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TUNNEL SPLITTING OF THE SPECTRUM AND BILOCALIZATION OF EIGENFUNCTIONS IN AN ASYMMETRIC DOUBLE WELL

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We consider the one-dimensional stationary Schrödinger equation with a smooth double-well potential. We obtain a criterion for the double localization of wave functions, exponential splitting of energy levels, and the tunneling transport of a particle in an asymmetric potential and also obtain asymptotic formulas for the energy splitting that generalize the well-known formulas to the case of mirror-symmetric potential. We consider the case of higher energy levels and the case of energies close to the potential minimums. We present an example of tunneling transport in an asymmetric double well and also consider the problem of tunnel perturbation of the discrete spectrum of the Schrödinger operator with a single-well potential. Exponentially small perturbations of the energies occur in the case of local potential deformations concentrated only in the classically prohibited region. We also calculate the leading term of the asymptotic expansion of the tunnel perturbation of the spectrum.

Keywords: tunneling, quasi-intersection of energy levels, one-dimensional Schrödinger equation, semiclassical approximation

1. Introduction

Interest in quantum tunneling is seen in many fields of contemporary physics (see, e.g., [1], [2]). One of the basic tunneling models is one-dimensional motion in a potential field with the shape of a generally asymmetric double well. The problem of investigating the spectrum and wave functions analytically in the case of a potential with two wells has a rich history: the first qualitative results were already obtained back in 1927 [3].

We consider the semiclassical asymptotic behavior of the wave functions of the one-dimensional stationary Schrödinger equation

$$\left(-\hbar^2\frac{d^2}{dx^2}+V(x)\right)\psi=E\psi,\quad 0<\hbar\ll 1,$$

where $\hbar$ is the small parameter of the semiclassical approximation.

We assume that the smooth real potential $V(x)$ has the shape of a double well (see Fig. 1), i.e., the classical region of particle motion ($V(x)<E$) consists of two finite intervals. There is a potential barrier between the two wells, and the energy E is not near the potential barrier peak. We assume that the energy spectrum is discrete near E. It is known that in the case of a mirror-symmetric potential, this spectrum consists of pairs of exponentially close points and the corresponding eigenfunctions are symmetric and antisymmetric [4]. This results in the effect of tunneling transport when a particle initially located in one of the wells can be discovered in the other well with a probability close to unity after a certain time.

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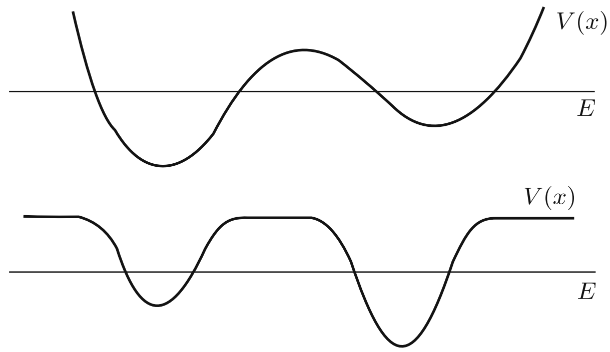

Fig. 1

An analogue of this result for a symmetric well was also obtained in the multidimensional case, namely, the asymptotic behavior of the splitting of the lower energy level is known [5].

Here, we study the case of an asymmetric potential $V(x)$. Such potentials are interesting from the physical standpoint (see [1], [6]), and the problem is significantly more complicated in the asymmetric case. But numerical calculations demonstrate that the double localization of eigenfunctions still occurs [1], [7], [8].

Considering numerically solved examples, we see that the spectrum of an operator with a double-well potential near the energy E, with a certain accuracy, consists of points E_ℓ and $E_{\rm r}$ corresponding to the spectra of the Schrödinger operator separately considered in the left and right potential wells. Let $\psi_{\ell,{\rm r}}$ be the wave functions localized in the respective left and right potential wells. If E_ℓ and $E_{\rm r}$ are close to each other, then the spectrum of the operator with a double-well potential contains a pair of close points or, as is usually said, the energy levels are quasidegenerate. The corresponding eigenfunctions in the first approximation then have the form of linear combinations of the functions ψ_ℓ and $\psi_{\rm r}$.

One of the methods used to determine the splitting value and the form of the eigenfunctions in the case of quasidegeneration is based on considering the restriction of the operator $\widehat{H}$ to the subspace spanned by the two vectors ψ_ℓ and $\psi_{\rm r}$ and subsequently diagonalizing $\widehat{H}$. This method, called the *two-level approximation*, is widely used in quantum mechanics problems (see the references in [2]). The matrix elements $\langle \widehat{H}\psi_i, \psi_j\rangle$, $i, j = \ell, {\rm r}$, are calculated in this method, the desired splitting value is determined as the distance between the eigenvalues of this matrix, and its eigenvectors approximate the coefficients of the linear expansion of the eigenvectors of $\widehat{H}$ in the system of eigenfunctions $\psi_{\ell,{\rm r}}$.

Because the subspace to which the operator is restricted is not invariant, this method gives only an approximate result whose accuracy depends on the proximity between this subspace and an invariant subspace, i.e., on the choice of ψ_ℓ and $\psi_{\rm r}$. A general mathematical justification of this method can be found in [9], [10]. This method in a somewhat modified form is presented in the appendix here along with some useful theorems from the theory of linear operators. Different modifications of this method were used to calculate the tunnel splitting of energy levels in the asymmetric case in [10]–[13].

In [10], [11], it was proposed to take the solution of the Schrödinger equations in a neighborhood Ω_ℓ of the left well not intersecting the right well as ψ_ℓ and E_ℓ and to impose the Dirichlet conditions on the boundary of the domain Ω_ℓ. The wave function $\psi_{\rm r}$ and the energy $E_{\rm r}$ are chosen similarly. It was shown that such a choice permits obtaining sufficiently exact expressions for the energies of the initial equations in terms of the solution of the Dirichlet problem for separate wells if sufficiently large neighborhoods Ω_i, $i = \ell, {\rm r}$, are considered. These neighborhoods must intersect and contain the “center” of the potential barrier. This method was used in [10] to obtain the asymptotic behavior of the splitting of a pair of lower energy levels in the case of a multidimensional asymmetric potential (without any explicit expression for the amplitude) in terms of the energies E_ℓ and $E_{\rm r}$ of the separate wells.

Here, we show that such a choice of domains Ω_i is not only a sufficient but also a necessary condition for the applicability of the two-level approximation method (see Secs. 6 and 7). Therefore, as shown in Sec. 7, the choice of the functions $\psi_{\ell,\mathrm{r}}$ used in [13] leads to a false result because the domains Ω_i are chosen to be nonintersecting. We simultaneously note the inaccuracy arising in [12] because the usual distance on the straight line was used to determine the center of the asymmetric barrier. In fact, it is necessary to determine the potential barrier center from the standpoint of the action in the instanton sense.[1]

In addition to permitting the calculation of the splitting of energy levels, the two-level approximation method permits determining the coefficients of the approximate expansion of the eigenfunctions of $\widehat{H}$ in ψ_ℓ and ψ_r. Because the eigenfunctions are determined up to a normalizing factor and are orthogonal, it suffices to know the asymptotic behavior of the probabilities $P_\ell(\hbar)$ and $P_\mathrm{r}(\hbar)$ to find the particle in the left and right wells for a pair of eigenfunctions. A wave function is said to be bilocalized if both the probabilities $P_i(\hbar)$ significantly differ from zero for sufficiently small $\hbar$, i.e., if $P_i(\hbar) = p_i + O(\hbar)$ and $p_i > 0$. It is easy to show that if one eigenfunction is bilocalized, then the other is also bilocalized. The effect of eigenfunction bilocalization is closely related to the value of the tunnel splitting of energy levels.

