Power-law energy splitting generated by tunnelling between non-smooth tori

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Abstract

We discuss the energy level splitting $\Delta\epsilon$ due to quantum tunnelling between congruent tori in phase space. In analytic cases, it is well known that $\Delta\epsilon$ decays faster than the power of $\hbar$ in the semiclassical limit. This is not true in non-smooth cases, specifically, when the tori are connected by a line on which the Hamiltonian is not smooth. Under the assumption that the non-smoothness depends only upon the x- or p-coordinates, the leading term in the semiclassical expansion of $\Delta\epsilon$ is derived, which shows that $\Delta\epsilon$ decays as $\hbar^{k+1}$ when $\hbar \to 0$ with k being the order of non-smoothness.

PACS numbers: 03.65.Sq, 03.65.Xp, 05.45.-a

1. Introduction

This paper is concerned with the splitting of classically degenerate energy levels. The near degeneracy (ND) classically corresponds to congruent tori in phase space while the quantum tunnelling between the tori causes the splitting[1]. A well known example occurs in the one-dimensional symmetric double-well potential, where the eigenenergies below the top of the barrier cluster into two-fold NDs where the energy difference vanishes as

$$\Delta\epsilon \sim \hbar^\alpha e^{-S/\hbar} \tag{1.1}$$

when $\hbar \to 0$. When turning to multi-dimensional cases, Wilkinson showed that $\Delta\epsilon$ vanishes normally in the same or, in certain situations, an even more singular manner than (1.1) [2]. However, is it always true that the energy level splitting resulting from quantum tunnelling is smaller than any power of $\hbar$ in the semiclassical limit? Let us see the following example.

Consider the system on a one-dimensional circle defined by any of the four Hamiltonians,

$$
\begin{aligned}
H_1 &= \frac{p^2}{2} + \cos^2 x & H_2 &= \frac{p^2}{2} + |\cos x| \\
H_3 &= |p| + \cos^2 x & H_4 &= |p| + |\cos x|.
\end{aligned}
\tag{1.2}
$$

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[1] In this paper, the word 'tunnelling' refers to the quantum transition between states that classically correspond to separate tori in phase space [1].

In classical mechanics, the above Hamiltonians determine similar phase space portraits, particularly the motion at $H \neq 1$ contains two symmetric closed orbits: the two vibrational orbits with $H < 1$ are connected by the transition $(x, p) \rightarrow (x + \pi, p)$ and the two rotational orbits with $H > 1$ are connected by the time reversal $(x, p) \rightarrow (x, -p)$. According to the Einstein–Brillouin–Keller (EBK) semiclassical quantization rule, this classical degeneracy implies a two-fold ND structure in the spectrum of H. We can verify this prediction by directly diagonalizing the Hamiltonians. In figure 1, $\Delta\epsilon$ is plotted as a function of the mean energy of the ND pair (ϵ). As expected, $\Delta\epsilon$ (open dots) is much smaller than the spacing of ϵ (approximately the dotted lines). However, in contrast with the exponential decay of $\Delta\epsilon$ with the increase of $|\epsilon - 1|$ in figure 1(a), non-exponential decay of $\Delta\epsilon$ in some cases is obvious. From the four illustrations, we can see that the 'exceptional' ND occurs when and only when the corresponding classically degenerate tori (closed orbits) in phase space are connected by line(s) where the Hamiltonian is not smooth. This fact suggests that tunnelling between the degenerate tori can be greatly enhanced by the passage of non-smoothness.

In fact, Berry showed this non-smoothness-enhanced quantum transition between classically degenerate states about two decades ago [3]. In studying the coefficient r for reflection above a barrier $V(x)$ in the semiclassical limit, Berry proved that $r \sim \hbar^k$ when $V(x)$ has a discontinuous kth derivatives, in contrast to the analytic case where r is exponentially small. Another interesting quantum manifestation of non-smoothness, the power-law localization of eigenstates, has also been discussed in more recent papers (e.g. [5–7]).

In this paper we shall investigate the energy level splitting resulting from the non-smoothness-enhanced tunnelling. We first consider the case where ND is related to the time reversal symmetry. Using a perturbation method, a relation between $\Delta\epsilon$ and the non-smoothness of the potential is derived. Based on a geometrical interpretation, this relation is applied to a class of non-smooth systems.

2. Power-law energy splitting

In this section we study systems where ND is related to the time reversal symmetry. The problem is more tractable since the projection of torus onto the coordinate space contains no singularity (caustic). By the perturbation method, we obtain an explicit power-law $\hbar$-dependence of the energy splitting.

Consider a mechanical system on a one-dimensional circle with Hamiltonian $H = E_k(p) + V(x)$, $V(x + 2\pi) = V(x)$. The kinetic energy $E_k(p)$ satisfies $E_k(-p) = E_k(p)$, and, for simplicity, we assume $E_k(0) = 0$, $E_k(\infty) = \infty$ and $\frac{d}{dp}E_k(p) > 0$ when $p > 0$. A familiar example of such kinetic energy is $\frac{1}{2}p^2$. Due to the time reversal symmetry, the two classical orbits at $H(x, p) = E > \max_x V(x)$, O_E^+ and O_E^-, one with $p > 0$ and the other with $p < 0$, yield an identical action integral, i.e.

