Coherent oscillations and incoherent tunneling in a one-dimensional asymmetric double-well potential

V. A. Benderskii[1,2] and E. I. Kats[3,4]

[1]*Institute of Problems of Chemical Physics, RAS, 142432 Moscow Region, Chernogolovka, Russia*

[2]*Laboratoire Spectrometrie Physique, UJF, Boîte Postale 87, St. Martin d'Heres Cedex, France*

[3]*Laue-Langevin Institute, F-38042 Grenoble, France*

[4] *L. D. Landau Institute for Theoretical Physics, 117940 Moscow, Russia*

(Received 21 July 2001; published 21 February 2002)

For a model one-dimensional asymmetric double-well potential we calculated the so-called survival probability (i.e., the probability for a particle initially localized in one well to remain there). We use a semiclassical (WKB) solution of the Schrödinger equation. It is shown that behavior essentially depends on transition probability, and on a dimensionless parameter Λ that is a ratio of characteristic frequencies for low-energy nonlinear in-well oscillations and interwell tunneling. For the potential describing a finite motion (double-well) one has always a regular behavior. For $\Lambda \ll 1$, there are well defined resonance pairs of levels and the survival probability has coherent oscillations related to resonance splitting. However, for $\Lambda \gg 1$ there are no oscillations at all for the survival probability, and there is almost an exponential decay with the characteristic time determined by Fermi golden rule. In this case, one may not restrict himself to only resonance pair levels. The number of levels perturbed by tunneling grows proportionally to $\sqrt{\Lambda}$ (in other words, instead of isolated pairs there appear the resonance regions containing the sets of strongly coupled levels). In the region of intermediate values of Λ one has a crossover between both limiting cases, namely, the exponential decay with subsequent long period recurrent behavior.

DOI: 10.1103/PhysRevE.65.036217 PACS number(s): 05.45.−a, 03.65.Sq

I. INTRODUCTION

Double level systems and models appear in various contexts in physics, chemistry, and biology. The recurrent interest in the topic is related mainly with fairly rich and interesting physics of the systems, and with the experimental activity on several classes of systems that can be viewed as good physical realization of double level models (including fashionable quantum dots, see, e.g., Ref. [1]). Among the possible types of behavior, we will particularly be concerned with coherent oscillations and incoherent (dissipativelike) tunneling. Our goal is to propose a simple mathematical model to illustrate crossover from coherent oscillations to dissipative tunneling (decay or relaxation), which are also related to incoherent transitions in multidimensional oscillator systems. In a certain sense this crossover reveals many features of chaotic behavior. It is a common fact now that classical chaos is defined as extreme complexity of the trajectories in phase space, with the trajectories being very sensitive to small changes in the initial conditions [2,3]. It is evident that the state vector (wave function) of a closed quantum system strictly speaking does not exhibit chaotic motion, as a consequence of the unitary nature of time evolution. But, in fact, since in quantum mechanics trajectories in the phase space cannot be introduced due to Heisenberg uncertainty principle, the standard classical concept of the stability becomes ambiguous (see, e.g., Refs. [4–8]).

We put forward a simple (but yet nontrivial) model of one-dimensional (1D)asymmetric double-well potential that can be used to describe under relatively weak assumptions a crossover from coherent oscillations (say mechanical behavior) to incoherent decay or dissipative tunneling (say ergodic behavior). The essential part of the model we will present is to illustrate this semiclassical quasichaotic behavior. In fact, the illustration was made long ago by Fermi, Pasta, and Ulam [9]. They performed computer studies of energy sharing and ergodicity for weakly coupled systems of N oscillators. Later on, the results of Ref. [9] were confirmed and refined (see, e.g., Refs. [10,11]). But all these papers were devoted to systems with many degrees of freedom [$(N \gg 1)$-dimensional phase space] for the cases where the motion is nearly integrable and irregular in different energy regions. Level statistics for such kind of mixed systems (i.e., when behavior is regular and chaotic in different phase space regions) changes gradually from Poisson to Wigner type of distributions [12–14]. Thus these systems become nonintegrable when the energy exceeds a certain critical value. On the contrary, we will propose and investigate in 1D a conservative system with time independent Hamiltonian that is evidently always integrable, and it does not generate classical chaos.

For the sake of completeness let us note that the tunneling in the mixed (i.e., regular-chaotic) systems has been studied as well for two-level systems when one of the levels interacts with a chaotic state [15,16] (see also review [17] and references therein). In the case of a resonance between the tunneling doublet and suitable chaotic states, the tunneling is enhanced (so-called chaos assisted tunneling) and has very strong resonance dependence on quantum numbers. Similar effects due to transverse vibrations take place for isolated Fermi resonances in tunneling systems [18].

Our paper has the following structure. Section II contains basic equations necessary for our investigation. Section III is devoted to the calculation of the so-called survival probability. We use the semiclassical approach [19] (see also Ref. [20] and references herein). Section IV contains the summary. The Appendix is devoted to the technical and methodical details of the calculations.