In [16], for two lower energy levels in a multidimensional potential, it was proved that if both the probabilities $P_{\ell,\mathrm{r}}(\hbar)$ have a positive lower limit as $\hbar \to 0$, then the splitting value Δ satisfies the estimate $\Delta = O(e^{-S/\hbar})$. This estimate was refined in [10] for a pair of lower energy levels.

Our main result here is the proof of a criterion for the double localization of eigenfunctions (Theorem 1) demonstrating that there is a relation between the amplitude of the energy level splitting and the probabilities p_ℓ and p_r. The theorem also proves a relation to the formula for the splitting of energy levels in terms of the solution of the spectral problem obtained separately for the right and left wells (a formula in the spirit of [10]). The corresponding formulas for the splitting are

$$\Delta = \frac{\delta}{2\sqrt{p_\ell p_\mathrm{r}}}\bigl(1 + O(\hbar)\bigr),$$

$$\Delta = \sqrt{(E_\mathrm{r} - E_\ell)^2 + \delta^2}\bigl(1 + O(\hbar)\bigr).$$

Here,

$$\delta = 2\hbar^2\left(\psi_\ell\frac{d\psi_\mathrm{r}}{dx} - \psi_\mathrm{r}\frac{d\psi_\ell}{dx}\right)_{x=c},$$

where c is the center of the potential barrier from the standpoint of the instanton action.

The asymptotic formula for δ for higher energy levels (see Sec. 2) has the form

$$\delta = \hbar\frac{\sqrt{\omega_\ell\omega_\mathrm{r}}}{\pi}\exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x_\mathrm{r}}|p|\,dx\right)\bigl(1 + O(\hbar)\bigr).$$

The formula for δ in the case of lower energy levels is given in Sec. 3.

The result obtained for higher energy levels is consistent with the result obtained in [4] for a symmetric potential; our result generalizes the result obtained in the case without any symmetry in [4].

The splitting amplitude for lower energy levels can be expressed in terms of the solution of the variational system for the instanton (see Sec. 3). A similar method was used in [17] for a pair of lower energies of the Schrödinger operator with a multidimensional symmetric potential.

In Sec. 6, we consider the problem of tunnel perturbations of the discrete spectrum of the Schrödinger operator with a single-well potential. The problem is to estimate the perturbation of the energy E_0 of the Schrödinger operator with a potential $V(x)$ to which a function $f(x)$ localized only in the classically

[1] Or in the sense of the Agmon metric [10], [14], [15].

forbidden region is added. It is not assumed that $f(x)$ is small in this case. We obtain the formula for the leading term of the asymptotic expansion of the tunnel perturbation

$$E - E_0 = \langle f(x)\psi_0, \psi_0\rangle\bigl(1 + o(1)\bigr),$$

where ψ_0 is the wave function corresponding to the energy E_0.

In Sec. 7, we prove that the problem of tunnel perturbation of the spectrum of a single-well potential is equivalent to the problem of the deformation of one side of the potential barrier of a double-well potential. In the case of deformation where the support of $f(x)$ is between the center of the potential barrier and the turning point, the double localization of eigenfunctions is destroyed, and the splitting satisfies the formula

$$\Delta = \langle f(x)\psi_i, \psi_i\rangle\bigl(1 + o(1)\bigr),$$

where $i = \ell$ or $i = \mathrm{r}$ for the deformation of the left or the right side of the barrier.

The problem of the deformation of one side of the potential barrier of a symmetric double-well potential for a pair of lower energy levels was considered in [18]. It was shown that a similar deformation destroys the double localization of eigenfunctions and the splitting value satisfies the estimate

$$\Delta = \exp\biggl(-\frac{2S + o(1)}{\hbar}\biggr),$$

where S is the action in the sense of an instanton between the turning point and the support of $f(x)$. A multidimensional generalization of this result was given in [15].

Our formula easily implies the estimates given in [18]. The obtained formula permits calculating not only the logarithmic limit but also the value of the splitting amplitude for specific functions $f(x)$.

2. Splitting value and the tunneling amplitude

In this section, we consider the case of higher energy levels. We assume that the energy E is greater than the minimums of the double-well potential and less than the peak of the potential barrier. The fact that the potential has two wells means that the equation $V(x) = E$ has four simple roots, i.e., turning points, and $V(x) > E + e$ for sufficiently large x and some $e > 0$.

We assume that there is a potential barrier between the turning points x_ℓ and x_r, i.e., $V(x) > E$ for $x_\ell < x < x_\mathrm{r}$. The point c is determined by the formula

$$\int_{x_\ell}^{c} |p(x)|\,dx = \int_{c}^{x_\mathrm{r}} |p(x)|\,dx,$$

where $p(x) = \sqrt{E - V(x)}$. The point c is the center of the potential barrier from the standpoint of the instanton action. We assume that points a and b are chosen such that

$$x_\ell < a < c < b < x_\mathrm{r}.$$

We introduce two smooth potentials $V_{\ell,\mathrm{r}}$ (see Fig. 2) satisfying the two conditions

$$V_\ell(x) \equiv V(x) \quad \text{for } x \le b, \qquad V_\mathrm{r}(x) \equiv V(x) \quad \text{for } x \ge a$$

and

$$V_\ell(x) > E + e \quad \text{for } x \ge b, \qquad V_\mathrm{r}(x) > E + e \quad \text{for } x \le a$$

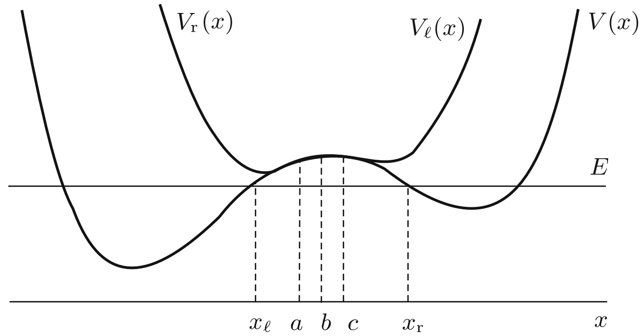

Fig. 2

for some $e > 0$.

We introduce the Schrödinger operators with the potentials $V_{\ell,\rm r}$ as

$$\widehat{H}_i = -\hbar^2 \frac{d^2}{dx^2} + V_i(x), \quad i = \ell, \rm r.$$

The potentials $V_{\ell,\rm r}$ are single-well potentials for the energy E because the classical region of a particle motion in each of the potentials $V_{\ell,\rm r}(x)$ is an interval. Therefore, the well-known results of the semiclassical analysis [4], [19] listed below hold for the spectra of the operators $\widehat{H}_i$.

I. The spectrum of the operator $\widehat{H}_i$ near the energy E is discrete and nondegenerate. The distance between neighboring points of the spectrum is of the order of $\hbar$.

II. Let E_i belong to the spectrum of the operator $\widehat{H}_i$, $i = \ell, \rm r$, and be close to E. Let ψ_i be the corresponding normalized eigenfunction. Then the asymptotic formulas

$$\psi_\ell(x) = \frac{C_\ell}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x} |p|\, dx\right)\big(1 + O(\hbar)\big),$$
$$\psi_{\rm r}(x) = \frac{C_{\rm r}}{\sqrt{|p|}} \exp\left(-\frac{1}{\hbar}\int_{x}^{x_{\rm r}} |p|\, dx\right)\big(1 + O(\hbar)\big)$$

are uniform in $x \in [a, b]$, and these asymptotic expansions are differentiable.