$$\oint_{O_E^+} p \, dx = \oint_{O_E^-} p \, dx = S(E). \tag{2.1}$$

Consequently, the EBK quantization condition $S(E) = 2n\pi\hbar$ predicts a two-fold degenerate level $E = \epsilon_n$. The two semiclassical eigenfunctions are given by

$$\Psi_n^\pm(x) = \frac{1}{\sqrt{T_n \dot{x}_n}} \exp[\pm i s_n(x)/\hbar] \tag{2.2}$$

where $s_n(x) = \int_0^x p_n(x') \, dx'$, $p_n(x) > 0$ is determined by $E_k(p) + V(x) = \epsilon_n$, $\dot{x}_n = \frac{d}{dp}E_k(p)|_{p=p_n(x)}$ is the classical velocity and the normalization constant $T_n = \int_0^{2\pi} \frac{dx}{\dot{x}_n}$ is the period of the corresponding classical orbit [4]. (The suffix 'n' of ϵ, Ψ, p, $\dot{x}$, T and s will be hereafter dropped for simplicity.)
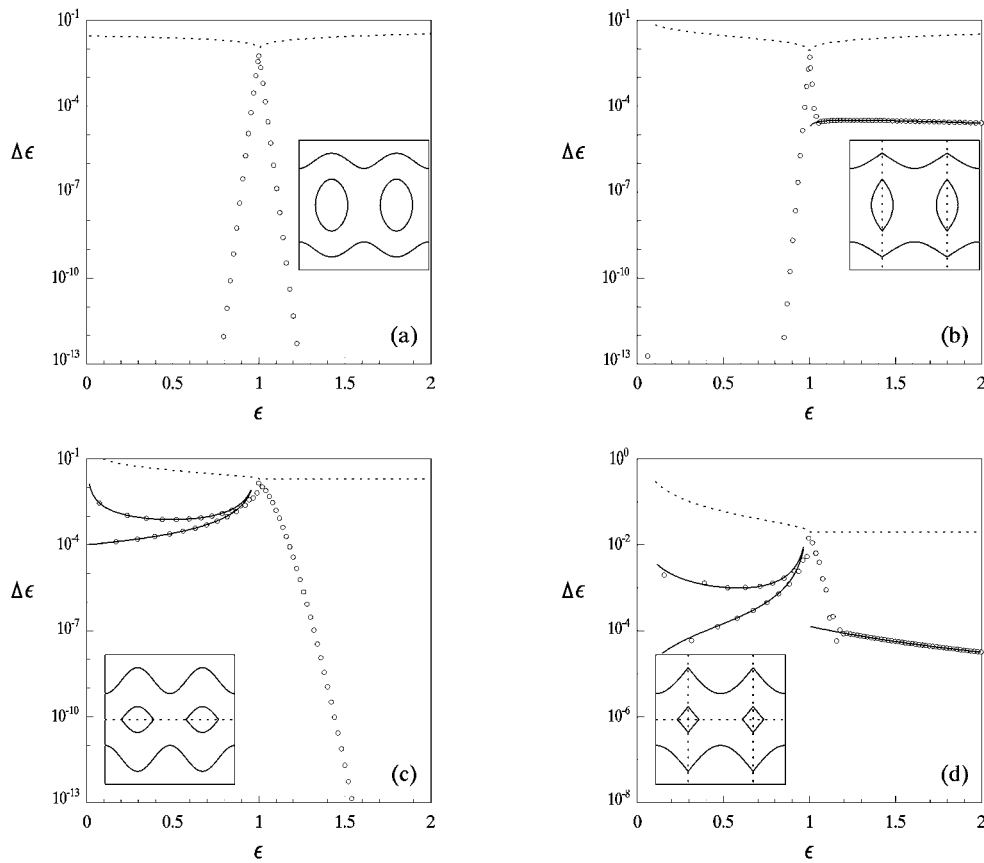
Figure 1. Splitting of nearly degenerate energy levels. (*a*)–(*d*) For $H = H_1$, H_2, H_3 and H_4, respectively. The numerical result of $\Delta\epsilon$ (open circles), the spacing of semiclassical levels (dotted curves) and the semiclassical approximation of $\Delta\epsilon$ (solid curves) are shown at $\hbar = 0.02$. The insets show the degenerate tori (solid curve) in phase space where H is not smooth on the dotted curves.

Of course, in general, the two levels do not exactly coincide. The difference between ϵ and the exact eigenenergy is of order $o(\hbar)$ in the semiclassical limit ($\hbar \to 0$, $n \to \infty$ while $n\hbar$ is fixed). In the case that $V(x)$ is not smooth (infinitely differentiable), we have seen in the last section (H_2 and H_4) that the splitting of energy levels ($\Delta\epsilon$) is not exponentially small. It is therefore possible that a non-vanishing $\Delta\epsilon$ will emerge from the higher-order semiclassical corrections. If we are only interested in the leading term in $\Delta\epsilon$, however, variational calculation in the space spanned by Ψ^+ and Ψ^- will give the result. We shall consider the simple case that $V(x)$ is a C^{k-1} function and

$$\bigwedge_x^k V(x) \equiv \lim_{x' \to x+0} \frac{\mathrm{d}^k}{\mathrm{d}x^k} V(x') - \lim_{x' \to x-0} \frac{\mathrm{d}^k}{\mathrm{d}x^k} V(x') \tag{2.3}$$

is well defined, which vanishes on $[0, 2\pi]$ except at discrete points x_j^*, $j = 1, \dots, N < \infty$. Then elementary calculations show that the energy splitting is given by (see the appendix)

$$\Delta\epsilon = \frac{\hbar^{k+1}}{2^k T} \left| \sum_{j=1}^{N} \frac{\exp(2is(x_j^*)/\hbar)}{p^{k+1} \frac{\mathrm{d}}{\mathrm{d}p} E_k|_{p=p(x_j^*)}} \bigwedge_x^k V(x_j^*) \right| + o(\hbar^{k+1}) \equiv \Delta\epsilon^{(0)} + o(\hbar^{k+1}). \tag{2.4}$$

Define a dimensionless measurement of ND by $\eta_n = 2\Delta\epsilon_n/(\epsilon_{n+1} - \epsilon_{n-1})$. Noticing that the semiclassical level spacing is $2\pi\hbar\frac{dE}{dS} = 2\pi\hbar/T$ and according to equation (2.4), we find

$$\eta = \frac{\hbar^k}{2^{k+1}\pi} \left| \sum_{j=1}^{N} \frac{\exp(2is(x_j^*)/\hbar)}{p^{k+1} \frac{d}{dp} E_k|_{p=p(x_j^*)}} \bigwedge_x^k V(x_j^*) \right| + o(\hbar^k) \equiv \eta^{(0)} + o(\hbar^k). \quad (2.5)$$

Example 2.1.
$H = \frac{1}{2}p^2 + V^{(k)}(x)$, where $V^{(1)}(x) = \max\{\cos x, 0\}$ and $V^{(k)}(x) = [V^{(1)}(x)]^k, k = 2, 3, \ldots$. According to equation (2.5), when $\epsilon > 1$,

$$\eta^{(0)} = \frac{k!\hbar^k}{2^k\pi(2\epsilon)^{\frac{k}{2}+1}} \left| \sin\left[\frac{(2\epsilon)^{\frac{1}{2}}\pi}{\hbar} + \frac{k\pi}{2} \right] \right|.$$

The comparison of η and $\eta^{(0)}$ is shown in figure 2.

