Decay Rate of Energy Eigenfunctions in Classically Energetically Inaccessible Regions *

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Classically energetically inaccessible parts of energy eigenfunctions in configuration space are studied by making use of a generalization of Brillouin-Wigner perturbation theory. Approximate formulas are proposed for describing local decaying rate of this part of energy eigenfunctions, which are useful in the study of quantum phenomena, such as tunnelling effect, and are tested in an anharmonic oscillator.

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Since the early times of quantum mechanics, it is well-known that energy eigenfunctions (EFs) generally decay exponentially in classically energetically inaccessible regions. One of the consequences of this property is the well-known tunnelling effect, which plays an important role in many quantum phenomena. However, a quantitative description of tunnelling effect is possible only in a limited number of cases. Techniques to dealing with the tunnelling effect, e.g., the Wentzel–Kramers–Brillouin (WKB) approximation, the most probable escape path, and the instanton methods,[1] often fail for systems with more than one degrees of freedom. Therefore, it is still of interest to seek effective techniques in describing properties of EFs in classically energetically inaccessible regions (see, e.g.,[2,3]).

In this Letter, we study the problem from a purely quantum mechanical point of view. As is known, exponential decay of long tails of EFs also exists for EFs expanded in unperturbed basis states, if the associated Hamiltonian matrices have band structure.[4] This phenomenon can be explained by a generalization of Brillouin-Wigner perturbation theory (GBWPT), even in the case of strong perturbation.[5]

We concentrate on the purpose to apply the GBWPT to EFs in configuration space. The basic observation is that the discretized stationary Schrödinger equation has a matrix form with a banded structure. It will be shown that the part of EFs in classically energetically inaccessible regions can be expressed in a convergent perturbative expansion, based on which approximate formulas for the decaying rate of the part of the EFs will be given.

Before discussing the GBWPT in configuration space, let us first give a brief recall of the main results of the GBWPT.[5] Consider a Hamiltonian $H = H^0 + V$, where H^0 is an unperturbed Hamiltonian and V is a perturbation. The eigenstates of the two Hamiltonians H^0 and H are denoted by $|k\rangle$ and $|\alpha\rangle$, respectively, $H^0|k\rangle = E_k^0|k\rangle$, $H|\alpha\rangle = E_\alpha|\alpha\rangle$. For simplicity, we assume that $V_{kk} = 0$. (If $V_{kk} \neq 0$ for some perturbation, one can change H_0 to include the diagonal part of V.)

In the GBWPT, for each state $|\alpha\rangle$, the set of the basis states $|k\rangle$ are divided into two subsets, denoted by P_α and Q_α, respectively (equivalently, P_α and Q_α can also be defined as sets of the labels k). For the sake of clearness, here we often use $|i\rangle$ to denote a basis state in P_α, use $|j\rangle$ to denote a basis state in Q_α, and $|k\rangle$ to denote a basis state that may be in either of the two sets.

We use the concept of path to express the main results of the GBWPT in a compact form. Firstly, for q basis states $|k_l\rangle$ in Q_α, $(l = 0, \cdots, q-1)$, and one basis state $|k_q\rangle$ in either Q_α or P_α, we term the sequence $k_0 \to k_1 \to \cdots \to k_{q-1} \to k_q$ *a path of q paces from* k_0 *to* k_q, denoted by s, if the direct coupling $V_{k_l,k_{l+1}}$ for each pace is non-zero. Secondly, to each pace $k_l \to k_{l+1}$ in a path s, we attribute a factor $D_\alpha^s(k_l \to k_{l+1})$ defined by $D_\alpha^s(k_l \to k_{l+1}) = V_{k_l,k_{l+1}}/(E_\alpha - E_{k_l}^0)$. Finally, we define the contribution of a path s by

$$f_\alpha^s(k_0 \to k_q) = \prod_{l=0}^{q-1} D_\alpha^s(k_l \to k_{l+1}). \tag{1}$$

In the GBWPT, the sets P_α and Q_α are chosen in such a way that for each pair of states $|j\rangle, |j'\rangle \in Q_\alpha$,

$$\lim_{q\to\infty} A_\alpha^q(j \to j') = 0, \tag{2}$$

where $A_\alpha^q(j \to j')$ is the total contribution of the paths with q paces from j to j', defined by $A_\alpha^q(j \to j') = \sum_{s_q} f_\alpha^{s_q}(j \to j')$, where s_q denotes paths with q paces from j to j'. Then, each component $C_{\alpha j} = \langle j|\alpha\rangle$ can be expressed in the following convergent perturbative