III. The normalization constants $C_{\ell,\rm r}$ can be chosen as

$$C_i = \frac{1}{2}\sqrt{\frac{\omega_i}{\pi}}, \quad i = \ell, \rm r,$$

where ω_i is the classical frequency of oscillations in the potential well $V_i(x)$ for the energy E.

Results I and II are general and hold for an arbitrary single-well potential, while assertion III holds only in the case of higher energy levels.

The operators $\widehat{H}_{\ell,\rm r}$ actually describe the left and right potential wells of the initial operator $\widehat{H}$. It is easy to show (see the proof of Theorem 1 below) that the spectrum of the operator $\widehat{H}$ near E can be obtained with an exponential accuracy when the spectra of $\widehat{H}_\ell$ and $\widehat{H}_{\rm r}$ are combined. If the energy E_ℓ is exponentially close to the energy $E_{\rm r}$, then the effect of the energy level quasidegeneration can arise in the case of such a combination. If there is no quasidegeneration, then the function ψ_ℓ or $\psi_{\rm r}$ can be chosen as an approximate eigenfunction of $\widehat{H}$. If the energy levels are quasidegenerate, then the spectrum of $\widehat{H}$ contains a pair of exponentially close points of the spectrum, and the eigenfunctions approximately have the form of linear combinations of the functions ψ_ℓ and ψ_{r}.

Let ψ be an eigenfunction of $\widehat{H}$. The probabilities $P_{\ell,\mathrm{r}}(\hbar)$ of discovering a particle in the left or right potential wells can be calculated as integrals of $|\psi(x)|^2$ for $x < c$ for the left well and for $x > c$ for the right well. The normalization condition for the wave functions implies the relation

$$P_\ell(\hbar) + P_{\mathrm{r}}(\hbar) = 1.$$

We can therefore take the probability ratio $P_{\mathrm{r}}(\hbar)/P_\ell(\hbar)$ as a quantity indicating where the wave function is concentrated.

We say that the wave function ψ has double localization if there is a number $\mu > 0$ such that

$$\frac{P_{\mathrm{r}}(\hbar)}{P_\ell(\hbar)} = \mu^2 + O(\hbar).$$

The probabilities $P_{\ell,\mathrm{r}}(\hbar)$ to find a particle in either the left or right potential well are then significantly different from zero and satisfy the asymptotic formulas

$$P_\ell(\hbar) = p_\ell\bigl(1 + O(\hbar)\bigr) = \frac{1}{1+\mu^2}\bigl(1 + O(\hbar)\bigr),$$

$$P_{\mathrm{r}}(\hbar) = p_{\mathrm{r}}\bigl(1 + O(\hbar)\bigr) = \frac{\mu^2}{1+\mu^2}\bigl(1 + O(\hbar)\bigr).$$

As is shown below in Sec. 4, the particle dynamics in the potential with two wells strongly depends on the value of μ.

We set

$$\delta(\hbar) = 4\hbar C_\ell C_{\mathrm{r}} \exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x_{\mathrm{r}}} |p|\,dx\right).$$

The quantity $\delta(\hbar)$ is the characteristic scale of exponential smallness for the tunnel effects in the double-well potential.

In the following theorem, we formulate a criterion for the resonant tunneling and obtain a relation between the splitting value Δ of the energy level, the tunneling amplitude μ, and the distance between E_ℓ and E_{r}.

Theorem 1. *For a fixed nonnegative number λ, the following three conditions are equivalent*:

1. *The operator $\widehat{H}$ has a bilocalized eigenfunction near the energy E, and the tunneling amplitude satisfies the formula*

$$\mu = \sqrt{1+\lambda^2} \pm \lambda.$$

2. *Near the energy E, the spectrum of the operator $\widehat{H}$ contains a pair of exponentially close points such that the distance between them satisfies the asymptotic formula*

$$\Delta = \sqrt{1+\lambda^2}\,\delta(\hbar)\bigl(1 + O(\hbar)\bigr).$$

3. *The distance between the points E_i satisfies the asymptotic formula*

$$|E_{\mathrm{r}} - E_\ell| = \delta(\hbar)\bigl(\lambda + O(\hbar)\bigr).$$

We first make several remarks and then prove the theorem.

This theorem generalizes the results obtained in the symmetric case. All three conditions are then obviously satisfied and $\lambda = 0$ in the case of a symmetric potential. The splitting then satisfies the Landau–Lifshits asymptotic formula

$$\Delta = \frac{\omega\hbar}{\pi} \exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x_{\mathrm{r}}} |p|\,dx\right)\bigl(1 + O(\hbar)\bigr).$$

In the general case, the number λ, just as μ, quantitatively characterizes the double localization of eigenfunctions. The number λ can uniquely be expressed in terms of μ because the plus sign is taken in the formula in condition 1 if $\mu > 1$ and the minus sign is taken if $\mu < 1$. There are two values $\mu = \mu_{1,2}$ and $\mu_1 = \mu_2^{-1}$ for each fixed λ. Two different values of μ correspond to a pair of eigenfunctions for a pair of close eigenvalues of $\widehat{H}$. The existence of one bilocalized eigenfunction with $\mu = \mu_1$ therefore implies that there is a second eigenfunction with the inverse exponent $\mu = \mu_2 = \mu_1^{-1}$. If one eigenfunction is more localized in the left well ($\mu_1 > 1$), then the other is more localized in the right well ($\mu_2 > 1$), and conversely.

If $\lambda = 0$, then $\mu = 1$, and tunneling transport occurs (see Sec. 4). For $\lambda = 0$, the splitting value satisfies the asymptotic formula

$$\Delta = \hbar\frac{\sqrt{\omega_\ell\omega_{\mathrm{r}}}}{\pi} \exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x_{\mathrm{r}}} |p|\,dx\right)\bigl(1 + O(\hbar)\bigr).$$

For an arbitrary $\lambda \geq 0$, the value $\delta(\hbar)$ can be calculated by the formula

$$\delta(\hbar) = 2\hbar^2\left[\psi_\ell\frac{d\psi_{\mathrm{r}}}{dx} - \psi_{\mathrm{r}}\frac{d\psi_\ell}{dx}\right]_{x=c},$$

which directly follows from the definition of δ and the asymptotic behavior of $\psi_{\ell,\mathrm{r}}(x)$.

Eliminating the constant λ from conditions 1 and 2 in Theorem 1, we can obtain the equation relating the energy level splitting Δ to the tunneling amplitude μ:

$$\Delta = \frac{1}{2}\left(\mu + \frac{1}{\mu}\right)\delta(\hbar)\bigl(1 + O(\hbar)\bigr).$$

We express μ in terms of $p_{\ell,\mathrm{r}}$, substitute the obtained expression for $\delta(\hbar)$, and obtain

$$\Delta = \frac{\delta(\hbar)}{2\sqrt{p_\ell p_{\mathrm{r}}}}\bigl(1 + O(\hbar)\bigr),$$

$$\Delta = \frac{\hbar}{2\pi}\sqrt{\frac{\omega_\ell\omega_{\mathrm{r}}}{p_\ell p_{\mathrm{r}}}} \exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{x_{\mathrm{r}}} |p|\,dx\right)\bigl(1 + O(\hbar)\bigr).$$

The quantity $\mu + \mu^{-1} = (p_\ell p_{\mathrm{r}})^{-1/2}$ is independent of any of the two eigenfunctions for which it is calculated.

