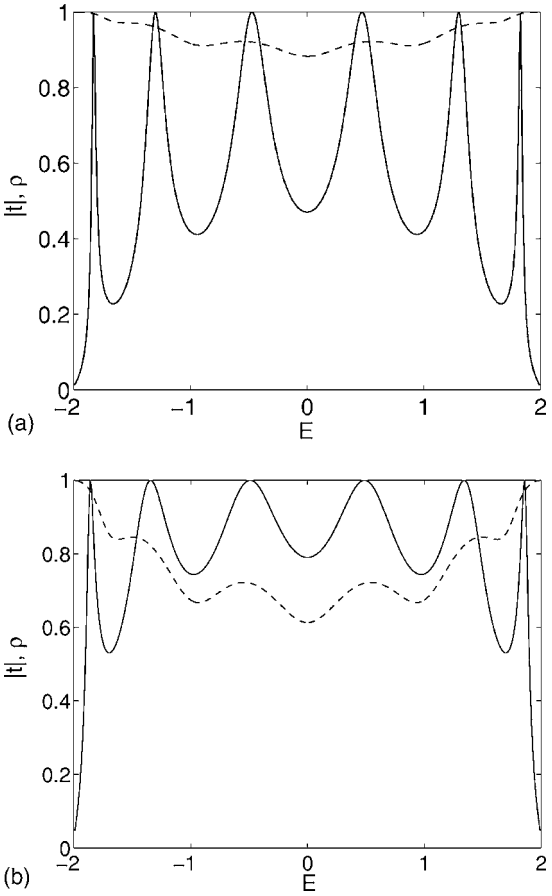

FIG. 1. The transmission $|t|$ (full lines) and phase rigidity $|\rho|$ (dashed lines) for a chain of six sites as a function of energy with $v=0.5$ (top) and $v=0.7$ (bottom). For the model see Ref. [27].

tails of the model are given in [27]. In Fig. 1, transmission $|t|$ and phase rigidity $|\rho|$ are shown as a function of energy for two different values of the external interaction v. The widths of the states in the middle $E=0$ of the spectrum are larger than those near to the thresholds $E=\pm 2$ as can be seen immediately from the profile of the transmission peaks. Therefore, also the degree of resonance overlapping increases towards the middle of the spectrum. The results show that the transmission increases with increasing overlapping of the resonances and, correspondingly, the phase rigidity decreases. The same result can be seen in comparing the two figures 1(a) and 1(b) which are calculated with different values of v. That means the transmission increases when one of the resonance states aligns with one scattering wave function that is expressed by the decrease of ρ.

B. Double quantum dot

Let us now consider a double quantum dot consisting of two identical single dots that are connected by an internal wire. Suppose both dots and the wire have one state each. For details of the model see [18]. In Fig. 2, the transmission $|t|$ and the landscape of the phase rigidity $|\rho|$ for such a double quantum dot are shown over energy E and coupling strength v. The internal interaction u is fixed in these calcu-