II. ASYMMETRIC 1D DOUBLE-WELL POTENTIAL

The simple model studied in this paper consists of a quantum particle in one-dimensional asymmetric double-well potential $U(X)$ with one-parameter dependent shape. Using the tunneling distance a_0 and the characteristic frequency of the oscillations around the left minimum Ω_0, we can introduced the so-called semiclassical parameter $\gamma \equiv m\Omega_0 a_0^2/\hbar \gg 1$ (m is a mass of a particle, and further we will set $\hbar=1$ measuring energies in the units of frequency), which is assumed to be sufficiently large, i.e., the tunneling matrix element should be small in Ω_0 scale. The choice of the model potential is dictated by the principle of minimal requirements. Our aim is to describe, in the framework of one universal model, the crossover from symmetric double-well potential to the so-called decay potential, and to do it we need a parameter to make the right well (R well) deeper and wider than the left well (L well).

Using Ω_0 and a_0 to set corresponding scales, the model potential satisfying these minimal requirements can be written in the following dimensionless form:

$$V(x)=\frac{1}{2}x^2(1-x)\left[1+\frac{1}{b^2}x\right], \tag{1}$$

where $V\equiv U/(\Omega_0\gamma)$, and $x\equiv X/a_0$. The dimensionless parameter b allows us to change the shape of the right well (R well), and to consider both limiting cases, namely, a traditional symmetric double-well potential (for $b=1$), and for $b\rightarrow\infty$ a decay potential (or, in other words, to change the level spacings from Ω_0^{-1} scale to zero). In fact, it can be shown (see below and the Appendix) that qualitatively all our results do not depend on the concrete form of the one parametric potential satisfying these requirements (only on the density of R states). Behavior in both limiting cases are well known, and for $b=1$ one has coherent quantum oscillations, typical for any two-level systems, while for $b\rightarrow\infty$ there is a continuum spectrum of eigenstates for $x\rightarrow+\infty$ and one can find an ergodic behavior (incoherent decay). Our main goal in this section is to study crossover between both limits at variations of b.

The general procedure for searching semiclassical solutions of the Schröedinger equation with the model potential (1) has a tricky point. The fact is that in the L well we have a discrete eigenvalue spectrum (stationary states) while for the R well in the case $b\gg1$ we have quasistationary states, which are characterized by wave functions $\Psi_n(X)$ exponentially increased in the region of $\varepsilon\gg V(X)$. Both kind of states are defined on different sheets of complex energetic surfaces [19], and to treat both kind of states one should use different tools, namely, the standard quantization of the stationary states from the discrete part of the spectra [19], and proposed long ago by Zeldovich [21] for quasistationary states the flux probability conservation law, which leads to the Lorentzian envelope for spectral distribution functions. Unlike Ref. [21], in our case, we get the Lorentzian envelope filled by δ peaks of the final states.

The procedure is described in the Appendix, and it includes three steps (see Refs. [19,21], and we will use notations from Ref. [20]).

(a) First, one should find the action W_L in the classically allowed region (i.e., W_L between turning points) in the left well (L well), and apply the semiclassical quantization. For the low-energy states in the L well it leads to the following relation:

$$\gamma W_L=\pi\left[n+\frac{1}{2}+\chi_n\right]\equiv\pi\varepsilon_n, \tag{2}$$

where, integer numbers n numerate eigenvalues, χ_n is determined by an exponentially small phase shift, and the last term on the right-hand side of Eq. (2) is in fact the definition for eigenvalues ε_n.

(b) Second, the same should be done for the right well (R well). The calculation is almost trivial in the limit $b\gg1$ [when the potential (1) becomes strongly asymmetric]

$$\gamma W_R=\gamma W_R^{(0)}+\pi\beta\varepsilon, \tag{3}$$

where the dimensionless energy ε is counted from the bottom of the L well, the action $W_R^{(0)}$ is

$$\gamma W_R^{(0)}=\frac{\pi}{16b}(b^2-1)^2(b^2+1), \tag{4}$$

and

$$\beta=\frac{b^2+1}{b}\simeq b \quad \text{for} \quad b\gg1. \tag{5}$$

Note that the parameter $\beta=2\Omega_0/\omega_R$ is proportional to the density of states in the R well (ω_R is the frequency of nonlinear oscillations in R well at $\varepsilon=0$), and, therefore, knowing the magnitude β one can compute the density of states in the R well, which grows proportional to b for $b\gg1$. It is convenient to rewrite Eqs. (3), (4) in the same form as Eq. (2),

$$\gamma W_R=\pi\left[n_R+\frac{1}{2}+\alpha_n+\beta\chi\right], \tag{6}$$

where n_R and α_n are integer and correspondingly fractional parts of the quantity

$$\frac{\gamma W_R^{(0)}}{\pi}+\beta\left(n+\frac{1}{2}\right)-\frac{1}{2}. \tag{7}$$

The physical meaning of α_n is the deviation from a resonance between the nth level in the L well and the nearest level in the R well. By the definition of a fractional part $|\alpha_n|<1/2\beta$.