Example 2.2.
$H = |p| + V^{(k)}(x)$.
When $\epsilon > 1$, the semiclassical level is given by $\epsilon_n = n\hbar + \alpha_k$ and according to equation (2.4)

$$\Delta\epsilon^{(0)} = \frac{k!\hbar^{k+1}}{2^k\pi\epsilon^{k+1}} \left| \sin\left(\frac{\alpha_k\pi}{\hbar} + \frac{k\pi}{2} \right) \right|$$

where

$$\alpha_k \equiv \frac{1}{2\pi} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos^k x \, dx = \frac{\Gamma\left(\frac{k+1}{2}\right)}{2\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{k}{2}+1\right)}.$$

The comparison of $\Delta\epsilon$ and $\Delta\epsilon^{(0)}$ is shown in figure 3.

3. Sum over transition paths

In this section we first give equation (2.4) a geometrical interpretation. We find the quantum transition between the semiclassical eigenstates can be classically described by the leaking of phase space points from one torus to the other via passage of non-smoothness. This picture will facilitate the generalization of equation (2.4).

The splitting of nearly degenerate energy levels is closely related to the transition probability between the corresponding semiclassical eigenstates. In the classical picture, Ψ^+ describes a particle moving on a circle with $p > 0$. After one classical period, due to quantum tunnelling, the particle has a non-zero probability to jump to the reflection wave Ψ^- with $p < 0$. Write $\exp(\frac{HT}{i\hbar})|\Psi^+\rangle = c|\Psi^+\rangle + \mathcal{A}|\Psi^-\rangle$. Simple calculations show that $\mathcal{A} \approx \frac{T}{\hbar}\langle\Psi^-|(H - \epsilon)|\Psi^+\rangle$ and $\Delta\epsilon \approx \frac{2\hbar}{T}|\mathcal{A}|$. According to equation (A.17), the leading term in $\mathcal{A}$ is the sum of contributions from each non-smooth point of $V(x)$, i.e.

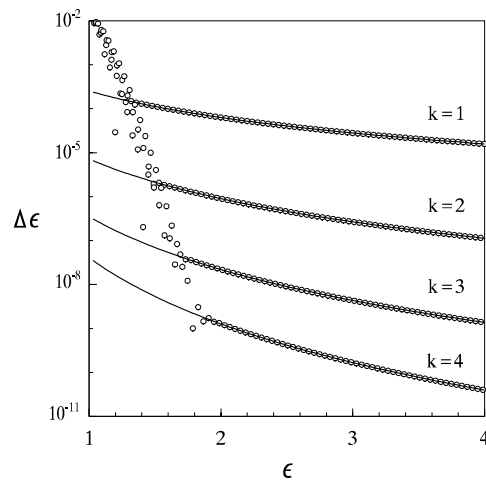$$\mathcal{A} \approx \mathcal{A}^{(0)} = \sum_{j=1}^{N} r_j \exp(i\phi_j) \quad (3.1)$$

with

$$r_j = \frac{(i\hbar)^k}{(2p_j^*)^{k+1}\dot{x}_j^*} \bigwedge_x^k V(x_j^*) \qquad \text{and} \qquad \phi_j = 2s(x_j^*)/\hbar \quad (3.2)$$
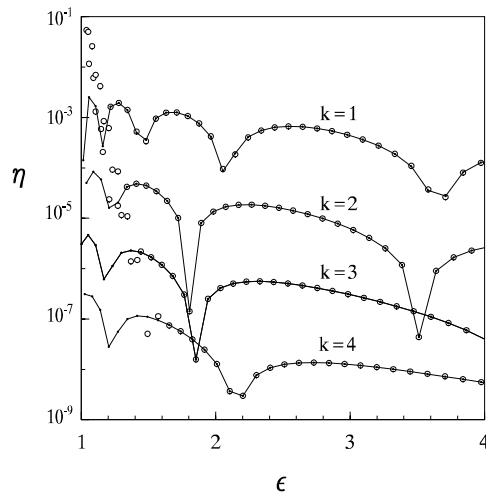
Figure 2. Scaled energy splitting η (open circles) and $\eta^{(0)}$ (connected solid dots) in example 2.1 at $k = 1$–4 and $\hbar = 0.05$.


Figure 3. Energy splitting $\Delta\epsilon$ (open circles) and $\Delta\epsilon^{(0)}$ (solid curves) in example 2.2 at $k = 1$–4 and $\hbar = 0.04$.

where $p_j^* \equiv p(x_j^*)$ and $\dot{x}_j^* \equiv \frac{\mathrm{d}}{\mathrm{d}p}E_k|_{p=p(x_j^*)}$. We note that r_j is exactly the reflection coefficient obtained by Berry[2].