The last formulas clearly show how fast the double localization of eigenfunctions disappears as the splitting Δ increases, i.e., one of the probabilities $p_{\ell,\mathrm{r}}$ tends to zero. The minimal splitting $\Delta \approx \delta(\hbar)$ corresponds to the maximal bilocalization $p_\ell = p_{\mathrm{r}} = 1/2$, and conversely.

We also note that Theorem 1 can be used to analyze tunneling in the case where the potential depends on $\hbar$. It is then necessary to recalculate the quantity $\delta(\hbar)$. Such a dependence can implicitly arise if the potential depends on an external parameter.

Proof of Theorem 1. Let a' and b' be independent of $\hbar$ and

$$x_\ell < a < a' < c < b' < b < x_{\mathrm{r}}.$$

We introduce two smooth cutoff functions $\sigma_{\ell,\mathrm{r}}(x)$ such that the conditions are satisfied:

$$\sigma_\ell(x) \equiv \begin{cases} 1, & x \le b', \\ 0, & x \ge b, \end{cases} \qquad \sigma_{\mathrm{r}}(x) \equiv \begin{cases} 1, & x \ge a', \\ 0, & x \le a. \end{cases}$$

Then the intersection of the supports of the functions $\sigma_{\ell,\mathrm{r}}$ is embedded in $[a,b]$ and necessarily contains the interval $[a',b']$ and hence the point c. It follows from the definition of $V_{\ell,\mathrm{r}}$ that

$$\sigma_i(x)[V(x) - V_i(x)] \equiv 0, \qquad \sigma_i(x)[\widehat{H} - \widehat{H}_i] = 0, \quad i = \ell, \mathrm{r},$$

where $\sigma_i(x)$ in the second equality is understood as the operator of multiplication by a function.

We first prove that any of the three conditions leads to quasidegeneration, i.e., there are energies E_i in the spectrum of the $\widehat{H}_i$, $i = \ell, \mathrm{r}$, such that the distance between them is exponentially small.

We assume that condition 1 is satisfied, ψ is the corresponding eigenfunction of $\widehat{H}$, and E is the corresponding eigenvalue. Let

$$u_i = \frac{\sigma_i \psi}{\sqrt{p_i}}, \quad i = \ell, \mathrm{r}.$$

Then

$$\|u_\ell\|^2 = \frac{1}{p_\ell} \int_{-\infty}^{b} |\sigma_\ell \psi|^2 \, dx = 1 + \frac{1}{p_\ell} \int_{c}^{b} |\sigma_\ell \psi|^2 \, dx \approx 1$$

because ψ is bilocalized by condition 1 and the integral over the interval $[c,b]$ is exponentially small and hence $p_\ell > 0$. We similarly have

$$\|u_{\mathrm{r}}\| \approx 1.$$

We show that u_i are quasimodes for the operators $\widehat{H}_i$ with an exponential accuracy. Interchanging the operators of differentiation and multiplication by the function $\sigma_i(x)$, we easily obtain the discrepancy

$$(\widehat{H}_i - E)u_i = \frac{-\hbar^2}{\sqrt{p_i}} \left(\sigma_i'' + 2\sigma_i' \frac{d}{dx} \right) \psi.$$

Because the supports of the functions $\sigma_i'(x)$ and $\sigma_i''(x)$ are embedded in the interval $[a,b]$ where the function $\psi(x)$ and its derivative are exponentially small, we see that u_i are quasimodes for $\widehat{H}_i$ with an exponential accuracy. We thus have proved that condition 1 implies that the spectrum is quasidegenerate.

We assume that condition 2 is satisfied, there are exponential split eigenvalues $E_{1,2}$ of $\widehat{H}$, and $\psi_{1,2}$ are the corresponding eigenfunctions. We can assume that $\psi_{1,2}$ are not bilocalized because condition 1 would otherwise be satisfied and this would imply quasidegeneration. The functions $\psi_{1,2}$ cannot be localized in one well, because this contradicts their orthogonality. For definiteness, we assume that ψ_1 is localized in the left well and ψ_2 is localized in the right well. We then write $\psi_{\ell,\mathrm{r}}$ and $E_{\ell,\mathrm{r}}$ instead of $\psi_{1,2}$ and $E_{1,2}$.

Let $u_i = \sigma_i \psi_i$. Then u_i are quasimodes for $\widehat{H}_i$ with an exponential accuracy, i.e.,

$$\|u_i\| \approx 1, \qquad (\widehat{H}_i - E_i)u_i = -\hbar^2 \left(\sigma_i'' + 2\sigma_i' \frac{d}{dx} \right) \psi_i.$$

We see that quasidegeneration follows from condition 2.

We now assume that condition 3 is satisfied. Then quasidegeneration obviously occurs because $\delta(\hbar)$ is exponentially small.

We have just proved that if any of the three conditions in the theorem is satisfied, then quasidegeneration occurs. Let at least one of the conditions in this theorem be satisfied for some λ. Quasidegeneration hence occurs. Let E_i be eigenvalues of $\widehat{H}_i$ and ψ_i be the corresponding eigenfunctions, $i = \ell, \mathrm{r}$. The quantity $|E_\mathrm{r} - E_\ell|$ is hence exponentially small.

We introduce the orthonormal functions

$$u_\ell(x) = \gamma_1 \sigma_\ell(x)\psi_\ell(x), \qquad u_\mathrm{r}(x) = \gamma_2\big(\sigma_\mathrm{r}(x)\psi_\mathrm{r}(x) + \gamma_3\sigma_\ell(x)\psi_\ell(x)\big),$$
$$\langle u_i, u_j\rangle = \delta_{ij}, \quad i,j = \ell, \mathrm{r}.$$

Because the functions $\psi_i(x)$, $i = \ell, \mathrm{r}$, are normed, we obtain

$$\gamma_{1,2} = 1 + O(\hbar).$$

The orthogonality condition for u_1 and u_2 implies

$$0 = \langle u_\ell, u_\mathrm{r}\rangle = \gamma_1\gamma_2 \int_a^b \sigma_\ell\sigma_\mathrm{r}\psi_\ell\psi_\mathrm{r}\,dx + \gamma_2\gamma_3\gamma_1^{-1}, \qquad \gamma_3 = O(\delta(\hbar)).$$

We calculate the asymptotic behavior of the discrepancy to show that u_i are quasimodes for $\widehat{H}$:

$$(\widehat{H} - E_\ell)u_\ell = \left[-\hbar^2\frac{d^2}{dx^2}, \sigma_\ell(x)\right]\gamma_1\psi_\ell(x) + \sigma_\ell(x)\gamma_1(\widehat{H}_\ell - E_\ell)\psi_\ell(x) =$$
$$= \hbar\sigma_\ell'(x)2C_\ell\sqrt{|p|}\exp\left(-\frac{1}{\hbar}\int_{x_\ell}^x |p|\,dx\right)\big(1 + O(\hbar)\big),$$
$$(\widehat{H} - E_\mathrm{r})u_\mathrm{r} = -\hbar\sigma_\mathrm{r}'(x)2C_\mathrm{r}\sqrt{|p|}\exp\left(-\frac{1}{\hbar}\int_x^{x_\mathrm{r}} |p|\,dx\right)\big(1 + O(\hbar)\big).$$

We introduce the notation

$$\varepsilon = \max\left[C_\ell\exp\left(-\frac{1}{\hbar}\int_{x_\ell}^{b'} |p|\,dx\right),\, C_\mathrm{r}\exp\left(-\frac{1}{\hbar}\int_{a'}^{x_\mathrm{r}} |p|\,dx\right)\right].$$

The quantity ε is exponentially small, and ε^2 is moreover exponentially less than $\delta(\hbar)$. We obtain the estimates

$$\|(\widehat{H} - E_i)u_i\| = O(\varepsilon), \quad i = \ell, \mathrm{r}.$$

Hence, u_ℓ and u_r are indeed quasimodes.