(c) And as the last step, again using the quantization rule, one can find the spectrum.

It turns out (see Appendix) that the spectrum and the behavior of the system depends crucially on the parameter $\Lambda \equiv \beta R_n$, where

$$R_n = \frac{2^{n+2}\gamma^{n+1/2}}{\pi^{1/2} n!}\exp(-2\gamma W_B), \tag{8}$$

is the β independent decay rate of the nth metastable state of the L well at $b\to\infty$ [W_B is the action in the classically forbidden (between turning points) region].

For $\Lambda \ll 1$, solving the quantization relation (A2), one can easily find

$$\varepsilon_{n\pm} = n + \frac{1}{2} \pm \frac{1}{2\beta}\left[\sqrt{\alpha_n^2 + \frac{4}{\pi^2}\Lambda} - \alpha_n\right]. \tag{9}$$

This expression (9) determines the resonance pairs of the levels, the so-called two-level systems.

Besides the same quantization rule (A2) we get analytically (i.e., for arbitrary values of Λ) eigenvalues for the R well in the vicinity of the resonance doublet

$$\varepsilon_{nm} = n + \frac{1}{2} + \frac{1}{2\beta}\left[\sqrt{(m-\alpha_n)^2 + \frac{4}{\pi^2}\Lambda} - (m-\alpha_n)\right],$$

$$m = \pm 1, \pm 2, \ldots . \tag{10}$$

These levels are numerated by the quantum number *m*.

For $\Lambda \ll 1$, all displacements of the levels due to tunneling are small, and two-level system approximation is valid [i.e., there is well defined isolated resonance pairs of levels with splitting $\propto (R_n/\beta)^{1/2}$]. The situation becomes completely different for $\Lambda \geqslant 1$. In the limit $\Lambda \gg 1$, we get almost equidistant spectrum of mixed L-R levels in the vicinity of the following values of χ (see Appendix for the details)

$$\chi \equiv \chi_{nm} = \pm \frac{m + 1/2 - \alpha_n}{\beta}\left[1 + \frac{1}{\pi\Lambda}\right]. \tag{11}$$

The expressions (10), (11) given above show that the number of levels perturbed by tunneling grows proportionally to $\sqrt{\Lambda}$. In Fig. 1 we have shown the displacements of the levels perturbed by tunneling. These displacements are decreased very rapidly for the levels with quantum numbers larger than $\sqrt{\Lambda}$. The scales in this figure are given by the semiclassical parameter γ that relates to the L well and the barrier. Once the scales are fixed the R well is characterized by the eigenfrequency $\propto 1/b$ at $\varepsilon = 0$ (or what is the same by the density of states or by the action W_R in the R well).

Summarizing the results of this section, we have shown that instead of isolated two-level systems taking place for $\Lambda \ll 1$, in the opposite limit $\Lambda \gg 1$ there appear the resonance regions containing the sets of strongly coupled levels. The resonance widths are determined by tunneling matrix elements [$H_{12}^2 = \omega_L \omega_R \exp(-2\gamma W_B)/4\pi^2 = R_n/\beta$]. In spite of the fact that for any finite values of Λ (and b) we have only the discrete spectrum of real eigenstates, we found above that mixing of L-R states very closely resembles the representation of quasistationary states in terms of eigenstates of a continuous spectrum. This behavior can be formulated, in other words, in terms of the so-called recurrence time, i.e., the characteristic time when the system returns to the initial state. For a finite motion (i.e., for a finite value of b) the behavior of the system remains regular. The recurrence time (i.e., in the case of merely coherent oscillation period) is proportional to $1/H_{12}$ for $\Lambda \ll 1$, while for $\Lambda \gg 1$ this time scales as $1/\omega_R$ (as a long-period time scale).

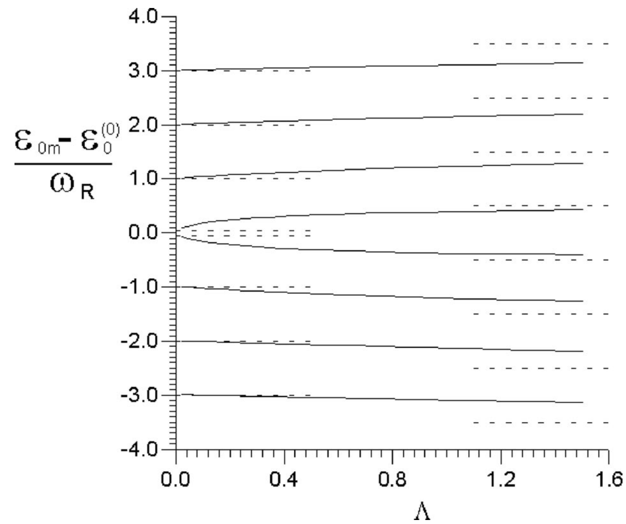

FIG. 1. The eigenvalues as functions of Λ for the zero-point level ($n=0$) of the L well. Dashed lines indicate the limits of $\Lambda \ll 1$, and $\Lambda \gg 1$; $\gamma = 10$, $\alpha_0 = 0$.