As the classical representation of Ψ^+ and Ψ^-, the tori O_ϵ^+ and O_ϵ^- are connected by the straight line $x = x_j^*$ where H is not smooth. We shall call the vector on $x = x_j^*$ that starts from O_ϵ^+ and ends at O_ϵ^- a *transition path* and denote it by γ_j (figure 4). Accordingly, we can say that $\Psi^+ \to \Psi^-$ is dominated by the tunnelling along the transition path(s). In fact, the reflection coefficient r_j is determined by the local properties of γ_j. Besides a constant, r_j consists of three ingredients. $\bigwedge_x^k V(x_j^*)$ can be regarded as the intensity of non-smoothness at γ_j. $1/(2p_j^*)^{k+1}$

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[2] Berry's calculation was based on $E_k = \frac{p^2}{2}$. However, the result (equation (27) in [3]) is essentially identical to equation (3.2).
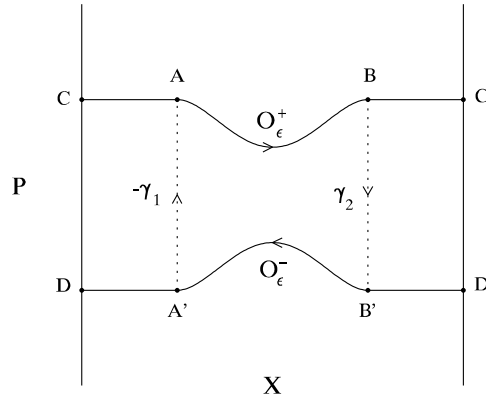
Figure 4. A schematic figure showing the transition paths γ_1 $(A \rightarrow A')$, γ_2 $(B \rightarrow B')$ and closed path γ_{21} $(B \rightarrow B' \rightarrow A' \rightarrow A' \rightarrow B')$. The EBK quantization rule guarantees that $\phi_2 - \phi_1 (\text{mod } 2\pi)$ is independent on the choice of real paths $B' \rightarrow A'$ on O_ϵ^- and $A \rightarrow B$ on O_ϵ^+.

describes a power-law decay with the increase of path length $2p_j^* = \hbar \frac{\partial \phi_j}{\partial x_j^*} \cdot \frac{1}{\dot{x}_j^*}$, which comes from the product of amplitude of semiclassical wavefunctions, gives a classical weight of the transition path: the longer the particle stays in the vicinity of the non-smooth point, the more probable is its jump to the other torus. In contrast to r_j, the phase ϕ_j is not determined by the local properties of γ_j. Since only the relative phase is of physical importance, i.e. gives rise to interference effect, we find

$$\phi_j - \phi_k = \frac{2}{\hbar}(s(x_j^*) - s(x_k^*)) = \frac{1}{\hbar} \oint_{\gamma_{jk}} p \, dx \tag{3.3}$$

where γ_{jk} is a closed path consisting of γ_j, $-\gamma_k$ (γ_k with opposite direction) and the segments of O_ϵ^+ and O_ϵ^- (real paths) that attached at their ends (see figure 4). If γ_{jk} is contractible, $\phi_j - \phi_k$ is simply the phase space area (in the unit of $\hbar$) enclosed by this closed path.

Behind the simple form of equation (3.2) there are two non-generic facts resulting from the assumption that $\frac{d}{dp}E_k(p) > 0$ when $p > 0$: the starting and end points of γ_j are symmetric with respect to $p = 0$ and the projection of O_ϵ^+ or O_ϵ^- onto the coordinate space contains no singularity. Now we ignore this assumption and require only $E_k(-p) = E_k(p)$ to guarantee the time reversal symmetry. Let $A_j = (x_j^*, p_j) \in O_\epsilon^+$ and $A_j' = (x_j^*, p_j') \in O_\epsilon^-$ be the starting and end points of γ_j. By adopting the general semiclassical eigenfunctions corresponding to the tori O_ϵ^+ and O_ϵ^- [4], similar calculations as those performed in the appendix show that equations (3.2), (3.3) should be modified as

$$r_j = \frac{(i\hbar)^k}{(p_j - p_j')^{k+1}\sqrt{|\dot{x}(A_j)\dot{x}(A_j')|}} \bigwedge_x^k V(x_j^*) \tag{3.4}$$

and

$$\phi_j - \phi_k = \frac{1}{\hbar} \oint_{\gamma_{jk}} p \, dx - M_{jk}\pi/2 \tag{3.5}$$

where M_{jk} is the sum of the Maslov indices of the segments of real paths on γ_{jk}. Having the contribution of each transition path, we need only to sum over all these paths to obtain the energy splitting $\Delta \epsilon^{(0)}$ or $\eta^{(0)}$.

Example 3.1.
$H = (p^2 - 1)^2 + V(x)$, where $V(x) = 1 - (\frac{x}{\pi})^2$, $|x| \leqslant \pi$.
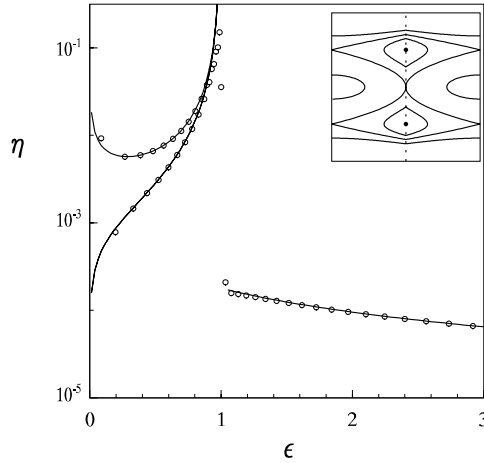
Figure 5. η (open circles) and $\eta^{(0)}$ (solid curves) in example 3.1 at $\hbar = 0.02$. The inset shows three types of tori in phase space. The tori encircling point $(0, 0)$ produce a semiclassically non-degenerate component of the energy spectrum at $1 < \epsilon \leqslant 2$, which has been excluded according to semiclassical criterion that the expectation value of p^2 at the corresponding eigenstates is less than unity.