We now assume that

$$|E_\mathrm{r} - E_\ell| = O(\varepsilon).$$

We can then use Theorem 6 (see the appendix). In what follows, we show that if the last relation does not hold, then all three conditions in the theorem are not satisfied.

We introduce the notation $L(\hbar) = (E_\mathrm{r} - E_\ell)/\delta$. The quantity L is introduced just as in condition 3 of the theorem, but we do not assume that this condition (the existence of the limit of $L(\hbar)$ as $\hbar \to 0$) is satisfied. Let $E = (E_\ell + E_\mathrm{r})/2$. We then have the estimate

$$\|(\widehat{H} - E)u_i\| \le \|(\widehat{H} - E_i)u_i\| + \frac{|E_\mathrm{r} - E_\ell|}{2}\|u_i\| = O(\varepsilon), \quad i = \ell, \mathrm{r}.$$

All conditions in Theorem 6 are hence satisfied. We calculate the matrix elements $m_{i,j} = \langle(\widehat{H} - E)u_i, u_j\rangle$, $i, j = \ell, \mathrm{r}$, as

$$m_{\ell,\ell} = \frac{E_\ell - E_\mathrm{r}}{2} + O(\varepsilon^2), \qquad m_{\mathrm{r},\mathrm{r}} = \frac{E_\mathrm{r} - E_\ell}{2} + O(\varepsilon^2),$$

$$m_{\ell,\mathrm{r}} = 2\hbar C_\ell C_\mathrm{r} \int_{b'}^{b} \sigma'_\ell(x) \exp\biggl(-\frac{1}{\hbar}\int_{x_\ell}^{x_\mathrm{r}} |p|\,dx\biggr)\bigl(1 + O(\hbar)\bigr)\,dx = -\frac{\delta}{2}\bigl(1 + O(\hbar)\bigr).$$

Hence,

$$m = \frac{\delta}{2}\begin{pmatrix} -L & -1 \\ -1 & L \end{pmatrix}\bigl(1 + O(\hbar)\bigr) + O(\varepsilon^2).$$

The eigenvalues m of the matrix are equal to

$$\mu_{1,2} = \pm\frac{\delta}{2}\sqrt{1 + L^2}.$$

The corresponding eigenvectors have the form

$$\begin{pmatrix} -1 \\ L + \sqrt{1 + L^2} \end{pmatrix}, \qquad \begin{pmatrix} L + \sqrt{1 + L^2} \\ 1 \end{pmatrix},$$

where the factor $1 + O(\hbar)$ is omitted for clarity. We determine the quantities

$$\widetilde{E}_1 = E + \mu_1 = \frac{E_\mathrm{r} + E_\ell}{2} + \frac{\delta}{2}\sqrt{1 + L^2},$$

$$\widetilde{E}_2 = E + \mu_2 = \frac{E_\mathrm{r} + E_\ell}{2} - \frac{\delta}{2}\sqrt{1 + L^2}.$$

By Theorem 6, we can construct the quasimodes $\tilde{u}_i$ for the energies $\widetilde{E}_i$ such that

$$\bigl\|(\widehat{H} - \widetilde{E}_i)\tilde{u}_i\bigr\| = O\biggl(\frac{\varepsilon^2}{\hbar}\biggr).$$

Their leading terms up to normalization are equal to

$$v_1 = -u_\ell + \bigl(L + \sqrt{1 + L^2}\bigr)u_\mathrm{r}, \qquad v_2 = \bigl(L + \sqrt{1 + L^2}\bigr)u_\ell + u_\mathrm{r}.$$

Each of the $O(\varepsilon^2/\hbar)$-neighborhoods of the energies $\widetilde{E}_1$ and $\widetilde{E}_2$ therefore contains one point of the spectrum of $\widehat{H}$. The distance between these points can be estimated as

$$\Delta = \sqrt{1 + L^2}\,\delta\bigl(1 + O(\hbar)\bigr) + O\biggl(\frac{\varepsilon^2}{\hbar}\biggr) = \sqrt{1 + L^2}\,\delta\bigl(1 + O(\hbar)\bigr).$$

The quantity $O(\varepsilon^2/\hbar)$ can be omitted because the ratio ε^2/δ is exponentially small. The smallness of ε^2/δ is ensured by the choice of the point c.

It follows from Theorem 5 (see the appendix) that the eigenfunction ϕ_i of $\widehat{H}$ corresponding to a point of the spectrum close to $\widetilde{E}_i$ satisfies the asymptotic formula

$$\phi_i = v_i(x) + O(\hbar^\infty).$$

The eigenfunction ϕ_i is therefore bilocalized only if there is a number λ such that

$$L(\hbar) = \lambda + O(\hbar).$$

Then the quantity μ corresponding to ϕ_1 can be written as

$$\mu = \sqrt{1+\lambda^2} - \lambda$$

and corresponding to ϕ_2 can be written as

$$\mu = \sqrt{1+\lambda^2} + \lambda.$$

The obtained results hold under the assumption that one of the conditions in the theorem is satisfied and $|E_{\mathrm{r}} - E_\ell| = O(\varepsilon)$. To prove the equivalence of all three conditions, we show that condition 3 implies conditions 1 and 2, and conversely.

We assume that condition 3 is satisfied, i.e., $L(\hbar) = \lambda + O(\hbar)$. It follows from the obtained formulas for μ and Δ that conditions 1 and 2 are satisfied.

We assume that condition 1 with some λ is satisfied. Because λ is uniquely determined by the number μ (recall that $\lambda \geq 0$), we have

$$|L(\hbar)| = \frac{|E_{\mathrm{r}} - E_\ell|}{\delta(\hbar)} = \lambda + O(\hbar),$$

and hence condition 3 is satisfied.

Condition 2 similarly implies condition 3 because if condition 2 is satisfied, then the quantity λ is uniquely determined by the ratio Δ/δ.

All the above reasonings were based on the assumption that

$$|E_{\mathrm{r}} - E_\ell| = O(\varepsilon).$$

We show that if this is not the case, then none of the three conditions in the theorem is satisfied. Condition 3 is not satisfied, because it implies $|E_{\mathrm{r}} - E_\ell| = O(\varepsilon)$.

Let $u_i = \sigma_i(x)\psi_i(x)$, $i = \ell, \mathrm{r}$. Then

$$\|(\widehat{H} - E_i)u_i\| = O(\varepsilon), \quad i = \ell, \mathrm{r}.$$

It follows from Theorem 4 (see the appendix) that there is an eigenvalue $\widetilde{E}_i$ of $\widehat{H}$ such that

$$|E_i - \widetilde{E}_i| = O(\varepsilon), \quad i = \ell, \mathrm{r}.$$

The corresponding eigenfunctions have the asymptotic behavior (see Theorem 5)

$$\tilde{\psi}_i = u_i + O(\varepsilon\Delta^{-1}),$$

where Δ is the distance between two close points of the spectrum of $\widehat{H}$. The estimate

$$\Delta = |E_\ell - E_{\mathrm{r}}| + O(\varepsilon)$$

is obvious. The ratio Δ/δ is hence unbounded, and condition 2 is not satisfied.

