Diabatic quasistationary states and unstable closed trajectories

A. K. Kazanskiĭ and V. N. Ostrovskiĭ

Leningrad State University

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Resonance states generated by unstable closed classical trajectories are discussed. In the framework of the parabolic-equation method it is shown that in the asymptotic limit $\hbar \to 0$ these states form series equally spaced along the imaginary energy axis. The physical meaning of these states in the case of the discrete spectrum becomes clear when one introduces a certain parameter determining the potential of the system in the vicinity of a closed trajectory. A characteristic pattern of pseudocrossings of levels arises, this pattern being connected with the diabatic quasistationary states. If the parameter varies rapidly with time the evolution of the system can be described as the decay of a quasistationary state, and this justifies the term "diabatic".

There exist three (not entirely independent) types of quasistationary states: a shape resonance, associated with tunneling through a potential barrier, a Feshbach resonance (quasibound states in the field of an excited core, e.g., autoionized states of the helium atom), and resonances associated with unstable closed trajectories. The latter type of resonance is the least well known and is associated with singularities (Lorentzian profiles) of the density of states in the theory of Gutzwiller[1] and Balian and Bloch.[2] These resonances are presently the subject of intense debate. In particular, in Ref. 3 it is shown that the Gutzwiller expansion for the density of states along closed trajectories (when corrected in accordance with Ref. 4) does not have a rigorous mathematical meaning and only relatively narrow resonances can be manifested physically.

Fundamental in this connection is the question of assigning a meaning to the quasistationary states in a system with a compact configuration space. We shall consider a one-dimensional system with the potential energy shown in Fig. 1. The state with energy ε_0, localized in the region A, becomes quasistationary in the limit $L \to \infty : \varepsilon = \varepsilon_0 - i\Gamma/2$. We shall assume that the problem contains a parameter λ, on which ε depends. If L is finite, instead of the quasistationary state there arises a characteristic pattern of levels: A band of levels is crossed by a sloping term, and the pseudocrossing parameters V are directly related, by virtue of "Fermi's golden rule", to the density of states dn/dE and the width Γ:

$$\pi V^2 \, dn/dE = \Gamma.$$

This relation is physically transparent: With comparatively rapid change of λ, when the system in region A has time to follow this change adiabatically but the time of the motion of the particle outside A is large, the evolution of the state localized in the region A can be described in terms of adiabatic passage through the pseudocrossing points in Fig. 2, but it is more natural to speak of the decay of a quasistationary state under the conditions $L \to \infty$. A similar method for calculating a charge-exchange process was proposed by Chibisov.[5] The mutually consistent character of these two descriptions is seen particularly clearly in the exactly solvable model of Demkov and Osherov[6] (see also Ref. 7). It is necessary to note the connection between this question and the problem (discussed intensively in papers of K. F. Fred, M. Bixon, and J. Jortner; see Ref. 7) of "practical irreversibility" in the theory of nonradiative transitions in complex systems. The picture described here makes it possible to introduce the concept of a diabatic quasistationary state (DQS). It appears to us that such states possess substantially greater "structural stability"[1)] than stationary states with complicated irregular wavefunctions that are unstable against small external perturbations and inaccuracies in the potential of the system. It is also important to bear in mind that an expansion in such stationary states presupposes that the observation time is long.

The principal condition that makes it possible to introduce the concept of a DQS is the existence of a small region of configuration space in which the particle spends a considerable time and in which its motion depends weakly on the behavior of the potential outside the region. In the framework of classical mechanics such conditions are created not only in the case of the above-mentioned shape resonance but also in the neighborhood of a point of unstable equilibrium or of an unstable closed trajectory (a hyperbolic limit cycle). The special role of closed trajectories in the analysis of nonintegrable systems was noted by Poincaré (see Ref. 8) in connection with the three-body problem. By virtue of the well known return theorems,[9] such trajectories form a very representative set, but only short-period and weakly unstable trajectories are capable of giving rise to a resonance structure of the density of states.[3] In quantum mechanics, closed trajectories were brought into consideration in Refs. 1 and 2, but the analysis here was carried out in terms of the density of states without consideration of the wavefunctions. As shown in papers of Heller[10] and Bogolmol'nyĭ, in the immediate vicinity of a closed trajectory one observes an appreciable increase of the wavefunction ("scars" appear), this being connected with the increase of the time spent by the particle in this region. Below we shall give a simple qualitative description of the behavior of the wavefunctions of resonance states and determine their width.