III. SURVIVAL PROBABILITY

The tunneling dynamics can be characterized by the time evolution of the initially prepared localized state $\Psi(0)$, and by the definition the survival probability of the state is

$$P(t) \equiv |\langle \Psi(0)|\Psi(t)\rangle|^2. \tag{12}$$

For the stationary states evidently $P(t)=1$, while for quasistationary (decaying states), the survival probability reads

$$P(t) = \exp(-\Gamma t), \tag{13}$$

where Γ is the decay rate that should be found, and we use ω_R^{-1} for the time scale.

The simplest case is the coherent tunneling dynamics of two-level states. Let us consider the $n-n'$ resonance region. The eigenfunctions of isolated R and L wells, Ψ_n^L, and $\Psi_{n'}^R$. If one has the initial state

$$\Psi(0) = \Psi_n^L,$$

the survival probability can be easily calculated

$$P(t) = \frac{1}{2}\left[1 + \cos\left(2t\sqrt{\frac{R_n}{\beta}}\right)\right]. \tag{14}$$

Normalized wave functions in the L well can be calculated trivially, and using standard semiclassical wave func-

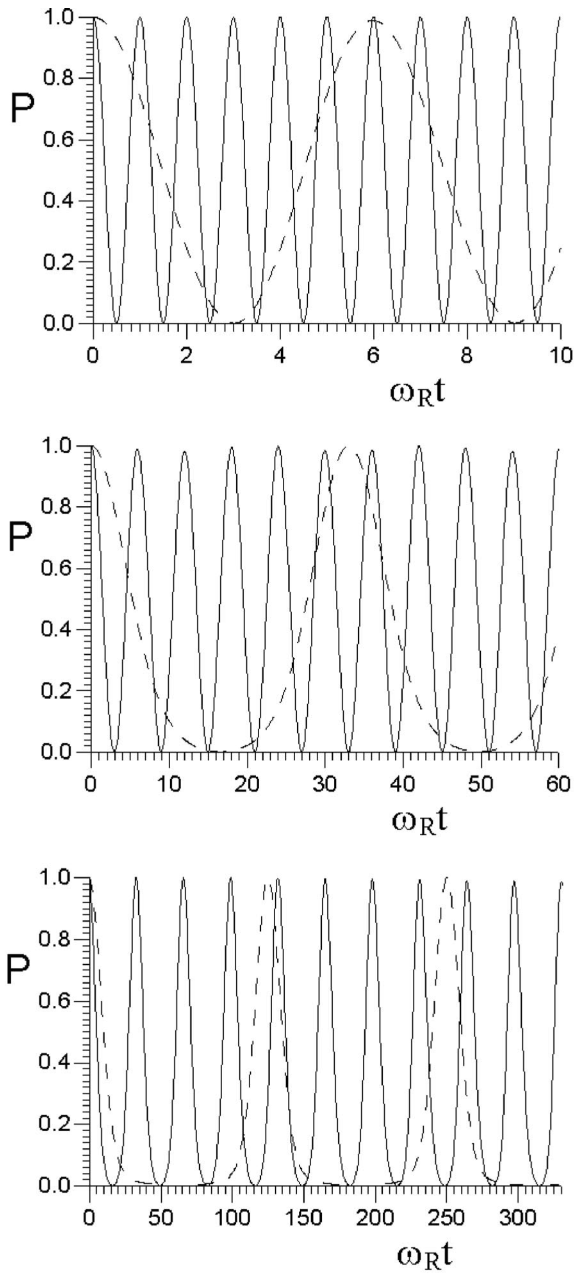

FIG. 2. The survival probability for different values of Λ and $\gamma = 10$. (a) $\Lambda = 0.02$, $b = 5$ (solid line); $\Lambda = 0.5$, $b = 116$ (dashed line); (b) $\Lambda = 0.5$, $b = 116$ (solid line); $\Lambda = 4.0$, $b = 929$ (dashed line); (c) $\Lambda = 4.0$, $b = 929$ (solid line); $\Lambda = 16.0$, $b = 3715$ (dashed line).

tions for the R well, we are in a position to compute the survival probability for a general case as a function of Λ. The results are shown in Fig. 2.