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expansion,[5]

$$C_{\alpha j} = \sum_{|i\rangle \in P_\alpha} A_\alpha(j \to i) C_{\alpha i}, \tag{3}$$

where

$$A_\alpha(j \to i) = \sum_s f_\alpha^s(j \to i), \tag{4}$$

with s denoting possible paths from j to i. We call the set of the components $C_{\alpha j}$ the Q-part of the EF of $|\alpha\rangle$. The Q-parts of EFs decay exponentially for Hamiltonians with band structure.[5]

Here we use the GBWPT to study the eigenproblem of the stationary Schrödinger equation in one-dimensional configuration space,

$$-\frac{\hbar^2}{2m_0}\frac{\partial^2\psi_\alpha(x)}{\partial x^2} + V(x)\psi_\alpha(x) = E_\alpha\psi_\alpha(x). \tag{5}$$

We assume that the variable x is restricted within the region (x_a, x_b) (in the limit $x_a \to -\infty$ and $x_b \to \infty$, one has $x \in (-\infty, \infty)$). We would mention that the results presented below are generalizable to EFs in more than one-dimensional configuration spaces.

We discretize the coordinate x, by dividing the interval (a, b) into N small sub-intervals and introducing, $x_k = a + k\Delta x$, with $k = 1, 2, 3, \cdots N-1$, where $\Delta x = (b-a)/N$. In the limit $N \to \infty$, Eq. (5) can be written as $\psi_{k+1} + \widetilde{E}_k^0\psi_k + \psi_{k-1} = \widetilde{E}\psi_k$, for $k = 2, 3, \cdots N-2$, where

$$\widetilde{E}_k^0 = -2 - \frac{2m_0}{\hbar^2}(\Delta x)^2 V(x_k),$$
$$\widetilde{E} = -\frac{2m_0}{\hbar^2}(\Delta x)^2 E_\alpha. \tag{6}$$

Here, for brevity, we use ψ_k to denote $\psi_\alpha(x_k)$. Then, equation (5) is equivalent to the eigenequation of the following Hamiltonian matrix with tridiagonal structure,

$$\widetilde{H}_{kk'} = \widetilde{E}_k^0\delta_{kk'} + \widetilde{V}_{kk'}, \quad \text{with} \quad \widetilde{V}_{kk'} = \delta_{k,k'+1} + \delta_{k,k'-1}. \tag{7}$$

For the Hamiltonian $\widetilde{H}$, the factor of a pace $k_l \to k_{l+1}$ in a path s is

$$D_\alpha^s(k_l \to k_{l+1}) = \left\{2 + \frac{2m_0}{\hbar^2}(\Delta x)^2[V(x_{k_l}) - E_\alpha]\right\}^{-1}. \tag{8}$$

Since $\widetilde{V}$ couples the nearest labels only, paths given by $\widetilde{V}$ have the following properties: (i) There is no path linking j and k, if there exists a label $i \in P_\alpha$ between j and k, e.g., $j < i < k$. (ii) As a result, the summation on the right-hand side of Eq. (3) is performed only over those labels $i \in P_\alpha$ that are successive to some $j' \in Q_\alpha$, with $|i - j'| = 1$.

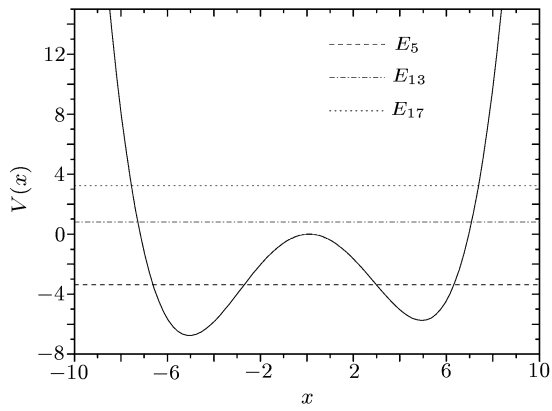

Fig. 1. Potential $V(x) = \mu_1 x - kx^2/2 + \mu_2 x^4$ in the Hamiltonian (17), with $k = 1, \mu_1 = 0.1$ and $\mu_2 = 0.01$, and positions of three eigenenergies E_α of $\alpha = 5, 13$, and 17.