When $\epsilon < 1$, the Maslov index of O_ϵ^+ (or O_ϵ^-), which encircles point $(\pi, 1)$ (or $(\pi, -1)$), is 2 and EBK quantization condition reads $S(\epsilon_n) = 2(n + \frac{1}{2})\pi\hbar$ (see the inset of figure 5). The straight line $x = \pi$ intersects O_ϵ^+ (or O_ϵ^-) at points $A_{1,2}$ (or $A'_{1,2}$) where $p = (1 \pm \epsilon^{\frac{1}{2}})^{\frac{1}{2}}$ (or $-(1 \pm \epsilon^{\frac{1}{2}})^{\frac{1}{2}}$). There exist four transition paths, i.e. γ_1 ($A_1 \rightarrow A'_1$), γ_2 ($A_2 \rightarrow A'_2$), γ_3 ($A_1 \rightarrow A'_2$) and γ_4 ($A_2 \rightarrow A'_1$). Moreover, the EBK quantization condition implies $\phi_j - \phi_1 = 0, n\pi, n\pi$ (mod 2π) for $j = 2, 3, 4$, respectively. According to equation (3.4), up to a phase

$$\mathcal{A}^{(0)} = \frac{i\hbar}{4\pi\epsilon^{\frac{1}{2}}} \left[\frac{1}{(1 + \epsilon^{\frac{1}{2}})^{\frac{3}{2}}} + \frac{1}{(1 - \epsilon^{\frac{1}{2}})^{\frac{3}{2}}} + (-1)^n \frac{4}{(1 + (1 - \epsilon)^{\frac{1}{2}})(1 - \epsilon)^{\frac{1}{4}}} \right].$$

When $\epsilon > 1$, only γ_1 survives so that

$$\mathcal{A}^{(0)} = \frac{i\hbar}{4\pi\epsilon^{\frac{1}{2}}(1 + \epsilon^{\frac{1}{2}})^{\frac{3}{2}}}.$$

Numerical results show that $\eta^{(0)} = |\mathcal{A}^{(0)}|/\pi$ is a good approximation of η when $\hbar$ is sufficiently small and ϵ is not too close to 1, the energy of the separatrix (figure 5).

The same treatment can be applied to non-smooth systems where ND is originated from spatial symmetries. By substituting $(p, -x) \rightarrow (x, p)$, relations (3.4), (3.5) can be directly transformed to systems where the non-smoothness that results in the transition path depends only upon the p-coordinate. Specifically, consider a transition path γ_j on the straight line $p = p_j^*$ with starting and end points at $A_j = (x_j, p_j^*)$ and $A'_j = (x'_j, p_j^*)$, the corresponding reflection coefficient should be

$$r_j = \frac{(i\hbar)^k}{(x'_j - x_j)^{k+1}\sqrt{|\dot{p}(A_j)\dot{p}(A'_j)|}} \bigwedge\nolimits_p^k H(x, p_j^*). \tag{3.6}$$

The phase difference is also given by equation (3.5), whereas the Maslov index should count the singularity of the projection of the torus onto the momentum space[3]. Despite this similarity,

[3] We use $\omega_1 = p\,dx$ instead of $\omega'_1 = -x\,dp$ based on two facts. Firstly, $\oint_{\gamma_{jk}} \omega_1 = \oint_{\gamma_{jk}} \omega'_1$ when γ_{jk} is contractible. Secondly, if the coordinate space has non-trivial topology, ω_1 is well defined while ω'_1 is not. We find that this choice is justified by numerical results.

interesting behaviour may occur when the configuration space has a non-trivial topology. We shall demonstrate this through some examples.

Suppose the configuration space is a circle, i.e. (x, p) and $(x + 2\pi, p)$ describe the same point. In this case, a path $(x, p) \rightarrow (x', p)$ implies a family of paths $(x, p) \rightarrow (x' + 2n\pi, p), n \in Z$. If we attribute the contribution of all these paths to a representative path, say, $(x, p) \rightarrow (x', p)$, the only change of equation (3.6) is that $1/(x'_j - x_j)^{k+1}$ should be replaced by

$$\sum_{q=-\infty}^{\infty} \frac{\exp(\mathrm{i}2q\pi p^*_j/\hbar)}{(x'_j - x_j + 2q\pi)^{k+1}} \equiv W_{k+1}(x'_j - x_j, p^*_j/\hbar). \tag{3.7}$$

W satisfies periodic condition $W_k(x, y + 1) = \mathrm{e}^{\mathrm{i}2\pi y} W_k(x + 2\pi, y) = W_k(x, y)$. When $y \in [0, 1]$,

$$W_2(x, y) = \frac{1}{4\sin^2 \frac{x}{2}}[1 + y(\mathrm{e}^{\mathrm{i}x} - 1)]\mathrm{e}^{-\mathrm{i}xy}$$

$$W_3(x, y) = \frac{1}{8\sin^3 \frac{x}{2}}\left[\cos\frac{x}{2} + \mathrm{i}2y\sin\frac{x}{2} - 2y^2\sin^2\frac{x}{2}\mathrm{e}^{\mathrm{i}\frac{x}{2}}\right]\mathrm{e}^{-\mathrm{i}xy} \tag{3.8}$$

and so on. We note that $\mathcal{A}^{(0)}$ is in general not invariant under the translation $(x, p) \rightarrow (x, p + \delta_p)$ when δ_p is not an integer multiple of $\hbar$, which is, however, always a symmetric transformation in classical mechanics. This difference reflects the discreteness of quantum momentum space.

Example 3.2.
$H = |p - p_c| + \cos^2 x.$
The symmetric double-well potential causes ND at $\epsilon < 1$. According to equations (3.6) and (3.7), the total contribution of the transition paths (on $p = p_c$) is given by

$$\mathcal{A}^{(0)} = \frac{\mathrm{i}\hbar}{\epsilon^{\frac{1}{2}}(1 - \epsilon)^{\frac{1}{2}}}\left[W_2\left(2x_c, \frac{p_c}{\hbar}\right) + W_2\left(2\pi - 2x_c, \frac{p_c}{\hbar}\right) + (-1)^n 2W_2\left(\pi, \frac{p_c}{\hbar}\right)\right]$$

where $x_c = \cos^{-1}\epsilon^{\frac{1}{2}}$. When $p_c = 0$, $\mathcal{A}^{(0)} = (\mathrm{i}\hbar/(2\epsilon^{\frac{1}{2}}(1 - \epsilon)^{\frac{1}{2}}))[\frac{1}{1-\epsilon} + (-1)^n]$. When $p_c = \frac{\hbar}{2}$, $\mathcal{A}^{(0)} = 0$. In fact, $\Delta\epsilon \equiv 0$ in this case because H is represented by the same matrix in the invariant subspaces spanned by functions $\{\mathrm{e}^{\mathrm{i}2nx}\}_n$ and $\{\mathrm{e}^{\mathrm{i}(2n+1)x}\}_n$, respectively.