For $\Lambda \ll 1$, $P(t)$ oscillates with characteristic time scales proportional to $H_{12}^{-1} = \sqrt{\beta/R_n}$. In the region $\Lambda \simeq 1$, these oscillations are strongly suppressed. The reason for the suppression of oscillations is related to interference of the states with energies in the resonance region. As a result of the interference the total probability for the system to return back from the R well is decreased, and low-frequency modulation of coherent tunneling is raised. The period of the modulation grows with β, and in the limit $\Lambda \gg 1$ we get the dense spectrum of states in the R well, and almost exponential decay for $P(t)$ with β independent relaxational time $\tau \propto R_n^{-1}$. In this case, the survival probability (i.e., the probability to keep the system in its initial state) for the time interval $\ll 1/\omega_R$ decays almost exponentially with time, and the characteristic relaxation time τ is determined by Fermi golden rule, i.e., $\tau^{-1} \propto H_{12}^2/\omega_R$. This result is also conformed to Van Hove statement [22] concerning quasichaotic behavior of semiclassical systems at time scales of the order of ω_R/H_{12}^2.

We can relate the phenomenom described above (i.e., almost vanishing probability for backflow from the R to L well) to the Fermi golden rule for a transition probability

$$W_{fi} = 2\pi |H_{fi}|^2 \rho_f, \tag{15}$$

where H_{if} is the matrix element between the initial state E_i and the final state E_f, and ρ_f is the density of final states. For our case ($H_{if} \equiv H_{12} = \sqrt{R_n/\beta}$, and $\rho_f = \beta/2$) we get easily

$$W_{if} = \pi R_n,$$

which does not depend on ρ_f. Therefore, the Fermi golden rule corresponds to the limit when the backflow from the R well is totally suppressed due to the interference.

The survival probability can be related also to spectral distribution of the initially localized in the L well states. Indeed, by the definition of the spectral distribution $S(E)$ of the initially prepared localized state is determined by the transition amplitudes in expansion over the eigenstates (Ψ_n, E_n),

$$S(E) = \sum_n |\langle \Psi(0) | \Psi_n \rangle|^2 \delta(E - E_n), \tag{16}$$

and, therefore,

$$\langle \Psi(0) | \Psi(t) \rangle = \int_{-\infty}^{+\infty} S(E) \exp(-iEt) dE. \tag{17}$$

For $\Psi(0) \equiv \Psi_i^L$ the spectral distribution is a set of δ peaks with Lorentzian envelope

$$S(E) = \frac{2}{\pi} \frac{\sqrt{R_i \beta}}{\beta(E - E_i)^2 + R_i} \delta(E - E_i). \tag{18}$$

Crossover from the coherent oscillations to exponential decay occurs when the Lorentzian envelope begins to fill up by δ peaks of the final states. Note that the width of the Lorentzian envelope (18) does not depend on the final state density (see Appendix and also Ref. [21]). We have shown the results of the calculation of the spectral distribution in Fig. 3.

IV. CONCLUSION

Let us sum up the results of our paper. We investigated the behavior of a quantum particle in 1D asymmetric double-well potential with one-parameter dependent shape, which

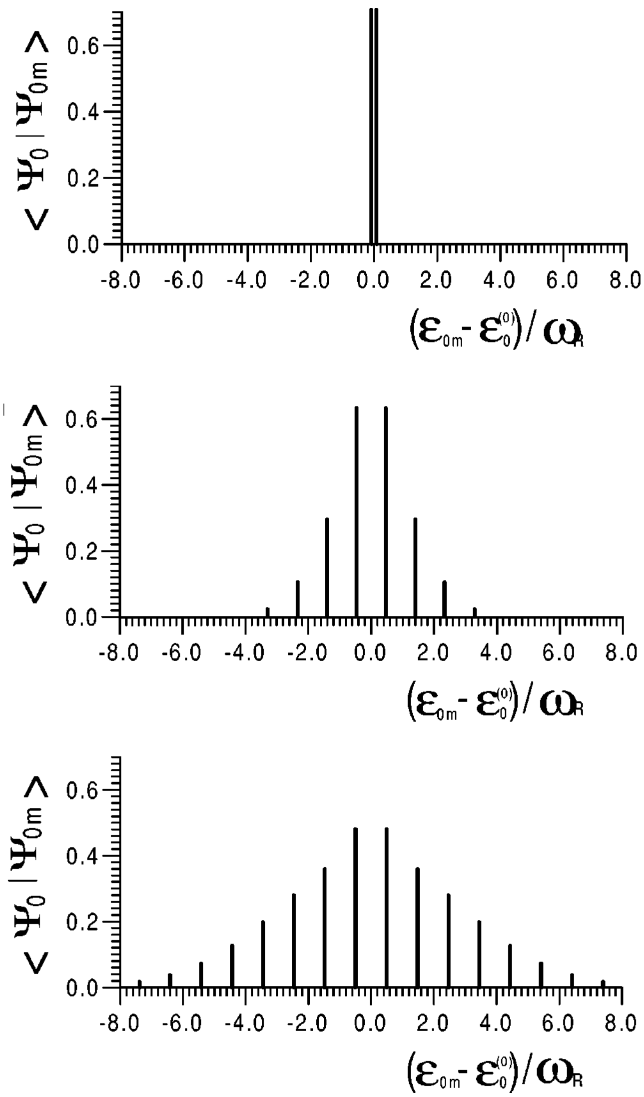

FIG. 3. The spectral distribution for different values of Λ and $\gamma=10$. (a) $\Lambda=0.02$, $b=5$; (b) $\Lambda=4.0$, $b=929$; (c) $\Lambda=20.0$, $b=4644$.