We assume that the double localization occurs. The double localization implies the existence of a limit $\mu^2 \neq 0$ for the probability ratio $p_{\mathrm{r}}(\hbar)/p_\ell(\hbar)$. Because the ratio Δ/ε is unbounded, the functions $\tilde{\psi}_i$ are close to u_i for a small $\hbar$. We see that the limit of the probability ratio, if it exists, is equal to either zero or infinity, which contradicts the definition of double localization. The proof of the theorem is complete.

3. The case of energy close to the potential minimum

An analogue of Theorem 1 holds for lower energy levels. It is only necessary to recalculate C_i and correspondingly change $\delta(\hbar)$. We must also distinguish the cases where both the local minimums of the potential $V(x)$ correspond to the same energy and where the values of $V(x)$ at the local minimums are different. As an example, we consider the case of coinciding values of $V(x)$ at the local minimum points.

Let $\xi_{1,2}$ be the coordinates of two nondegenerate local minimums of a double-well potential $V(x)$. We assume that

$$V(\xi_i + x) = \omega_i^2 x^2 \bigl(1 + O(x)\bigr), \quad i = 1, 2.$$

If the nth level $E_\ell^{(n)}$ of the left well is close to the mth level $E_{\mathrm{r}}^{(m)}$ of the right well in this case, then δ satisfies the asymptotic formula

$$\delta = 4\hbar \frac{\sqrt{\omega_1\omega_2}}{\sqrt{\pi n! m!}} \left(\frac{2}{\hbar}\right)^{n+m/2} J_1^{n+1/2} J_2^{m+1/2} \exp\biggl(-\frac{1}{\hbar}\int_{\xi_1}^{\xi_2} \sqrt{V(x)}\,dx\biggr)\bigl(1 + O(\hbar)\bigr),$$

where

$$J_1 = \sqrt{\omega_1} \lim_{t\to\xi_1+0} \biggl\{(t-\xi_1)\exp\biggl(\omega_1 \int_t^c \frac{dx}{\sqrt{V(x)}}\biggr)\biggr\},$$

$$J_2 = \sqrt{\omega_2} \lim_{t\to\xi_2-0} \biggl\{(\xi_2 - t)\exp\biggl(\omega_2 \int_c^t \frac{dx}{\sqrt{V(x)}}\biggr)\biggr\}.$$

If the conditions in Theorem 1 are satisfied, then $|E_{\mathrm{r}}^{(m)} - E_\ell^{(n)}|$ is exponentially small, and the first terms of the expansion of these energies in $\hbar$ hence coincide:

$$\omega_1(2n+1) = \omega_2(2m+1).$$

The ratio of the oscillation frequencies of the classical particle in the left and right wells is hence a rational number. The origination of tunnel effects in a double-well potential is therefore often called the *resonant tunneling*. This term is not quite good, because the rationality of the frequency ratio is only a weak necessary condition for effects such as tunneling transport and the double localization of eigenfunctions.

Following the method presented in [17], we express the limits J_1 and J_2 in terms of the asymptotic behavior of the solution of the variational system.

We consider the Hamilton system determining an instanton,

$$\dot q = 2p, \qquad \dot p = V'(q),$$

with the boundary conditions $q(-\infty) = \xi_1$, $q(0) = c$, and $q(\infty) = \xi_2$. This system is obtained by changing the sign of the potential. The instanton can be given by the implicit formula

$$2t = \int_c^q \frac{dx}{\sqrt{V(x)}}.$$

We consider the corresponding variational system

$$\ddot z = 2V''(q(t))z,$$

$$z(\pm\infty) = 0, \qquad z(0) = 1.$$

Its solution has the form

$$z(t) = \sqrt{\frac{V(q(t))}{V(c)}}.$$

We investigate the asymptotic behavior of the solution of the variational system as $t \to -\infty$:

$$z(t) \sim \frac{1}{\sqrt{V(c)}}\,\omega_1(q - \xi_1).$$

The definition of J_1 implies

$$q - \xi_1 \sim J_1 \omega_1^{-1/2} \exp\biggl(\omega_1 \int_c^q \frac{dx}{\sqrt{V(x)}}\biggr), \qquad z(t) \sim J_1 \frac{\sqrt{\omega_1}}{\sqrt{V(c)}}\, e^{2\omega_1 t}.$$

We similarly obtain the asymptotic behavior of the solution of the variational system as $t \to \infty$:

$$z(t) \sim J_2 \frac{\sqrt{\omega_2}}{\sqrt{V(c)}}\, e^{-2\omega_2 t}.$$

We have thus determined the relation between the limits $J_{1,2}$ and the asymptotic behavior of the solution of the variational system for the instanton.

4. Dynamics of a particle in the case of resonant tunneling

We consider the operator

$$\widehat{H} = -\hbar^2 \frac{d^2}{dx^2} + V(x),$$

where $V(x)$ is a smooth real function with the shape of a double potential well.

We consider the dynamics of a particle in a double-well potential for energy close to a pair of quasidegenerate stationary energy levels. We assume that the conditions in Theorem 1 are satisfied, two energy levels $E_{1,2}$ of the operator $\widehat{H}$ are exponentially close to each other, and the corresponding eigenfunctions $\psi_{1,2}$ are bilocalized.

With the orthogonality condition for the functions ψ_i taken into account, we obtain (see the proof of Theorem 1)

$$\psi_1 = u_\ell + \mu u_{\mathrm{r}} + O(\hbar^\infty), \qquad \psi_2 = \mu u_\ell - u_{\mathrm{r}} + O(\hbar^\infty),$$

where $u_{\ell,\mathrm{r}}$ are concentrated only in the respective left and right potential wells.

We consider the Cauchy problem with the initial state localized in the left well:

$$i\hbar \frac{\partial u}{\partial t} = \widehat{H}u, \qquad u|_{t=0} = u_\ell.$$

The solution of this Cauchy problem with an accuracy of $O(\hbar^\infty)$ has the form

$$u = \frac{1}{1+\mu^2}(e^{-iE_1 t/\hbar}\psi_1 + \mu e^{-iE_2 t/\hbar}\psi_2).$$

We substitute the expressions for ψ_1 and ψ_2 and obtain

$$u = \frac{e^{-iE_1 t/\hbar}}{1+\mu^2}\bigl(u_\ell + \mu u_{\mathrm{r}} + e^{-(i/\hbar)(E_2 - E_1)t}\mu(\mu u_\ell - u_{\mathrm{r}})\bigr) =$$

$$= \frac{e^{-iE_1 t/\hbar}}{1+\mu^2}\bigl((\mu^2 e^{-(i/\hbar)(E_2 - E_1)t} + 1)u_\ell + \mu\bigl(1 - e^{-(i/\hbar)(E_2 - E_1)t}\bigr)u_{\mathrm{r}}\bigr).$$

The total tunneling transport means that there is an instant $t = T$ when the solution is concentrated in the well other than the well where the initial condition is concentrated. The total transport therefore occurs if the coefficient of u_ℓ vanishes. Because μ is a positive number, we obtain $\mu = 1$. Only a partial transport arises for positive values $\mu \neq 1$.

We can see that the transport is a periodic process and the transport half-period T is the time of the particle transport into the other potential well. The quantity T is exponentially large and has the form

$$T = \frac{\pi\hbar}{E_2 - E_1}.$$

We use the formulas for μ and Δ in Theorem 1 to obtain the maximal probability of finding the particle in the right well

$$\max_t P_{\mathrm{r}}(t) = \left(\frac{\delta}{\Delta}\right)^2 + O(\hbar^\infty).$$

5. Examples of asymmetric transport

A fourth-degree polynomial is a classical example of the double-well potential. We can use special functions to study the exact solution in this case (see [7]).