By counting the number of paths with q paces and using that the denominator on the right-hand side of Eq. (8) is larger than 2 for points x satisfying $V(x) > E_\alpha$, one can show that the part of an EF in any classically energetically inaccessible region is a Q-part of the EF. The region of x associated with a Q-part of an EF is called a *Q-region* of the EF. Suppose that (x_c, x_d) is a Q-region of an EF α, then,

$$\psi_j = A_\alpha(j \to c)\psi_c + A_\alpha(j \to d)\psi_d, \quad c < j < d. \tag{9}$$

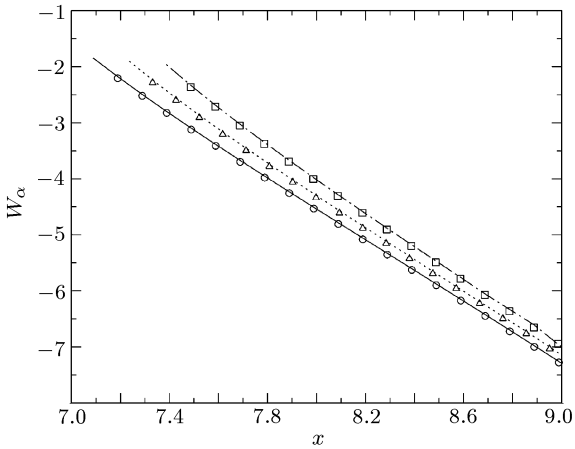

Fig. 2. Comparisons between the values of $W_\alpha(x)$ calculated from Eqs. (14)–(16) for $\alpha = 13$ (circles), $\alpha = 15$ (triangles), and $\alpha = 17$ (squares), and the values of $W_\alpha(x)$ calculated directly from numerical solutions of the eigenfunctions of $\alpha = 13$ (solid curve), $\alpha = 15$ (dashed curve), and $\alpha = 17$ (dashed-dot curve), respectively. The Hamiltonian is the one in Eq. (17), with $m_0 = 1, k = 1, \hbar = 1, \mu_1 = 0.1$ and $\mu_2 = 0.01$.

In applying the above results, let us first discuss tails of EFs in classically energetically inaccessible regions. For right tails, $\psi_d = 0$ in Eq. (8), while $\psi_c = 0$ for left tails. Without loss of generality, we discuss right tails in the Q-region (x_c, x_b). Taking an arbitrary point $x_j > x_c$, the region (x_j, x_b) is also a Q-

region, since it is also classically energetically inaccessible. Then, for any $j' > j$,

$$\psi_{j'} = A_\alpha(j' \to j)\psi_j. \tag{10}$$

The quantity we are to discuss is $W_\alpha(x) = [d\psi_\alpha(x)/dx]/\psi_\alpha(x)$. This quantity gives the local decay rate of $\psi_\alpha(x)$, which is useful in the study of decaying behavior of eigenfunctions, such as tunnelling effect. Taking $x_{j'} = x_j + \Delta x$, i.e., $j' = j+1$, and letting $\Delta x \to 0$, we have

$$W_\alpha(x) = \lim_{\Delta x \to 0}[A_\alpha(j+1 \to j) - 1]/\Delta x, \tag{11}$$

with $x = \lim_{\Delta x \to 0} x_j$. Since $\psi_\alpha(x + \Delta x)$ approaches $\psi_\alpha(x)$ when $\Delta x \to 0$, from Eqs. (4), (8), and (10) we have

$$\lim_{\Delta x \to 0} A_\alpha(j+1 \to j) = \sum_s (1/2)^{q_s} = 1, \tag{12}$$

where q_s is the number of paces of the path s from $j+1$ to j. Substituting Eqs. (4), (8) and (12) into (11), we have

$$W_\alpha(x) = -\lim_{\Delta x \to 0} \sum_s \left(\frac{1}{2}\right)^{q_s} \left\{ \left[\sum_{l=0}^{q_s - 1} \frac{m}{\hbar^2}(V(x_{k_l}) - E_\alpha) \right] \Delta x + O((\Delta x)^3) + \cdots \right\}, \tag{13}$$

where s indicates all the paths starting at $j+1$ and ending at j. We write the right-hand side of Eq. (13) in an integral form, the limit $x_b \to \infty$,

$$W_\alpha(x) = -\int_x^\infty u(y) g(x,y) dy, \tag{14}$$

where $u(y) = (2m_0/\hbar^2)[V(y) - E_\alpha]$ and $g(x,y)$ is determined by the summations in Eq. (13).

It is difficult to derive an explicit expression for the function $g(y)$ from Eq. (13). Instead, we give a conjecture on its form, based on the following properties: (i) $g(x,y)$ gives a measure for the weight of $u(x)$, i.e., the probability for $u(x)$ to appear in the summations in Eq. (13); (ii) for long paths with large q_s, most of the paths can be viewed as random walks under the restriction of starting at $j+1$ and ending at j, therefore $g(x,y)$ may have a form such as $\exp(-\alpha'(y-x)^2)$. The quantity α' should have the same dimension as $1/x^2$. Note that the quantity $u(y)$ has this dimension, hence the simplest choice for $g(x,y)$ is

$$g(x,y) = \mathcal{N} e^{-u(y)\cdot(y-x)^2}, \tag{15}$$

with

$$\mathcal{N} \int_x^\infty \sqrt{u(y)} e^{-u(y)\cdot(y-x)^2} dy = 1, \tag{16}$$

where the term $\sqrt{u(x)}$ is introduced for balancing the dimension of dy.