allows us to consider in the framework of one universal model the crossover from the traditional symmetric double-well potential to the decay one. We have shown that behavior essentially depends on transition probability, and on a dimensionless parameter Λ that is a ratio of characteristic frequencies for low-energy nonlinear in-well oscillations and inter-well tunneling. For the potential describing a finite motion (double well), strictly speaking, one has always a regular behavior. For $\Lambda \ll 1$, there are well defined resonance pairs of levels and the survival probability has coherent oscillations related to resonance splitting. However, for $\Lambda \gg 1$ there are no oscillations at all for the survival probability, and there is almost an exponential decay with the characteristic time determined by Fermi golden rule. In this case, one may not restrict himself to only resonance pair levels. The number of levels perturbed by tunneling grows proportionally to $\sqrt{\Lambda}$ (in other words, instead of isolated pairs there appear the resonance regions containing the sets of strongly coupled levels). In the region of intermediate values of Λ one has a crossover between both limiting cases, namely, the exponential decay with subsequent long period recurrent behavior.

However, a number of remarks related to our results are in order. Many features often classified as evidences of quantum chaos, in fact, as we have illustrated in our model, can occur for well defined states possessing only discrete energy levels. The deviation from two-level system behavior, taking place for $\Lambda \gg 1$, has nothing to do with random or chaotic properties of the system. It means only that due to well known phenomenom of level repulsion the two-level approximation is not adequate. Lorentzian envelope (see Fig. 3) we found arises from the interaction of a single level in L well with a set of levels in the R well and not with appearance of level widths (imaginary self-energy contributions).

One should distinguish between short-time and long-time behavior, and the boundary between them depends on the parameter Λ. Short-time returns ($\propto \beta$) are governed by one or a small number of semiclassical paths, while long-time returns ($\propto R_n^{-1}$) arise from interference between many paths. In the limit $\Lambda \ll 1$, exponential decay occurs for short-time dynamics, while the system remains regular for long-time scales, in contrast with chaotic models we discussed in the Introduction. Nevertheless, the tunneling in the limit of $\Lambda \gg 1$ can induce vibrational relaxation for localized R levels. The relaxation appears due to tunneling recurrences, and results in redistribution of initial energy over all levels coupled with a single L level.

The main physical idea of our paper, namely, that specific quasichaotic behavior is associated with the fact that one level in L well in a certain condition ($\Lambda \gg 1$) is coupled to a set of almost dense levels in the R well, was discussed in the literature long ago [22] (see also Ref. [21]), mainly qualitatively. Our achievement is that we have proposed a concrete and tractable analytical model to illustrate and to investigate explicitly and quantitatively this statement.

In this respect our results are quite different from numerical investigations of billiard-type systems (see, e.g., review paper [17]), showing universal behavior of level spacings in finite chaotic systems. Our results (for the totally integrable 1D model) demonstrate that level spacing distribution is not a specific feature of quantum systems with chaotic classical counterpart limit. Our finding of the equidistant regular level distribution is a result of the interaction of the single L level with several (of the order of ten for our particular choice of the parameters) R levels (which in own turn are regular ones). We should also distinguish our model from the dynamic tunneling ones [23,24]. The latter assumed strong coupling of the tunneling system with an environment that destroys the coherence, whereas in our model the coherence is destroyed by the tunneling itself due to the high density of R states, breaking two-level approximation.

Note also at the very end of the paper that results presented here are not only interesting in their own right (at least in our opinion), but they might be directly tested experimentally since there are many molecular systems where the 1D asymmetric potential investigated in the paper is a reasonable model for the reality. And not only molecular systems, for instance, recently as a controllable two-level system, double quantum dots have also been proposed for realizing a single quantum bit in solid state systems. Experimentally [1], in these systems two distinct regimes characterizing the nature of low-energy dynamics have been observed: (i) relaxational regime, when an excited-state electron population decays exponentially in time with a rate correctly given by Fermi golden rule; (ii) vibronic regime, when the population oscillates for some number of cycles before decaying.