Consider a spin system defined in classical and quantum mechanics by respectively $\{J_j, J_k\} = \varepsilon_{jks}J_s$ and $[J_j, J_k] = \mathrm{i}\hbar\varepsilon_{jks}J_s$, $j, k = 1, 2, 3$. When $J^2 = J_1^2 + J_1^2 + J_3^2$ is fixed, the classical mechanics is confined within a sphere $\mathcal{S}_J$. Restricting the $su(2)$ Poisson structure to $\mathcal{S}_J$ yields a symplectic two form $\omega_2 = J\sin\theta\,\mathrm{d}\phi \wedge \mathrm{d}\theta$, where (θ, ϕ) is the conventional sphere coordinate. In quantum mechanics, $J^2 = j(j+1)\hbar^2$, $j = \frac{1}{2}, 1, \frac{3}{2}, \ldots$. An eigenspace of J^2 is associated with a classical sphere $\mathcal{S}_J$, in which we shall assume $J = (j + \frac{1}{2})\hbar$ so that its phase space area (the integral of ω_2 on $\mathcal{S}_J$) in units $2\pi\hbar$ is $2j + 1$, which directly corresponds to the dimension of the eigenspace. In our treatment of non-smooth systems, a prerequisite is that the phase space is the direct product of the coordinate and momentum spaces. To meet this requirement, we write $(J\cos\theta + p_0, \phi) = (p, x)$, in which $\omega_2 = \mathrm{d}p \wedge \mathrm{d}x$, and regard (x, p) as the natural coordinate of the phase space of a mechanical system on a circle. Moreover, to ensure the right spectrum of $J_3 = p - p_0$, we choose $p_0 = 0$ (or $\frac{1}{2}\hbar$) in the case of j is an integer (or half integer). By this transformation in classical mechanics, we can treat the non-smoothness-enhanced tunnelling in some spin systems.
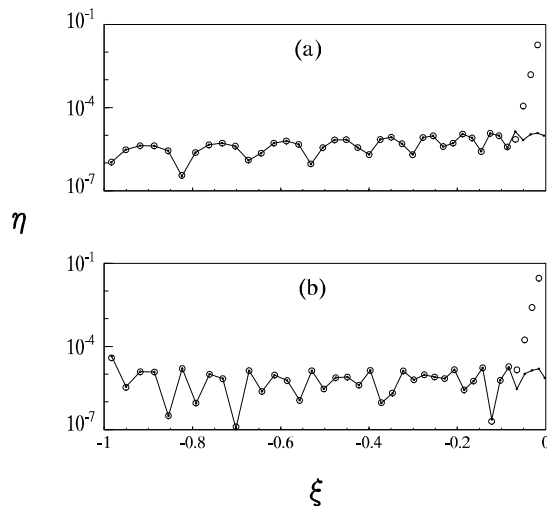
Figure 6. η (open circles) and $\eta^{(0)}$ (connected dots) in example 3.3 at (a) $j = 100$ and (b) $j = 99\frac{1}{2}$.

Example 3.3.

$$H(J_1, J_2, J_3) = \begin{cases} J_1^2 - J_2^2 + J_3^2 & J_3 \geqslant 0 \\ J_1^2 - J_2^2 & J_3 < 0. \end{cases}$$

The corresponding classical system on a circle is

$$H(x, p) = \begin{cases} [J^2 - (p - p_0)^2]\cos 2x + (p - p_0)^2 & p \geqslant p_0 \\ [J^2 - (p - p_0)^2]\cos 2x & p < p_0. \end{cases}$$

From phase space portrait we know that energy levels in $(-J^2, 0)$ consist of two-fold ND and according to equations (3.6) and (3.7),

$$\mathcal{A}^{(0)} = \frac{-\hbar^2}{J^2 \sin 2x_c} \left[W_3\left(2\pi - 2x_c, \frac{p_0}{\hbar}\right) + W_3\left(2x_c, \frac{p_0}{\hbar}\right) e^{2i(\phi - \frac{\pi}{2})} + 2W_3\left(\pi, \frac{p_0}{\hbar}\right) e^{i(\phi - \frac{\pi}{2})} \right]$$

where $x_c = \frac{1}{2}\cos^{-1}\xi$ with $\xi \equiv \epsilon/J^2$ and $\phi = \pi J(1 - \sin x_c)/\hbar = \pi(j + \frac{1}{2})[1 - (\frac{1-\xi}{2})^{\frac{1}{2}}]$. When j is an integer,

$$|\mathcal{A}^{(0)}| = \frac{|\cos \phi|}{2(j + \frac{1}{2})^2(1 - \xi)^2}$$

and when j is a half integer,

$$|\mathcal{A}^{(0)}| = \frac{1}{4(j + \frac{1}{2})^2(1 - \xi^2)^{\frac{1}{2}}} \left| \frac{3 + \xi}{\sqrt{2}(1 - \xi)^{\frac{3}{2}}} \sin \phi + \frac{1}{2} \right|.$$

(In this case, $\frac{1}{j + \frac{1}{2}}$ can be regarded as an effective $\hbar$.) These relations give a good description of the energy splitting when $j \gg 1$ (figure 6).

