Tunneling Effect and the Natural Boundary of Invariant Tori

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The invariant torus of nonintegrable systems breaks up in complexified phase space. The breaking border is expected to form a natural boundary (NB) along which singularities are densely condensed. The NB cuts off the instanton orbit controlling the tunneling transport from a quantized invariant torus, which might result in a serious effect on the tunneling process. In the present Letter, we provide clear evidence showing that the presence of the NB is observable as an anomalous enhancement of the tunneling wave amplitude in the immediate outer side of the NB.

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Poincaré showed in his well-known theorem of nonintegrability that if an integrable system is perturbed there are no analytic integrals of motion other than energy, and he considered it as a ''fundamental problem of mechanics'' to clarify what is happening after the perturbation destroys the integrals of motion [1]. As was proved by Kolmogorov, Arnold, and Moser (KAM), most of the tori which conserve quasiperiodic motion and the very prototype in the integrable limit, survive if the perturbation strength is weak enough [2].

However, surviving tori are no longer analytically entire objects but they break up in general in the complexified phase space since there appears the *natural boundary* (NB) along which singular points densely accumulate [3]. In the nearly integrable regime, in which the measure of a chaotic set is exponentially small, the really problematic aspect of the fundamental problem manifests itself as the NB which is hardly visible from the real phase space.

However, it might be of crucial significance in quantum tunneling problems even in the nearly integrable regime: the torus satisfying the EBK condition is quantized, and the fully real part of the torus semiclassically well reproduces the principal part of the corresponding eigenfunction, but a serious problem arises in the tunneling components. The subset of the complexified tori contributing to the tunneling component in general encounters the NB and the tunneling tail loses its semiclassical support beyond the NB. If this effect is not only mathematical but also physically meaningful, the presence of the NB, which is hardly visible from the real phase space, could be observed in tunneling phenomena.

The serious problem caused by the NB was first noticed by Creagh [4], in the application of Wilkinson's formula to nearly integrable systems [5]. He also showed that the presence of the NB seems to give a non-negligible effect on the radiation pattern from microcavities [6]. The present authors showed that, in the time domain semiclassics, the major tunneling orbits called the ''Laputa chains'' [7], which are guided by complexified stable and unstable manifolds (CSUM), are significantly influenced by the NB if the perturbation is not very weak [8]. There have been several authors who mention the possible role of the NB, but to the authors' knowledge, no direct evidence revealing the crucial effect of the NB on the tunneling effect has been presented [9–12]. The objective of the present Letter is just to provide it.

The model we treat in the present Letter is the quantum map

$$U = e^{-ip^2/4\hbar} e^{-iV(q)/\hbar} e^{-ip^2/4\hbar}, \tag{1}$$

with a cubic potential $V(q) = \epsilon(2q^2 + q^3/3)$, which has a barrier with the height $V_{\max} = 32\epsilon/3$ [8]. The classical map of the above model, $(q', p') = (q + p + V'(q + p/2)/2, p + V'(q + p/2))$, is conjugate to the well-known Hénon map, while in the limit $\epsilon \to 0$, the system (1) is well approximated by the standard one-dimensional model of barrier tunneling: $U_1 = e^{-i\epsilon H_1/\hbar}$ with $H_1 = p^2/(2\epsilon) + V(q)$, which is completely integrable.

In the KAM region, the invariant tori satisfying the EBK quantization condition $\oint p dq/2\pi = (n + 1/2)\hbar (n = 0, 1, \cdots)$ in the present case form quantum resonances with finite lifetime due to tunneling. With ϵ increasing, the KAM region becomes surrounded by chaotic regions developed around the homoclinic orbits of the saddle point $S = (-4, 0)$ on the top of the potential barrier, and complex tunneling orbits guided by CSUM, which can be roughly identified with the *Julia set*, dominate the tunneling process [8]. On the contrary, the tunneling lifetime of the integrable model H_1 can be evaluated by using instanton.