And what's more, at short times the averaged excited-state populations oscillate but have a decaying envelope. The similarity with the behavior we found in the paper is evident.[1]

ACKNOWLEDGMENTS

The research described in this publication was made possible in part by RFFR Grants 97-03-33687a and 00-02-11785. The numerical results were obtained in collaboration with E.V. Vetoshkin, whose contribution is gratefully acknowledged.

APPENDIX

The semiclassical wave function is represented in the well known WKB form[2]

$$\Psi = \exp(iW).$$

The action W should satisfy to the WKB equation

$$\frac{1}{2}\left(\frac{dW}{dX}\right)^2 = \frac{\varepsilon}{\gamma} - V(X), \tag{A1}$$

and two turning points, which are boundaries of classically allowed regions, are situated near zeros of $V(X) - \varepsilon/\gamma$.

For the asymmetric double-well potential (1) the Bohr-Sommerfeld [19] quantization equations read

$$\tan(\gamma W_L)\tan(\gamma W_R) = 4\exp(2\gamma W_B), \tag{A2}$$

where W_B is the action in the classically forbidden region in between the turning points X_1, X_2 in the left and right wells, and $W_{L,R}$ are the coordinate independent actions in the classically allowed regions inside of the L (respectively R) well. Using the following expansion:

$$\tan z = \sum_{m=0}^{\infty} 2z\left[z^2 - \pi^2\left(m + \frac{1}{2}\right)^2\right]^{-1},$$

one gets the almost equidistant spectrum of the mixed L-R levels, and in this condition the solution of Eq. (A2) leads to the expressions (9), (10) presented in the main text of the paper.

The time evolution of any initially prepared state can be described by a superposition of the eigenfunctions of the discrete and continuous spectra with time dependent phases. For the potential (1) with $b \gg 1$ the initial finite motion, i.e., the initial density distribution

$$\rho(t) = \int_{X_1}^{X_2} |\Psi(X,t)|^2 dX, \tag{A3}$$

concentrated in the L well at $t=0$ decreases exponentially with time

$$\rho(t) = \rho(0)\exp(-\eta t). \tag{A4}$$

Equation (A4) signifies that the wave functions of quasistationary states have the form

$$\Psi_n(X,t) = \Psi_n(X)\exp[(-i\varepsilon_n - \eta_n/2)t], \tag{A5}$$

and the eigenvalues are complex and lies on the lower half-space of (ε, η) plane. The quantization of the stationary states of a discrete spectrum is performed by the requirement [19]

$$|\Psi(X,t)|^2 \to 0 \quad \text{at} \quad |X| \to \infty.$$

This condition is impossible to impose on quasistationary states, since the wave function $\Psi_n(X)$ is exponentially increased in the region of $\varepsilon \gg V(X)$. The physically meaningful boundary condition noted first by Zeldovich [21] for quasistationary states can be written as a conservation law for the flux probability from the L well through the barrier. The difference between stationary and quasistationary states disappears as it should at $\eta \to 0$.

The expansion of the initially quasistationary state is dominated by the continuum spectrum eigenfunctions with the energies close to the real parts of the eigenvalues ε_n. These eigenfunctions have the form

$$\Psi_k(X) = \left(\begin{array}{cc} A(k)\phi_k^0(X), & X < X_m \\ \sqrt{\dfrac{2}{\pi}}\sin(kX + \delta(k)), & X > X_m \end{array}\right), \tag{A6}$$

where X_m is the left turning point of the R well, the localized wave function ϕ_k^0 is normalized to unity, and the phase is given as

$$\delta(k) = \delta_0 - \arctan\frac{k_2}{k - k_1}, \tag{A7}$$

and δ_0 is a k-independent component, $k_1 = \sqrt{2m\varepsilon_n}$, $k_2 = k_1\eta_n/4\varepsilon_n$. For the eigenfunctions with the energies ε and ε' close to ε_n we get

[1]All characteristics of our model are not specific only for the 1D case. For $\Lambda \gg 1$, one can expect similar behavior for multidimensional systems.

[2]Equivalently, it can be represented in the so-called instanton or minimum action tunneling path formalism [25] (see also Ref. [20]) in the form of $\Psi = \exp(-\gamma W_E)$, which is more efficient for classically inaccessible parts of phase space.

$$\int_{-\infty}^{X}\phi_k(X')\phi_{k'}(X')dX' = \frac{1}{2m}\left(\frac{1}{\varepsilon-\varepsilon'}\right)\left(\phi_k'\frac{d\phi_k}{dX}-\phi_k'\frac{d\phi_k'}{dX}\right). \quad \text{(A8)}$$

From Eqs. (A6), (A7), and (A8) in the limit $\varepsilon-\varepsilon'\to 0$ we get

$$A^2(k)=\frac{2}{\pi}\sqrt{\frac{2\varepsilon_n}{m}}\frac{\eta_n}{4(\varepsilon-\varepsilon_n)^2+\eta_n^2}. \quad \text{(A9)}$$