We begin with a simple remark. It is clear that in classical mechanics a particle with energy close to the top of a barrier remains in the vicinity of the top for a considerable time. In quantum mechanics this region can be described in terms of states with purely imaginary energy. In fact, after the change of variables

$$(x, \rho) = (x', \rho') \exp(i\pi/4)$$

the Hamiltonians of the problems for one- and two-dimensional barriers (Δ_2 is the two-dimensional Laplacian opera-

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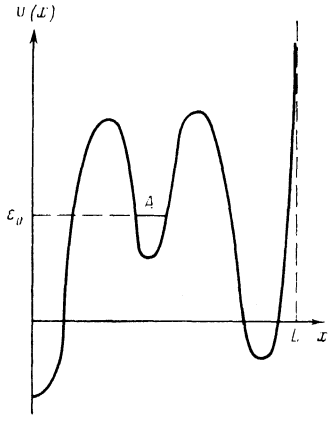

FIG. 1. Potential in a one-dimensional model. Bound states in the central well become quasistationary as $L\to\infty$. The parameter λ, which is discussed in the text, can characterize, e.g., the depth of the central well.

tor, $\hat{L}_3$ is the operator of the corresponding orbital angular momentum, ρ are cylindrical coordinates, and α and μ are parameters)

$$\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2}-\frac{\alpha^2}{2}x^2\right)\psi=E^{(1)}\psi \tag{1}$$

and

$$\left(-\frac{\hbar^2}{2}\Delta_2+\mu\hat{L}_3-\frac{\alpha^2}{2}\rho^2\right)\psi=E^{(2)}\psi \tag{2}$$

go over into oscillator Hamiltonians, while their eigenfunctions, containing only outgoing waves, go over into the decaying solutions of the self-adjoint problems that arise. Therefore, the radiation condition for the Hamiltonians (1) and (2) gives the spectrum

$$E_n^{(1)}=i\alpha\hbar(n+{}^1/_2),\qquad E_{n,m}^{(2)}=\mu\hbar m-i\hbar\alpha(2n+|m|+1). \tag{3}$$

It is important to stress that the eigenfunctions constructed for the Hamiltonians (1) and (2) play the role of the basis in the description of the decay of an initial state of the Gaussian type.

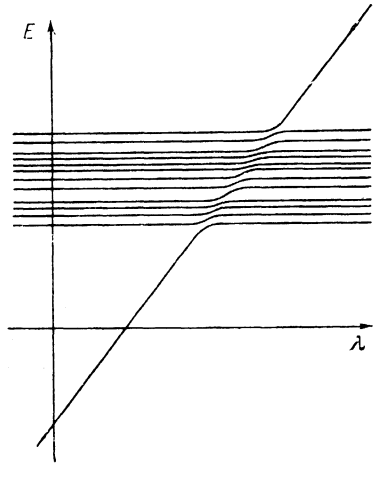

FIG. 2. Characteristic dependence of the energy levels (terms) on the parameter λ.

We shall consider now the case of a hyperbolic limit cycle. We introduce a natural system of coordinates, tied to the trajectory. In such a coordinate system the problem reduces in the limit $\hbar\to 0$ to the time-dependent Schrödinger equation in the subspace orthogonal to the trajectory, and it is possible to approximate the Hamiltonian of this Schrödinger equation by a quadratic Hamiltonian. This assertion constitutes the basic content of the parabolic-equation method,[12] which generalizes the semiclassical approximation of Keller and Rubinov (see Ref. 13). In the framework of this approach the wavefunction ψ describing a state with energy E (differing from the energy E_0 of the motion along the trajectory) has the form

$$\psi=v_{E_0}(t)^{-1/2}\exp(iS_{E_0}(t)/\hbar)\Phi(q_1, q_2, \ldots, q_{n-1}, t), \tag{4}$$

where S_{E_0} and v_{E_0} are the action and the velocity of the motion along the trajectory, q_i are the coordinates in the transverse space, and t is a parameter having the meaning of the time of the motion along the trajectory. The closed character of the trajectory leads to periodicity of the Hamiltonian in the parabolic equation, and this makes it possible to characterize the functions ψ by a definite quasi-energy ε. The requirement that the wavefunction ψ be single-valued after passage around the trajectory gives the quantization condition[2)]

$$E-E_0-\varepsilon-S_{E_0}(T)/T=2\pi n\hbar/T, \tag{5}$$

where T is the period of the motion around the trajectory. The parabolic-equation method assumes that the motion along the trajectory is semiclassical, i.e., that $S_{E_0}(T)/\hbar\gg 1$.