First of all, we take the classical invariant torus as a basis of our argument. It is parametrized by the angle variables θ through the conjugation function $(q, p) = (Q(\theta), P(\theta))$ according to the KAM theorem. The conjugation function, which is a 2π-periodic function, is written as $Q(\theta) = [q(\theta + \omega/2) + q(\theta - \omega/2)]/2$, $P(\theta) = q(\theta + \omega/2) - q(\theta - \omega/2)$ by using a standard representation of the position function $q(\theta)$ satisfying the functional equation $q(\theta + \omega) + q(\theta - \omega) - 2q(\theta) = -V'(\theta)$. This is equivalent to the classical mapping rule, where ω denotes the irrational rotation number of a given torus. The function $q(\theta)$ is usually expanded as the Fourier series $q(\theta) = \sum_n a_n e^{in\theta} = \sum_n a_n z^n$ with $a_{-n} = a_n \in \mathbb{R}$, where $z = e^{i\theta}$. The Fourier expansion has the radius of convergence $\rho = 1/\overline{\lim}_{n\to\infty} a_n^{1/n}$, if there exists a singular point at $|z| = \rho$. The singular point propagates with the irrational rotation number ω, and as a result the singular points are distributed densely along the circle $|z| = \rho$, which forms the NB [3]. If the invariant torus satisfies the quantization condition, $\int_0^{2\pi} P(\theta)Q'(\theta)d\theta/2\pi = (n + 1/2)\hbar$, then the subset $\mathcal{T}$ of the torus which semiclassically contributes to the q − represented eigenfunction is given by

$$\mathcal{T} = \{(q, p) = (Q(\theta), P(\theta)) | \mathrm{Im}Q(\theta) = 0, |\mathrm{Im}\theta| < \log\rho\}, \quad (2)$$

which is represented by the blue lines on the complex θ-plane illustrated in Fig. 1(b). We further define $\mathcal{T}_r$ and $\mathcal{T}_i$ as $\mathcal{T}_r = \{(q, p) | (q, p) \in \mathcal{T}, \mathrm{Im}p = 0\}$ and $\mathcal{T}_i = \mathcal{T} \setminus \mathcal{T}_r$, respectively. As indicated in Fig. 1, $\mathcal{T}_r$ is the *real torus* corresponding to the invariant circle on the real qp-plane bouncing between the turning points q_2 and q_1, which semiclassically contributes to the principal part of the wave function. On the other hand, the remaining part of $\mathcal{T}$, i.e., $\mathcal{T}_i$, is the *instanton* supporting the tunneling part of the wave function. Since $Q(\theta) = Q(-\theta)$ and $P(\theta) = -P(-\theta)$, blue lines $\theta = -i\eta$ and $\theta = \pi - i\eta$ ($\eta(>0) \in \mathbb{R}$) on the complex θ-plane in Fig. 1 are obviously contained in $\mathcal{T}_i$. The set $\mathcal{T}_i$ is not confined in the real qp-plane, and its projection onto the real qp-plane is shown in Fig. 1(a) as the two blue lines along $q = 0$

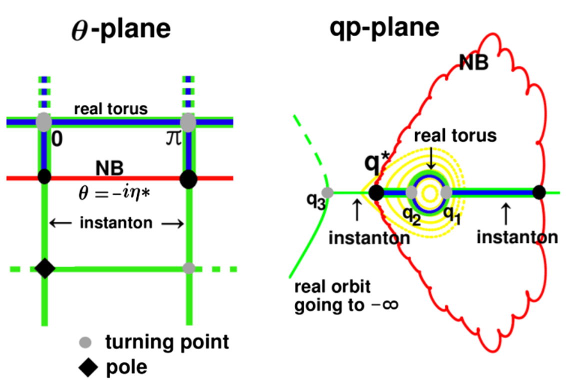

FIG. 1 (color online). An example of the set $\mathcal{T}$ on the complex θ plane (left), and its projection onto the real qp-plane computed for $\epsilon = 0.05$ (right). See the text. The yellow curves are the Poincaré plot. (The dotted lines do not contribute because of the Stokes phenomenon.)

emanating from the classical turning points $q = q_2 = Q(\pi)$ and $q_1 = Q(0)$.

To discuss the crucial role of the NB, indicated by the red line in Fig. 1, we consider the integrable limit H_1. The instanton branches (and also the real torus component as well) of the integrable model are indicated by green lines, and they are almost indistinguishable from the set $\mathcal{T}$ of the nonintegrable model if ϵ is small. The instanton branches of the integrable model are complete in the sense that they support the tunneling tails extending toward $+\infty$ and $-\infty$ from the two classical turning points $q = q_1$ and q_2, respectively; the second branch is particularly important because it corresponds to the instanton orbit responsible for the tunneling transport toward $q = -\infty$ going through the potential barrier. Indeed, as η increases along the second branch, $(q, p) = (Q(\theta), P(\theta))$ passes through the classically forbidden region and reaches the third turning point $q_3(<q_2)$, from which a real branch emanates and ends at a pole of $q(\theta)$, which provides a real orbit going toward $q = -\infty$ on the qp-plane and supports the tunneling tail extending toward $q = -\infty$.