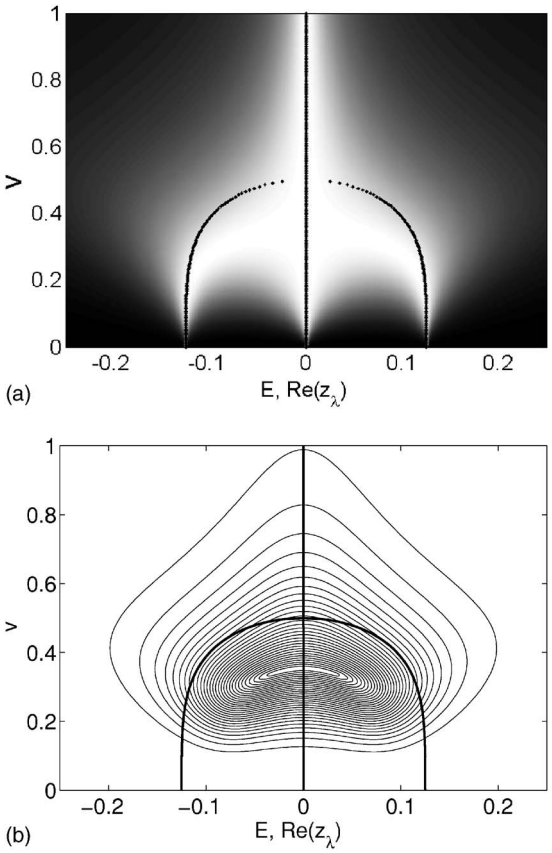

FIG. 2. The transmission $|t|$ (top) and the landscape of the phase rigidity $|\rho|$ (bottom, thin lines) for a double quantum dot over energy E and coupling strength v. The distance between the contour lines is $\Delta|\rho|=1/30$. The minimal value $\rho=0$ is surrounded by a high density of contour lines. The highest shown contour line corresponds to $|\rho|=1-1/30$. The $\mathrm{Re}(z_\lambda)$ of the three eigenstates (thick lines in both panels of the figure) are calculated at $E=0$. The branch point is at $v_c=1/2$, $E_c=0$. $u=\sqrt{2}/16$. Around $v=0.345$, the phase rigidity is minimal and the transmission maximal with a plateau $|t|=1$ (for the plateau compare Fig. 4 in Ref. [18]).

lations. At $v=v_c$, the eigenvalues z_λ and $z_{\lambda'}$ of the effective Hamiltonian coalesce and a branch point in the complex energy plane appears [18,19]. When $v<v_c$, the states repel each other in energy while widths bifurcation starts beyond the branch point where $v>v_c$. The smallest value of $|\rho|$ ($\rho=0$) is reached when the transmission is maximal with a plateau $|t|=1$ (for the plateau compare Fig. 4 in [18]). At $v=v_c$, $|\rho|$ is relatively large due to the fact that the contributions of the two states λ and λ' (almost) cancel each other. Beyond v_c, the phase rigidity increases slowly further up to its maximal value 1.

C. Sinai billiard

In Fig. 3, we show $|t|$ and $|\rho|$ calculated for a realistic chaotic system with many states and many avoided level crossings. The calculations are performed in the tight-binding lattice model, for details see [29]. The high correlation between the two values $|t|$ and $1-|\rho|$ can be seen also under these conditions. In some energy intervals, $|t|$ is near 1.

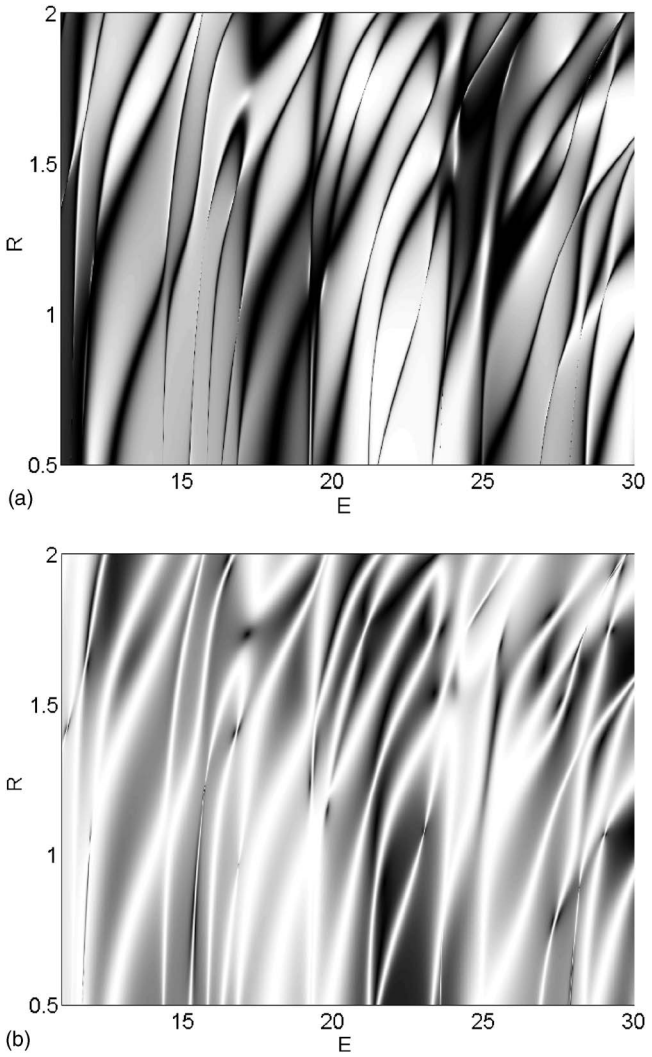

FIG. 3. The transmission $|t|$ (top) and phase rigidity $|\rho|$ (bottom) for a Sinai billiard over energy E and radius R of the circular disk (size of the billiard: $x=4$, $y=5$ in units of the width of the leads). The calculations are performed in the tight-binding lattice model [29].

Here $|\rho|$ is small, in agreement with the results shown in Fig. 2.