The spectrum of the quasi-energies ε is determined by the eigenstates of the evolution operator over a time equal to one period. To find these states it is necessary[14] to diagonalize the classical monodromy matrix Λ. We shall assume that the eigenstates of this matrix are nondegenerate. The following sets of eigenvalues are possible[14]: $\exp(\pm i\omega T)$, $\exp(\pm\alpha T)$, $\exp(\pm i\mu T\pm\alpha T)$ (in the latter case there are four values). It should be noted that for a unique determination of the parameters ω it is necessary to supplement the definition of the logarithm of the monodromy matrix:

$$\ln\hat{\Lambda}=\int_0^T\hat{\mathscr{L}}(t)^{-1}\dot{\hat{\mathscr{L}}}(t)\,dt,$$

where $\mathscr{L}$ is the fundamental matrix of the classical system. Obviously, the parameters α are directly related to the exponents of the Lyapunov linear instability of the trajectory. The proper subspaces of each set give rise to a set of canonical normal coordinates. In each subspace the evolution operator over one period can be represented[14] in the form $\exp(i\hat{H}T)$, where $\hat{H}$ is a quadratic Hamiltonian. For the above-described eigenvalues of the operator $\hat{\Lambda}$ this will be, respectively, a Hamiltonian of the oscillator type (with a certain frequency ω_j) or else a Hamiltonian of the form (1) or (2) with certain parameters α_j and μ_j. Therefore, by virtue of (3) we obtain for the operator of the quasi-energies of the system

$$\varepsilon(\{n\},\{m\})=\sum_{j_1}\omega_{j_1}(n_{j_1}+{}^1/_2)-i\sum_{j_2}\alpha_{j_2}(n_{j_2}+{}^1/_2)+\sum_{j_3}(\mu_{j_3}m_{j_3}-i\alpha_{j_3}(2n_{j_3}+|m_{j_3}|+1)), \tag{6}$$

where n_i and m_i are integers, n_i being non-negative, and the summation is taken over all the eigenvalues of the matrix $\hat{\Lambda}$. The eigenfunctions Φ can be expressed in terms of Hermite functions.

The formulas (5) and (6) constitute the main content of the paper. Turning to the discussion of the results obtained, we stress that the quadratic approximation requires[12] localization of the wavefunctions in the vicinity of the trajectory, while the resonance functions constructed above do not possess this property. Therefore, we must consider the problem after making a transformation $q = q'\exp(i\pi/4)$ in the transverse space, after which the resonance wavefunctions become decaying. (The method of rotation of the coordinates in the complex plane in order to determine the resonance states is well known and can be applied to the analysis of rather complicated systems.[15]) The relationship of such states to the problem of the decay of the initial state was indicated above.

The formula (6) assumes that the n_i are not large, since otherwise the solution lies outside the limits of applicability of the quadratic approximation. Nevertheless, it should be stressed that resonance states of the type discussed form a series with equal spacing along the imaginary axis of the complex energy plane. Therefore, these resonances differ fundamentally from shape resonances and Feshbach resonances. In particular, in the absorption curves associated with resonances of this type, due to unstable trajectories, simple Lorentzian profiles will not always be observed. It is more natural to expect structures in the form of Fano contours, analogous to the structures in the curves for sub-barrier absorption for a Coulomb center in a uniform electric field.[16]

The question arises of the possibility of going beyond the framework of the quadratic approximation that we have used. In principle, the passage from a time-independent quantum problem to a time-dependent problem in a space of fewer dimensions is well known in collision theory[17] and does not require the assumption that the Hamiltonian in the transverse subspace is quadratic. Thus, our approach, which reduces the problem of finding the resonance states to the problem of determining the quasi-energies, can be applicable to considerably more-general situations. However, such problems require special, and far from universal, analysis.