The contributing set of the nonintegrable model (1) almost overlaps with that of the integrable model, but a crucial difference is that the instanton branches of the nonintegrable model intersect with the NB at a certain $\eta = \eta^*$, which corresponds to $q = q^* \equiv Q(\pi + i\eta^*)$ on the qp-plane. Until the intersection $q = q^*$ the tunneling tail can be well approximated by the semiclassical wave function $\Psi = A(q)\exp\{iS(q)/\hbar\}$ (the Maslov index is omitted), where $A(q) = 1/|Q'(\theta)|^{1/2}$ and $S(q = Q(\pi + i\eta)) = \int_0^\eta iP(i\eta' + \pi)Q'(i\eta' + \pi)d\eta'$. But beyond the intersection, there is no analytic continuation of the invariant torus, meaning that we lose the semiclassical basis for tunneling tails.

The NB is certainly a strict border at which analyticity is broken, and quite important when one argues the mathematical nature of given functions. But it is not obvious that any physical reality is significantly influenced by the NB and it could be that the NB is a purely mathematical phenomenon. Therefore, the fundamental question here arising is whether the interruption by the NB is physically significant or not. However, we do not have any theoretical method to predict how serious the question is in classical mechanics, so even more in quantum mechanics: to answer the question we have to go beyond the KAM theory.

If the NB is not critical in quantum mechanics, it will be possible to go over the NB by a suitably devised approximation which can formally eliminate the nonintegrable part of U. As a powerful approximation we here employ a Baker-Hausdorff-Campbell type expansion which is a very efficient algorithm transforming U into a unitary transformation of a one-dimensional Hamiltonian with H_1 as the lowest order term. Let us define the effective Planck constant $k = \hbar/\sqrt{\epsilon}$ and the new momentum $p' = -ikd/dq$, then $U = e^{-i\mu p'^2/4}e^{-i\mu V(q)}e^{-i\mu p'^2/4}$, where

$\mu = \sqrt{\epsilon}/k = \epsilon/\hbar$. Then the Baker-Hausdorff-Campbel-type expansion leads to

$$U \sim \exp\{-i\sqrt{\epsilon}\sum_{\ell=0}^{\infty}(i\mu)^{2\ell}H_{\ell+1}(q,p')/k\}, \qquad (3)$$

where $H_{\ell+1}(q,p')$ is a polynomial of q and p', and $H_{\rm eff}^{(m)}(q,p') = \sum_{\ell=0}^{m}(-\mu^2)^{\ell}H_{\ell+1}(q,p')$ is classically an integrable one-dimensional Hamiltonian, but note that this expansion is of course only a formal asymptotic expansion. If ϵ is small (practically $|\epsilon| < 0.1$), the classical invariant set $H_{\rm eff}^{(m)}(q,p') = E$ approximates the real torus $\mathcal{T}_r$ of Eq. (1) at the precision of $O(\mu^{2m+3})$. We executed the expansion up to $m = 9$ by using a computer algebra system.

We can expect that the semiclassical approximation based on $\mathcal{T}_i$ of the effective Hamiltonian $H_{\rm eff}^{(m)}$ reproduces very well the tunneling tail of the exact eigenstates of U at least in the range up to the intersection with the NB, namely $q^* < q < q_2$. Moreover, $\mathcal{T}_i$ of $H_{\rm eff}^{(m)}$ has no singularities in $\mathcal{T}_i$ and so it can be extended beyond $q < q^*$. As is shown in Fig. 2(a), if ϵ is small but $\hbar$ is not very small, the fully extended semiclassical approximation reproduces the whole of the tunneling component of the exact eigenfunction. These observations allow us to use the $\mathcal{T}$ given by $H_{\rm eff}^{(m)}(q,p') = E$ as a pseudoextension of the exact $\mathcal{T}$ beyond the NB, which will provide a nicely improved instanton approximation to tunneling components, if a properly large m is chosen. (In practice we take $m = 8$ or 9.)

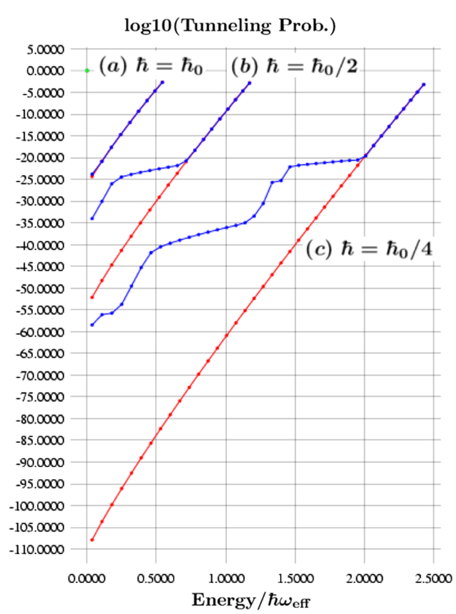

FIG. 2 (color online). Exact tunneling amplitude (blue) compared with instanton approximation (red) of $H_{\rm eff}^{(m)}$, where $\omega_{\rm eff} = 2\pi/\sqrt{\epsilon}$. The amplitude is computed in the quasistationary regime far from the barrier, i.e., $q \ll q_3$. See the text and Ref. [14].