4. Discussion

When the non-smooth system is controlled by a parameter λ, e.g. $V(x) \to \lambda V(x)$, it is easy to obtain a zero of $\mathcal{A}^{(0)}$ when λ is continuously varied. One can naturally ask whether the zero of $\mathcal{A}^{(0)}$ predicts an exact degeneracy of the energy level or if it merely corresponds to a minimum of $\Delta\epsilon$. The answer turns out to be dependent upon the symmetry of the system. If the eigenstates involved in ND can be distinguished by different symmetries irrespective of the parameter, the energy difference between the two eigenstates should be a smooth function of λ, which is approximately given by $\frac{2\hbar}{T}\mathcal{A}^{(0)}$ or a similar expression. In this case, the zero of $\mathcal{A}^{(0)}$ indicates a nearby exact degeneracy. Of course, because of the symmetry of H, this conclusion cannot be regarded as a violation of the well known theorem of von Neumann and Wigner, which states that generically we must vary two parameters to create a degeneracy [8]. On the other hand, if the eigenstates cannot be restricted within different parameter-independent invariant subspaces, e.g., when $H = p^2/2 + \cos x + \lambda|\sin x|$, the zero of $\mathcal{A}^{(0)}$ generally corresponds to a minimum of $\Delta\epsilon$ where we must take the higher order corrections into account.

Acknowledgments

Appendix. Semiclassical calculation of energy splitting

We first consider the conventional Hamiltonian $H = \frac{1}{2}p^2 + V(x)$. Direct calculation show that

$$\left(-\frac{\hbar^2}{2}\frac{d^2}{dx^2} + V(x)\right)\Psi^\pm(x) = (\epsilon + Q(x))\Psi^\pm(x) \tag{A.1}$$

with $Q = -\frac{\hbar^2}{2}p^{1/2}(p^{-1/2})''$, where the prime denotes derivation with respect to x at fixed ϵ. Because $\langle\Psi_+|\Psi_+\rangle = \langle\Psi_-|\Psi_-\rangle = 1$ and $\langle\Psi_-|\Psi_+\rangle \sim 0$, the energy splitting calculated in the space spanned by Ψ^+ and Ψ^- is given by

$$\Delta\epsilon = 2|\langle\Psi^-|Q|\Psi^+\rangle| = \frac{\hbar^2}{2T}\left|\int_0^{2\pi}\left[\frac{V''}{p^3} + \frac{5(V')^2}{2p^5}\right]\exp(i2s(x)/\hbar)\,dx\right|. \tag{A.2}$$

Before evaluating $\Delta\epsilon$ according to equation (A.2), it is helpful to recall a useful mathematical result on the asymptotic behaviour of the Fourier coefficients of a non-smooth function. Let $f(x)$ be a sufficiently regular 2π-periodic function on R. How its Fourier coefficients, defined by

$$\hat{f}(n) = \int_0^{2\pi} f(x)\exp(inx)\,dx \qquad n \in Z \tag{A.3}$$

decay when $n \to \pm\infty$ is basically determined by the analytic property of $f(x)$. If it is smooth, then $\hat{f}(n)$ for large n will approach zero faster than any power of $|n|^{-1}$, i.e. $\lim_{|n|\to\infty}\hat{f}(n)|n|^\alpha = 0$ for arbitrary $\alpha > 0$. On the other hand, if $f(x)$ is not smooth, the decay of $\hat{f}(n)$ may follow a power law. In the simple case when $f(x)$ is the union of N smooth segments on intervals $[x_i^*, x_{i+1}^*]$, $x_1 < x_2 \cdots < x_{N+1} = x_1+2\pi$, $\hat{f}(n)$ can be expressed by the asymptotic series

$$\hat{f}(n) = \sum_{l=0}^\infty \frac{i^{l+1}}{n^{l+1}}\sum_{j=1}^N \exp(inx_j^*)\bigwedge_x^l f(x_j^*). \tag{A.4}$$

Letting $s(x) = n\hbar\theta(x)$, we rewrite equation (A.2) as

$$\Delta\epsilon = \frac{\hbar^2}{2T} \left| \int_0^{2\pi} \left[\frac{V''}{p^3} + \frac{5(V')^2}{2p^5} \right] \frac{n\hbar}{p} \exp(\mathrm{i}2n\theta) \, \mathrm{d}\theta \right|. \tag{A.5}$$

Noticing the integrand apart from $\exp(\mathrm{i}2n\theta)$ is unchanged in the semiclassical limit, according to equation (A.4), we have

$$\Delta\epsilon = \frac{\hbar^{k+1}}{2^k T} \left| \sum_{j=1}^{N} \frac{\exp[2\mathrm{i}s(x_j^*)/\hbar]}{p^{k+2}(x_j^*)} \bigwedge_x^k V(x_j^*) \right| + \mathrm{o}(\hbar^{k+1}). \tag{A.6}$$

Then we consider Hamiltonian $H = E_k(p) + V(x)$. In order to evaluate energy splitting according to $\Delta\epsilon = 2|\langle\Psi^-|H - \epsilon|\Psi^+\rangle|$, it is instructive to go into some detail about the momentum representation of $\Psi^\pm$. Write

$$\Psi^\pm = \sum_{r=-\infty}^{\infty} \phi_r^\pm |r\rangle \qquad \langle x|r\rangle = \frac{1}{\sqrt{2\pi}} \exp(\mathrm{i}rx) \tag{A.7}$$

with

$$\phi_r^\pm = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \Psi^\pm(x) \exp(-\mathrm{i}rx) \, \mathrm{d}x. \tag{A.8}$$