We consider the operator $\widehat{H}$ with the potential

$$V(x, s) = (x-1)^2(x+1)^2 + sx,$$

where s is a parameter characterizing the asymmetry. We study the spectrum of $\widehat{H}$ near E, where $0 < E < 1$. The parameter s varies in the range $(0, s_0)$, where $s_0 = s_0(E)$ is chosen such that the equation $V(x, s_0) = E$ has four simple roots. The case of higher energy levels is hence considered.

Just as in Sec. 2, we introduce the operators $\widehat{H}_i$ and constants $c = c(s)$ and $\delta = \delta(s, \hbar)$. We assume that $E_i^{(n)}$ are points of the spectrum of $\widehat{H}_i$, $i = \ell, \mathrm{r}$. The quantum numbers $n = n(\hbar)$ are chosen such that $E_i^{(n)}$ are near E. The energy levels $E_i^{(n)}$ and the corresponding eigenfunctions depend continuously on s for a fixed small $\hbar$.

For $s = 0$, the operator $\widehat{H}_\ell$ differs from $\widehat{H}_{\mathrm{r}}$ by the change of x to $-x$. This implies that $E_\ell^{(n)} = E_{\mathrm{r}}^{(n)}$. It follows from Theorem 1 that the eigenfunctions are bilocalized. As the parameter s increases, the energy level $E_\ell^{(n)}$ decreases, and $E_{\mathrm{r}}^{(n)}$ increases with an accuracy of $O(\hbar^2)$. This follows because they approximately satisfy the Planck–Bohr–Sommerfeld discretization rule [4]. The continuous dependence on s implies that there is an s_1 such that

$$E_\ell^{(n+1)} = E_{\mathrm{r}}^{(n)} \quad \text{for } s = s_1.$$

If $s = s_1$, then the eigenfunctions of $\widehat{H}$ corresponding to the eigenvalues with numbers $2n$ and $2n+1$ are bilocalized, and transport occurs. A similar example can also be considered in the case of lower energies.

6. Tunnel perturbation of the spectrum

In this section, we determine the asymptotic behavior of a perturbation of the discrete spectrum of the Schrödinger operator with a single-well potential and with an added perturbed potential completely concentrated outside the region of motion of the classical particle. We consider the problem in a neighborhood of a certain energy. Obviously, the spectrum perturbation is exponentially small even for a nonsmall perturbing potential (for the energy in question). The main goal is to obtain the leading term of the asymptotic expansion. We assume that after the perturbation is added, the potential remains a single-well potential for the given energy.

We assume that the initial single-well potential $V(x)$ and the corresponding operator $\widehat{H}_0$ are given. Let E_0 be an eigenvalue of $\widehat{H}_0$ and ψ_0 be the corresponding wave function. Let (x_1, x_2) be the region of classical motion, i.e., $V(x) < E_0$ for $x \in (x_1, x_2)$. To the initial operator, we add a perturbation in the form of a continuous function $f(x)$ completely localized in the classically forbidden region:

$$\widehat{H} = \widehat{H}_0 + f(x), \qquad \operatorname{supp} f(x) = [a, b], \quad x_2 < a < b.$$

The wave function $\psi_0(x)$ for $x \in [a, b]$ satisfies the WKB expansion

$$\psi_0(x) = \frac{C}{\sqrt{|p|}} \exp\biggl(-\frac{1}{\hbar} \int_{x_2}^{x} |p|\, dx\biggr)\bigl(1 + O(\hbar)\bigr).$$

Therefore,

$$\bigl\|(\widehat{H} - E_0)\psi_0\bigr\|^2 = \|f(x)\psi_0\|^2 = \int_a^b f^2(x)\psi_0^2(x)\, dx = \varepsilon^2,$$

and ε satisfies the estimate

$$\varepsilon \le C_1 e^{-S/\hbar},$$

where S is the action in the sense of an instanton from the turning point to the support of $f(x)$:

$$S = \int_{x_2}^{a} \sqrt{V(x) - E}\, dx.$$

This estimate implies that $\widehat{H}$ has a spectrum point E such that the distance from this point to E_0 is exponentially small (does not exceed ε). If the potential for energies close to E_0 remains a single-well potential after the addition of $f(x)$, then ψ_0 can be considered an approximation of the eigenfunction of $\widehat{H}$ (see Theorem 5) because the distance between neighboring levels for an operator with a single-well potential has the order $\hbar$.

We determine the next term of the expansion of E in ε. Because we do not assume that the function $f(x)$ is small, the formulas of the usual perturbation theory are inapplicable. We only have the weak estimate $|E - E_0| \le \varepsilon$.

To construct the asymptotic behavior of the energy E, we proposed using the perturbation theory to seek the spectrum of $\widehat{H}$, where the unperturbed operator is not the operator $\widehat{H}_0$ but a certain specially constructed operator. These ideas are close to the ideas used to prove Theorem 6.

Theorem 2. *Let $f(x) \to 0$ as $x \to a$. Then the energy E of the operator $\widehat{H}$ satisfies the asymptotic formula*

$$E - E_0 = \langle f(x)\psi_0, \psi_0\rangle\bigl(1 + o(1)\bigr).$$

Proof. Let Π be the operator of projection on ψ_0, and let $\Pi' = 1 - \Pi$. We consider the operators

$$A = \widehat{H}_0 + \Pi' f(x)\Pi', \qquad B = f(x)\Pi + \Pi f(x) - \Pi f(x)\Pi,$$

which satisfy the relations

$$A + B = \widehat{H}_0 + f(x) = \widehat{H}, \qquad \|B\| = O(\varepsilon),$$

$$A\psi_0 = E_0\psi_0, \qquad B\psi_0 = f(x)\psi_0.$$

If we assume that $V + f(x)$ remains a single-well potential for energies close to E_0, then the operator $\widehat{H}$ has a unique point E of the spectrum that is exponentially close to E_0, and the other points of the spectrum are at a distance of the order of $\hbar$. To seek the asymptotic behavior of E, we therefore need to apply the formula of the perturbation theory for an isolated point of the spectrum:

$$E = E_0 + \langle B\psi_0, \psi_0\rangle + \sum_{k=1}^{+\infty} \frac{\langle B\psi_0, \phi_k\rangle^2}{E_0 - \lambda_k} + O\biggl(\frac{\varepsilon^3}{\hbar^2}\biggr),$$

where $\psi_0, \phi_1, \phi_2, \dots$ is the orthonormal set of eigenfunctions of the operator A and $E_0, \lambda_1, \lambda_2, \dots$ are the corresponding eigenvalues. The terms of the sum for which the energy λ_k is close to E_0 do not contribute to the asymptotic behavior, because the corresponding functions ϕ_k are exponentially small on the support of $f(x)$. Therefore,

$$E = E_0 + \langle f(x)\psi_0, \psi_0\rangle + O(\varepsilon^2).$$

It remains to prove that

$$\varepsilon^2 = \langle f(x)\psi_0, f(x)\psi_0\rangle = o(\langle f(x)\psi_0, \psi_0\rangle).$$

These estimates hold because only a small neighborhood of a contributes to the integral $\langle f(x)\psi_0, f(x)\psi_0\rangle$ and the function $f(x)$ is small in this neighborhood.

Theorem 2 permits obtaining several important consequences.