For smaller $\hbar$, the fully quantum eigenstate for $H_{\rm eff}^{(m)}$ has a tunneling amplitude much smaller than the numerically attainable precision, and so we use the semiclassical instanton approximation instead of the rigorous eigenstate of $H_{\rm eff}^{(m)}$. Since $H_{\rm eff}^{(m)}$ is integrable, the semiclassical approximation works very well in the small limit of $\hbar$.

The improved instanton approximation using the integrable model $H_{\rm eff}^{(m)}$ works very well, but an extensive numerical investigation reveals that as $\hbar$ is reduced there exists a threshold of $\hbar$ below which the exact tunneling amplitude starts to deviate markedly from the semiclassical one. A quite interesting and paradoxical fact is that the threshold value of $\hbar$ decreases as the quantum number n decreases. Therefore, if $\hbar$ is fixed at a relatively small value, such a transition takes place as we move from the highest classically bounded state $n = n_{\max}$ to the ground state. Note here that we take a sufficiently small value $\epsilon = 0.05$ such that no nonlinear resonances with quantum mechanically recognizable size, i.e., $\sim\sqrt{\hbar}$) are visible on the Poincaré plot. As mentioned above, at a relatively large value $\hbar = \hbar_0 \equiv \sqrt{\epsilon}/1.5$ the tunneling amplitude follows exactly the instanton amplitude, as shown in Fig. 2(a), but when $\hbar$ is halved, $\hbar = \hbar_0/2$, as in Fig. 2(b) there emerges a state with the quantum number n_c beyond which the tunneling amplitude is drastically enhanced from the instanton amplitude. As $\hbar$ is halved further, the drastic transition is more evident [see Fig. 2(c)]. This sudden transition implies that the tunneling process due to the instanton is overwhelmed by some other coexistent process. This shares some features with the crossover from the instanton to the CSUM mechanism reported for a multidimensional scattering-tunneling process [13]. But the transition reported in it is smooth and is not so sharp as in the present case, which might reflect the analyticity of the perturbation. We note that the sharp transition demonstrated above is observed by the tunneling rate defined as the imaginary part of the eigenangle, because it is proportional to the square of the tunneling amplitude far from the potential barrier.

Next, we focus our attention on the relation between the observed drastic increase of tunneling amplitude and the NB. As shown in Fig. 1, the instanton branch always intersects with the NB, and moreover, until the intersection, the instanton approximation based on the existing set $\mathcal{T}_i$ of the quantum map should work well. Therefore, the increase of the tunneling amplitude should occur out of the intersection, that is, $q < q^*$. Indeed, as demonstrated above, the instanton wave function of the effective Hamiltonian $H_{\rm eff}^{(m)}$ approximates the exact tunneling tail at least up to q^*, and moreover, it approximates well the exact tunneling rate if the transition does not take place. Therefore, we use $\mathcal{T}_i$ of $H_{\rm eff}^{(m)}$ as the quasiextension of the exact $\mathcal{T}_i$ beyond $q = q^*$ and use the instanton wave function $\Psi_n^{\rm inst}(q)$ of $H_{\rm eff}^{(m)}$ as the reference for the comparison