Expressions (A7) and (A9) are valid for a continuous spectrum, for discrete levels the phase shift as well is governed by the probability flux from the R well into classically forbidden region, and instead of Eq. (A7) it leads to

$$\delta=\arctan\sqrt{R_n\beta}\,\frac{1}{\varepsilon_n-\varepsilon_{nm}}, \quad \text{(A10)}$$

and instead of Eq. (A9) one can easily find

$$A^2(\varepsilon_{nm})=\frac{2}{\pi}\frac{\sqrt{R_n\beta}}{\beta(\varepsilon_n-\varepsilon_{nm})^2+R_n}. \quad \text{(A11)}$$

Note that Eq. (A11) has almost the same form as Eq. (A9), although it depends on discrete energy levels, and besides it has a different coefficient due to different normalization condition.

The relation (A9) shows that the probability density of the continuous spectrum eigenstates exhibits the Lorentzian distribution around the real part of the quasistationary eigenvalues ε_n. Expressions (A9)–(A11) are equivalent to the spectral distribution (18) presented in the main body of the paper.

A few words concerning numerical results have been presented in the captions of Figs. 1–3. The calculations have been performed to check: (i) semiclassical approximation for the model potential (1); (ii) the spectral distribution (18).

We used the numerical diagonalization of the Hamiltonian matrix in the basis set of trial functions, which includes: so-called instanton wave functions of the L well (see Ref. [20]), and the WKB functions of R well. This basis was orthonormalized by using standard Schmidt method [26]. For the L well, highly excited states near the barrier top have also been included. In all numerical calculations we set the value of α_0 (so-called defect of a resonance) as zero. All results presented in the figures do not depend on this particular choice.

The numerical results confirm that Eq. (18) is quite accurate in the whole range of Λ where the transition from coherent oscillations to exponential decay occurs. Note that since R levels with the negative energy are not mixed with L levels, and besides the resonance region is sufficiently narrow ($R_n=0.01$), we need not diagonalize huge matrices. For our purposes the diagonalization of the matrix 3000×3000 is more than sufficient to find eigenvalues in the resonance region around the $n=0$ L level.

[1] H.S. Yang *et al.*, Physica B **263**, 476 (1999).
[2] G.M. Zaslavsky, Phys. Rep. **80**, 157 (1980).
[3] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer, New York, 1983).
[4] Y. Weissman and J. Jortner, J. Chem. Phys. **77**, 1469 (1982); *ibid.* **77**, 1486 (1982).
[5] M. V. Berry, in *Chaotic Behavior of Deterministic Systems* edited by G. Iooss, R. Helleman, and R. Stora (North-Holland, Amsterdam, 1983).
[6] M.V. Berry, Proc. R. Soc. London, Ser. A **423**, 219 (1989).
[7] K. Nakamura, *Quantum Chaos* (Kluver, Dordrecht, 1997).
[8] L. Kaplan and E.J. Heller, Phys. Rev. E **62**, 409 (2000).
[9] E. Fermi, J. Pasta, and S. Ulam, Los Alamos Scientific Laboratory Report No. LA-1940, 1955 (unpublished).
[10] E.A. Jackson, J. Math. Phys. **4**, 686 (1963).
[11] J. Ford and J. Waters, J. Math. Phys. **4**, 1293 (1963).
[12] M.V. Berry and M. Robnik, J. Phys. A **17**, 2413 (1984).
[13] E. Caurier and B. Grammaticos, Europhys. Lett. **2**, 417 (1986).
[14] T. Zimmermann, H.D. Meyer, H. Koppel, and L.S. Cederbaum, Phys. Rev. A **33**, 4334 (1986).
[15] S. Tomsovic and D. Ullmo, Phys. Rev. E **50**, 145 (1994).
[16] D.A. Steck, W.H. Windell, and M.G. Raizen, Science **293**, 274 (2001).
[17] O. Bohigas, S. Tomsovich, and D. Ullmo, Phys. Rep. **223**, 43 (1993).
[18] V.A. Benderskii, E.V. Vetoshkin, and H.P. Trommsdorf, Chem. Phys. Lett. **244**, 273 (1999).
[19] L. D. Landau and E. M. Lifshits, *Quantum Mechanics (Non-Relativistic Theory)* (Pergamon Press, New York, 1965).
[20] V.A. Benderskii and E.V. Vetoshkin, Chem. Phys. **257**, 203 (2000).
[21] Ya.B. Zeldovich, [Sov. Phys. JETP **12**, 542 (1961)].
[22] L. Van Hove, Physica, **21**, 517 (1955).
[23] M. Wilkinson, J. Phys. A **21**, 1173 (1988).
[24] S.D. Frischat and E. Doron, Phys. Rev. E **57**, 1421 (1998).
[25] A.M. Polyakov, Nucl. Phys. B **129**, 429 (1977).
[26] P. M. Morse and M. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).