It is also interesting to apply this approach to problems in which unstable classical trajectories have been found. There are quite a few such problems,[16,18–20] but we shall not analyze them here. We note only that our approach is most convenient in application to nonintegrable systems. In this case, a particle that has left the neighborhood of an unstable trajectory returns to the vicinity of the trajectory, intersects the trajectory, and does not experience recapture (we recall in this connection the homoclinic structure that arises upon splitting of separatrices[9]). Therefore, the resonance structure can be destroyed as a result of interference phenomena only after a very long time. In integrable systems, on the other hand, the repeated captures are repeated in a regular manner, and this destroys the resonance structure. Therefore, in the analysis of integrable systems we must monitor the fulfillment of the principal condition for the formation of a DQS: The time of the motion in the outer part of the configuration space should exceed the times associated with the DQS. If the configuration space is noncompact, the difference between an integrable and a nonintegrable system is less important.

[1)] I.e., these states make it possible to use ordinary perturbation theory for the calculation.

[2)] Strictly speaking, in the framework of the parabolic-equation method of Ref. 12 the object of quantization in (5) is the Planck constant.

[1]M. C. Gutzwiller, J. Math. Phys. **12**, 343 (1971).
[2]R. Balian and C. Bloch, Ann. Phys. (N.Y.) **85**, 514 (1974).
[3]A. Voros, J. Phys. A **21**, 685 (1988).
[4]W. H. Miller, J. Chem. Phys. **63**, 996 (1975).
[5]M. I. Chibisov, Pis'ma Zh. Eksp. Teor. Fiz. **24**, 56 (1976) [JETP Lett. **24**, 46 (1976)]; R. K. Janev and P. S. Krstić, J. Phys. B **21**, 485 (1988).
[6]Yu. N. Demkov and V. I. Osherov, Zh. Eksp. Teor. Fiz. **53**, 1589 (1967) [Sov. Phys. JETP **26**, 916 (1968)].
[7]E. S. Medvedev and V. I. Osherov, *Theory of Nonradiative Transitions in Polyatomic Molecules*, Nauka, Moscow (1983).
[8]V. Szebehely, *Theory of Orbits*, Academic Press, London (1967) [Russ. transl., Nauka, Moscow (1982)].
[9]G. M. Zaslavskiĭ, *Chaos in Dynamic Systems*, Harwood Academic, Chur, Switzerland (1985) [Russ. original, Nauka, Moscow (1984)].
[10]E. J. Heller, Phys. Rev. Lett. **53**, 1515 (1984).
[11]E. B. Bogomol'nyĭ, Pis'ma Zh. Eksp. Teor. Fiz. **44**, 436 (1986) [JETP Lett. **44**, 561 (1986)].
[12]V. M. Babich and V. S. Buldyrev, *Asymptotic Methods in Problems of Diffraction of Short Waves* [in Russian], Nauka, Moscow (1982).
[13]A. I. Baz', Ya. B. Zel'dovich, and A. M. Perelomov, *Scattering, Reactions and Decay in Nonrelativistic Quantum Mechanics*, Israel Program for Scientific Translations, Jerusalem; Wiley, New York (1969) [Russ. original (2nd ed.), Nauka, Moscow (1971)].
[14]I. A. Malkin and V. I. Man'ko, *Dynamical Symmetries and Coherent States of Quantum Systems* [in Russian], Nauka, Moscow (1979).
[15]B. R. Junker, Int. J. Quantum Chem. Symp. **17**, 53 (1980).
[16]V. D. Kondratovich and V. N. Ostrovskiĭ, Zh. Eksp. Teor. Fiz. **83**, 1256 (1982) [Sov. Phys. JETP **56**, 719 (1982)]; V. D. Kondratovich and V. N. Ostrovsky, J. Phys. B **17**, 1981, 2011 (1984).
[17]E. E. Nikitin and S. Ya. Umanskiĭ, *Theory of Slow Atomic Collisions*, Springer, New York (1984).
[18]U. Fano, Phys. Rev. A **22**, 2660 (1980).
[19]H. Klar, Z. Phys. D **6**, 107 (1987).
[20]D. Wintgen, J. Phys. B **20**, L511 (1987).

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