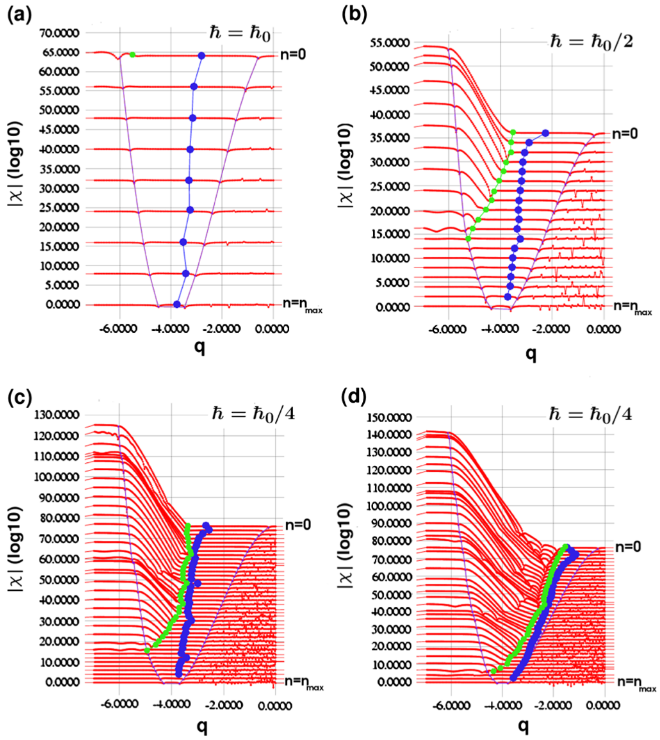

FIG. 3 (color online). The red curves show $|\chi_n(q)|$ (log scale) vs q for eigenstates from $n = 0$ to $n = n_{\max}$. The curves are shifted constantly with n, and almost straight parts in each curve in the range $q > -2$ indicate $|\chi_n(q)| \approx 1$. Blue and green lines show $q^*(n)$ and $q^c(n)$, respectively. The positions of q_3 and q_2 are drawn as purple lines. $\epsilon = 0.05$ for (a–c), which correspond to the cases shown in the three figures of Fig. 3. The value of ϵ is taken to be larger in (d): $\epsilon = 0.15$.

with the exact wave function $\Psi_n(q)$. To clarify quantitatively the expected increase beyond $q = q^*$, we define the ratio

$$\chi_n(q) = \Psi_n(q)/\Psi_n^{\mathrm{inst}}(q), \tag{4}$$

as a function of q. Since q^* is the projection of the intersection of the instanton branch with the NB onto the q-coordinate, and varies with the quantum number n, we here introduce $q^*(n)$ to show explicitly its n dependence. The position of q^* is most distant from the turning point q_2 at the ground state ($n = 0$), but it comes closer to q_2 as we move from the ground state $n = 0$ toward the classically bounded highest excited state (see Fig. 3). We also denote by $q = q^c(n)$ the characteristic q beyond which $|\chi_n(q)|$ increases notably from unity. What we are most interested in is the relation between $q^c(n)$ and $q_n^*(n)$.

In Fig. 3, we show how the ratio $|\chi_n(q)|$ deviates from unity as a function of q for n scanned from 0 to $n_{\max}$. Fig. 3(a) corresponds to Fig. 2(a), where $\hbar = \hbar_0$ is relatively large and no transition from the instanton tunneling amplitude occurs. Then $\chi_n(q)$ is almost equal to 1, indicating that the instanton approximation works very well. As $\hbar$ is halved the transition from the instanton happens as Fig. 2(b) depicts, and there emerges the threshold quantum number n_c below which $\chi_n(q)$ exhibits an exponential increase at a certain $q = q^c(n)$. The increase saturates beyond q_3.

For $n < n_c$, the threshold $q^c(n)$ moves toward the point $q = q^*(n)$. As $\hbar$ is halved further, the curve $q^c(n)$ overall shifts toward q^* and quickly reaches just the outer side of $q = q^*(n)$ as n decreases from n_c. With further decrease in n, the curve runs almost in parallel with $q^*(n)$. In Fig. 3(d), we show the same result for a larger ϵ ($\epsilon = 0.15$) and the same $\hbar$ as in Fig. 3(c), where $q^c(n)$ moves more closely to $q^*(n)$ with n, implying a more serious effect of NB.

The result of numerical studies summarized as (i) $n_{\max} - n_c$ is insensitive to $\hbar$, but it increases as ϵ decreases, (ii) as n is reduced from n_c, the distance $|q^c(n) - q^*(n)|$ tends to a finite value and (iii) the distance $|q^c(n) - q^*(n)|$ goes to zero as $\hbar \to 0$. These results mean that, if $\hbar$ is sufficiently small, in most of the eigenstates with a quantum number less than n_c, drastic enhancement from the instanton tunneling amplitude occurs immediately outside of the intersection $q = q^*(n)$ with the NB.

We have demonstrated clear evidence revealing a critical role of the NB in the tunneling problem. In particular, the observed transition from the instanton tunneling process is shown to be closely related with the presence of the NB. It is not necessary to make $\hbar$ "extremely small" in order to observe the effect of the NB, which manifests itself as a remarkable enhancement of tunneling amplitude just in the outer side of the NB. This fact implies that the enhancement beyond the NB is not due to a mechanism such as resonance assisted tunneling caused by some particular nonlinear resonances. These facts strongly suggest that the "fundamental problem of mechanics" has a particular meaning in the quantum tunneling problem. Detailed theoretical analyses of the transition process will be given in a forthcoming paper.

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