It is easy to check that Eqs. (14)–(16) give correct results for the case of $V(x)$ being a constant in the region (x_c, ∞). What is of more interest is to test these equations for more complicated potentials. We have studied the system

$$H = \frac{1}{2m_0}p^2 - \frac{1}{2}kx^2 + \mu_1 x + \mu_2 x^4. \tag{17}$$

The shape of the potential in this system is shown in Fig. 1. Its EFs can be obtained numerically, by which the values of $W_\alpha(x)$ can be calculated directly. In Fig. 2, we present the predictions of Eqs. (14)–(16) for $W_\alpha(x)$ of the right tails of $\psi_\alpha(x)$ of $\alpha = 13, 15$, and 17, in comparison with direct numerical calculations.

Next, we study the values of $W_\alpha(x)$ in regions with the tunnelling effect. Suppose $V(x) = E_\alpha$ at four points $x_{c'} < x_c < x_d < x_{d'}$. For x in the regions $(x_{c'}, x_c)$ and $(x_d, x_{d'})$, the potential $V(x)$ is lower than the eigenenergy E_α; while for x in the other regions, $V(x) > E_\alpha$. For $x \in (x_c, x_d)$, $\psi_\alpha(x)$ is given by Eq. (9).

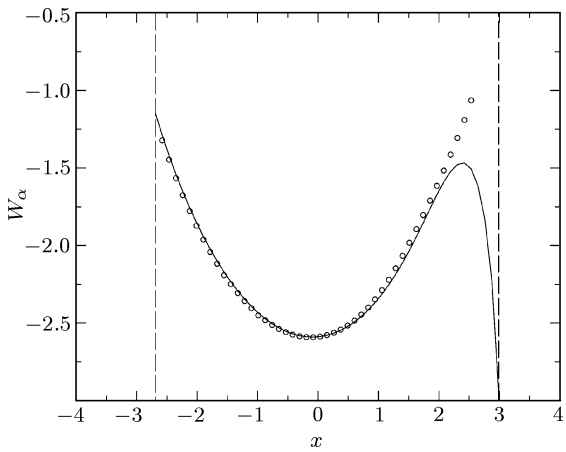

Fig. 3. Comparison of $W_\alpha(x)$ calculated from Eqs. (14), (18) and (19) for $\alpha = 5$ (circles) and those calculated directly from the numerical solution of the eigenfunction $\psi_5(x)$ (solid curve). The two vertical dashed lines indicate the boundary of the region with the tunnelling effect.

In the tunnelling phenomena, $|\psi_\alpha(x)|$ at one of the two points x_c and x_d is much larger than the other, say $|\psi_\alpha(x_c)| \gg |\psi_\alpha(x_d)|$, then, Eq. (9) gives $\psi_\alpha(x) \approx A_\alpha(x \to x_c)\psi_\alpha(x_c)$, for x not close to the point x_d. Following the arguments leading to Eq. (14), we are led to the same expression for $W_\alpha(x)$ in this case. However, the form of the function $g(x,y)$ in Eq. (15) is unsuitable here, since it gives $g(x, x_d) = \mathcal{N}$, which is in confliction with the above interpretation of $g(x,y)$ requiring that $g(x,y)$ be very small at $y = x_d$. For this reason, we have the following assumption for $g(x,y)$,

$$g(x,y) = \mathcal{N} e^{-u(y)\cdot(y-x)^2}(1 - e^{-u(y)\cdot(y-x)^2}), \tag{18}$$

$$\mathcal{N}\int_{x}^{x_{d'}}\sqrt{u(y)}e^{-u(y)\cdot(y-x)^2}(1-e^{-u(y)\cdot(y-x)^2})dy=1. \tag{19}$$

We have tested the above predictions in Eqs. (14), (18), and (19) for the Hamiltonian in Eq. (17), whose EFs with $\alpha \leq 11$ have the tunnelling effect. The results are presented in Fig. 3 for $\alpha = 5$, showing good agreement with direct calculations, at x not close to x_d, the right border of the tunnelling region.

In summary, we have presented a convergent perturbation expansion for EFs in classically energetically inaccessible regions in one-dimensional configuration space. Based on the analysis of the form of the expansion, conjectures are given on approximate expressions for the modulus of the gradient of EFs, which have been tested numerically. The approach developed here can be used in the study of the tunnelling effect, which is completely different from other approaches, e.g., no imaginary eigenenergy appears in our approach. It would be of interest to carry out a direct comparison of the method here and other methods, such as the instanton method (see, e.g.,[6]) in the future.

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