IV. CONCLUSIONS

From the results obtained, we conclude that $|\rho|<1$ characterizes the scenario of overlapping resonances in which the resonance states interact with one another and avoided (and true) crossings appear, generally. In this scenario, the system cannot be described by a Hermitian Hamilton operator that provides rigid phases of its eigenfunctions ($r_\lambda=1$). Rather, H_{eff} is non-Hermitian, its eigenfunctions are biorthogonal and r_λ varies with energy and coupling strength. Since the scattering wave function and the eigenfunctions of the effective Hamiltonian are related to one another according to Eq. (11), also ρ varies between 1 and 0 in the regime of overlapping resonances. That means, the reduction of the phase rigidity ρ of the scattering wave function is caused, at least partly, by the mutual perturbation of neighboring resonances. It is an internal property of an open quantum system in the overlapping regime and cannot be avoided.

The reduction of the phase rigidity ρ is, in the one-channel transmission, an expression for the (partial) alignment of two of the eigenfunctions $\phi_{\lambda,\lambda'}$ of the effective Hamiltonian H_{eff} with the two scattering wave functions $\xi^E_{C=R,L}$ in the overlapping regime. Due to this alignment (described by $r_{\lambda,\lambda'}<1$), the transmission through the system is enlarged in a certain energy region around the energies $E_{\lambda,\lambda'}$ of the two resonance states. As can be seen from Fig. 2 and the corresponding discussion in [18], the profile of the transmission is, when $\rho\approx 0$, completely different from that through two isolated resonance states. It is plateaulike. This result explains the correlation between $|t|$ and $1-|\rho|$ which can be seen in all our numerical studies (Figs. 1–3). Both values are, according to Eqs. (5) and (11), characterized by the contributions from a sum of overlapping resonance states.

Since the variation of r_λ and $|\rho|$ with energy follows from the interaction of the resonance states via the common continuum of scattering wave functions, it is related, generally, to the profile of Fano resonances. The relation is, however, unique only with respect to r_λ. For example, the mutual influence of neighboring resonances is, according to the results presented in [5,30], maximum when two eigenvalues of the effective Hamiltonian coincide. The line profile of two completely overlapping resonance states is, in the one-channel case and up to the background term, given by [5,31]

$$S = 1 - 2i\frac{\Gamma_d}{E - E_d + \frac{i}{2}\Gamma_d} - \frac{\Gamma_d^2}{\left(E - E_d + \frac{i}{2}\Gamma_d\right)^2}, \qquad (12)$$

where $E_1=E_2\equiv E_d$ and $\Gamma_1=\Gamma_2\equiv\Gamma_d$. According to this equation, the line profile of the two resonances differs strongly from that of isolated resonances [5] (determined by the rigid value $r_\lambda=1$). In correspondence to this result, we have $r_\lambda=0$ in the one-channel case when two resonance states completely overlap. However, $|\rho|$ might be large in this case as for weakly overlapping resonance states, as discussed above. This result underlines once more the difference between the value r_λ characteristic of a special resonance state λ of the system, and ρ characteristic of the behavior of a sum of resonance states in the overlapping regime.

Thus the avoided crossings of resonance states represent one of the sources for the dephasing [8] observed in experimental data. The variation of r_λ and $|\rho|$ between 0 and 1 is characteristic of an open quantum system with overlapping resonance states, as stated above. Therefore dephasing and dissipation should be equivalent in terms of their effect on the Fano profile. Such a result is observed experimentally, indeed [6].

As to averaged values, we mention the following results obtained earlier. The distributions of $|\rho|$ with energy and ensemble averaging calculated for large chaotic cavities do not depend on the concrete shape of the cavity [32] since the averaging smears the different contributions to $|\rho|$. As a re-

sult, the distribution of $|\rho|$ is characterized, in such a case, only by the number of channels [11].

We underline that the interaction of neighboring resonance states via the common continuum which is considered here as a source for the dephasing [8], is fundamentally different from, e.g., the electron-electron interaction or the interaction due to some radiation. It is rather of nonlinear geometrical origin, related to branch points in the complex energy plane, as can be seen in the following manner. On the one hand, the branch points determine the physical properties of an open quantum system in the overlapping regime as discussed in [18,19,28]. They are, generally, related to the avoided crossings of resonance states which demonstrate the mutual perturbation of resonance states. On the other hand, as shown in the present paper, the mutual interaction of neighboring resonance states is accompanied by phase changes of the eigenfunctions ϕ_λ of $H_{\rm eff}$ as well as of the scattering wave functions Ψ_C^E inside the cavity. In any case, the interaction of neighboring resonance states via the common continuum and the resulting reduction of the phase rigidity (dephasing) cannot be neglected in an open quantum system in the regime of overlapping resonances.

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