Since $\phi_{-r}^- = \phi_r^{+*}$, we shall focus on Ψ^+. The semiclassical limit of equation (A.8) should be calculated in two separate cases. In the classically permissible region (CPR), where $p(x) - r\hbar = 0$ is satisfied by some $x \in [0, 2\pi)$, the stationary phase approximation can be adopted, which gives

$$\phi_r^+ \approx \sqrt{\frac{\hbar}{T}} \sum_m \frac{1}{\sqrt{|V'(x_m)|}} \exp[\mathrm{i}(s(x_m)/\hbar - rx_m - \sigma_m\pi/2)] \tag{A.9}$$

where $\{x_m\}$ are solutions of $p(x) - r\hbar = 0$ and $\sigma_m = \mathrm{sign}(V''(x_m))$. When $r\hbar$ is beyond CPR, by using expansion (A.4), we find

$$\phi_r^+ \approx \frac{(\mathrm{i}\hbar)^{k+1}}{\sqrt{2\pi T}} \sum_{j=1}^N \frac{\exp[\mathrm{i}(s(x_j^*)/\hbar - rx_j^*)]}{(p - r\hbar)^k \frac{\mathrm{d}}{\mathrm{d}p} E_k} \frac{\mathrm{d}}{\mathrm{d}p} \left[\frac{-1}{(p - r\hbar)\sqrt{\frac{\mathrm{d}}{\mathrm{d}p} E_k}} \right] \Bigg|_{p=p(x_j^*)} \bigwedge_x^k V(x_j^*). \tag{A.10}$$

From equations (A.9) and (A.10) we conclude that Ψ^+ consists of the main part distributed within CPR and two power-law-like long tails beyond CPR. (As the non-smoothness of the eigenfunction resulted via the eigenequation from $V(x)$, this picture is also true for the exact eigenfunction.) Furthermore, if the semiclassical momentum representation of $V\Psi^+$ is calculated using a similar procedure, one can find that the main part of Ψ^+ within CPR, but its long tail approximately satisfies the eigenequation $(E_k(p) + V(x))\Psi = \epsilon\Psi$, i.e.

$$\sum_{m=-\infty}^{\infty} (E_k(r\hbar)\delta_{m,0} + V_m)\phi_{r+m}^+ \approx \epsilon\phi_r^+ \tag{A.11}$$

when $r\hbar \in$ CPR, where

$$V_m = \langle 0|V|m\rangle \approx \frac{i^{k+1}}{2m^{k+1}\pi} \sum_{j=1}^N \exp(\mathrm{i}mx_j^*) \bigwedge_x^k V(x_j^*) \qquad (|m| \to \infty). \tag{A.12}$$

Based on the above discussion, we know that

$$\langle\Psi^-|E_k(p)|\Psi^+\rangle = \sum_{r=-\infty}^{\infty}\phi_{-r}^+ E_k(r\hbar)\phi_r^+ \approx \sum_{|r\hbar|\in\text{CPR}}\phi_{-r}^+ E_k(r\hbar)\phi_r^+$$

$$\approx \left(\sum_{v\hbar\in\text{CPR}}\sum_{\mu=-\infty}^{\infty} + \sum_{-\mu\hbar\in\text{CPR}}\sum_{v=-\infty}^{\infty}\right)\phi_{-v}^+(\epsilon\delta_{v,\mu} - V_{\mu-v})\phi_\mu^+. \tag{A.13}$$

Compare the last expression with

$$\langle\Psi^-|\epsilon - V|\Psi^+\rangle = \sum_{\mu,v=-\infty}^{\infty}\phi_{-v}^+(\epsilon\delta_{v,\mu} - V_{\mu-v})\phi_\mu^+. \tag{A.14}$$

The main contribution of equation (A.14) consists of three parts coming from different regions: (1) $\mu\hbar, v\hbar \in \text{CPR}$, (2) $-\mu\hbar, -v\hbar \in \text{CPR}$ and (3) $\mu\hbar, -v\hbar \in \text{CPR}$, respectively. Equation (A.13) contains only the former two parts while we can screen the last contribution by making a high-frequency cut off of $V(x)$, i.e. replacing it by

$$V^{(0)}(x) = \sum_{|m|\leqslant k_c} V_m \exp(-\mathrm{i}mx) \tag{A.15}$$

where k_c is a large but fixed integer so that $V^{(1)}(x) = V(x) - V^{(0)}(x)$ is negligibly small. Therefore, $\langle\Psi^-|E_k(p)|\Psi^+\rangle \approx \langle\Psi^-|\epsilon - V^{(0)}|\Psi^+\rangle$, and consequently

$$\langle\Psi^-|H - \epsilon|\Psi^+\rangle \approx \langle\Psi^-|V^{(1)}|\Psi^+\rangle = \frac{1}{T}\int_0^{2\pi}\frac{V^{(1)}}{\frac{\mathrm{d}}{\mathrm{d}p}E_k|_{p=p(x)}}\exp(2\mathrm{i}s(x)/\hbar)\,\mathrm{d}x. \tag{A.16}$$

Observing that $V^{(1)}(x) \approx 0$ and $\bigwedge_x^j V^{(1)}(x) = \bigwedge_x^j V(x)$ for arbitrary $x \in [0, 2\pi)$ and $j \geqslant 0$, by partial integration of equation (A.16) for successive $k+1$ times we obtain

$$\langle\Psi^-|H - \epsilon|\Psi^+\rangle = \frac{(\mathrm{i}\hbar)^{k+1}}{2^{k+1}T}\sum_{j=1}^{N}\frac{\exp(2\mathrm{i}s(x_j^*)/\hbar)}{p^{k+1}\frac{\mathrm{d}}{\mathrm{d}p}E_k|_{p=p(x_j^*)}}\bigwedge_x^k V(x_j^*) + \mathrm{o}(\hbar^{k+1}) \tag{A.17}$$

which immediately leads to equation (2.4).

Finally, it is worth pointing out that although the exact eigenstates have power-law tails beyond CPR, the leading term of $\Delta\epsilon$ does not actually rely on this detail. In fact, equation (A.16) essentially equals

$$\sum_{\mu\hbar,-v\hbar\in\text{CPR}}\phi_{-v}^+ V_{\mu-v}\phi_\mu^+$$

which is controlled by the power-law decay of $\{V_m\}$. Therefore, equation (A.16) can be reproduced from the highly localized semiclassical eigenfunctions corresponding to the smoothed Hamiltonian $H^{(0)} = E_k(p) + V^{(0)}(x)$.

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