Corollary 1. *The formula for the leading term of the asymptotic expansion coincides with the formula in the classical perturbation theory, but the value of the correction can be much greater than the small parameter ε and significantly depends on how the function $f(x)$ tends to zero as $x \to a$.*

Corollary 2. *The estimate*

$$E - E_0 = \exp\biggl(-\frac{2S + o(1)}{\hbar}\biggr)$$

holds.

The simple perturbation theory gives the significantly weaker estimate

$$|E - E_0| \le \varepsilon = \exp\biggl(-\frac{S + o(1)}{\hbar}\biggr)$$

and does not permit calculating the order of the error.

7. Application of the tunnel perturbation method

As shown in Sec. 6, a variation in the potential in the classically forbidden region leads to an exponentially small perturbation of the spectrum. These corrections are rather interesting if the problem contains an exponential quasidegeneration of the spectrum because a small perturbation of the energies can then result in a significant variation in the eigenfunctions and hence in the system dynamics. The simplest example of such a system is the double-well potential. With the results in Sec. 2 taken into account, we can reduce studying the double-well potential to studying a pair of single-well potentials to which Theorem 2 is applicable.

We first consider the influence of the potential barrier deformation on the tunneling. We use the obtained results to construct a counterexample to [13] and then independently prove the correctness of condition 3 in Theorem 1 relying on the estimates in Corollary 2.

We consider the influence of the potential barrier deformation on the resonant tunneling in the double-well potential. We assume that the double-well potential $V(x)$ satisfies the requirements of Theorem 1, $E_{1,2}$ is a pair of quasidegenerate eigenvalues of the operator $\widehat{H}$, and the corresponding eigenfunctions are bilocalized. To the potential V, we add a function $f(x)$ such that the support of $f(x)$ lies between the potential barrier center and the turning point. For definiteness, we assume that the perturbation occurs on the right-hand side of the barrier.

We then use the results in Theorems 1 and 2 to prove the following theorem.

Theorem 3. *In the case of a smooth deformation of one side of the potential barrier, the right side for definiteness, the double localization of eigenfunctions is destroyed, and the splitting value satisfies the formula*

$$\Delta = \langle f(x)\psi_{\mathrm{r}}, \psi_{\mathrm{r}}\rangle\bigl(1 + o(1)\bigr).$$

A similar problem in the case of a symmetric potential was considered in [18], where only the exponent such as in the estimate in Corollary 2 was obtained.

We now use the formula for the tunnel perturbation to show that the results presented in [13] are not true.

The double-well asymmetric potential for energies close to the equilibriums of the potential was considered in [13]. It was assumed that the potential is exactly quadratic in a neighborhood of the domains of classical motion, i.e., in some finite neighborhoods of the potential minimums. The splitting can be calculated by the two-level approximation method. As the potentials of the left and right potential wells, we take oscillators with the corresponding frequencies.

The error is that under such a choice of the potentials of the left and right potential wells, the result obtained for the splitting turns out to be less than the error of this method. This approach implies that the localization of the eigenfunctions and the transport existence are independent of the choice of the smooth part of the potential barrier connecting the domains where the potential is quadratic. Similar calculations lead to a false result because the potential barrier deformation outside the domains where the potential is quadratic destroys the tunneling (Theorem 3). The splitting is exponentially greater than that obtained in [13]. As a counterexample, we can consider any symmetric double-well potential satisfying all conditions in [13] with an asymmetric perturbation of the potential barrier added to this potential.

We further consider an independent proof that the conditions in Theorem 1 are well posed using the formula for the tunnel perturbation of the spectrum. Condition 3 in Theorem 1 is formulated in terms of the spectra of the operators $\widehat{H}_{\ell,\mathrm{r}}$ with single-well potentials $V_{\ell,\mathrm{r}}(x)$. It follows from the conditions imposed on the potentials $V_{\ell,\mathrm{r}}$ that the choice of $W_{\ell,\mathrm{r}}$ is not unique. Otherwise, the chosen potentials $W_{\ell,\mathrm{r}}$ can differ from the initial potentials $V_{\ell,\mathrm{r}}$ only in the classically forbidden region. As follows from Theorem 1, the condition for the existence of a number λ such that $|E_{\mathrm{r}} - E_\ell| = \delta(\hbar)\bigl(\lambda + O(\hbar)\bigr)$ is independent of the freedom in choosing $V_{\ell,\mathrm{r}}$ and characterizes the double-well potential V. We prove this directly using the formula for the tunnel perturbation.

Let

$$\widehat{K}_i = -\hbar^2\frac{d^2}{dx^2} + W_i(x), \quad i = \ell, \mathrm{r}.$$

We assume that the eigenvalues $E_{\ell,\mathrm{r}}$ of $\widehat{H}_{\ell,\mathrm{r}}$ satisfy condition 3 in Theorem 1, i.e., there is a λ such that

$$\|E_{\mathrm{r}} - E_\ell\| = \delta(\hbar)\bigl(\lambda + O(\hbar)\bigr).$$

Let $\psi_{\ell,\mathrm{r}}$ be the eigenfunctions corresponding to the eigenvalues $E_{\ell,\mathrm{r}}$. We must prove that the operators $\widehat{K}_{\ell,\mathrm{r}}$ have eigenvalues $k_{\ell,\mathrm{r}}$ that are close to $E_{\ell,\mathrm{r}}$ and satisfy the condition

$$|k_\mathrm{r} - k_\ell| = \delta(\hbar)\big(\lambda + O(\hbar)\big).$$

We introduce the notation

$$f_i(x) = W_i(x) - V_i(x), \quad i = \ell, \mathrm{r}.$$

Then the conditions imposed on the potentials V_i and W_i imply

$$f_\ell(x) \equiv 0 \quad \text{for } x \le b, \qquad f_\mathrm{r}(x) \equiv 0 \quad \text{for } x \ge a.$$

We set

$$S_\ell = \int_{x_\ell}^{b} |p(x)|\, dx, \qquad S_\mathrm{r} = \int_a^{x_\mathrm{r}} |p(x)|\, dx.$$

Applying the estimate in Corollary 2, we obtain

$$k_i - E_i = \exp\bigg(-\frac{2S_i + o(1)}{\hbar}\bigg).$$

Because the points a and b are chosen such that $a < c < b$ and the point c is the center of the potential barrier from the action standpoint,

$$\int_{x_\ell}^{c} |p|\, dx = \int_c^{x_\mathrm{r}} |p|\, dx,$$

we see that $|k_i - E_i|$ is exponentially less than $\delta(\hbar)$. Therefore,

$$\frac{|k_\mathrm{r} - k_\ell|}{\delta} = \frac{|E_\mathrm{r} - E_\ell|}{\delta} + O(\hbar) = \lambda + O(\hbar),$$

as required.

Appendix: Several theorems in the theory of linear operators

The following assertions are widely known.

Lemma 1 (norm of resolvent)**.** *Let Γ be a Hilbert space, and let an operator A be self-adjoint. In this case, if $\lambda \notin \mathrm{Spectre}(A)$, then*

$$\|(A-\lambda)^{-1}\| = \frac{1}{d(\lambda, \mathrm{Spectre}(A))},$$

where d is the distance on the line.

Lemma 2. *Let Γ be a Hilbert space, and let an operator A be self-adjoint. If a quasimode u such that*

$$\|u\| = 1, \qquad \|(A-\lambda)u\| \le \varepsilon$$

is given, then

$$d(\lambda, \mathrm{Spectre}(A)) \le \varepsilon.$$

Theorem 4 (equality between the number of modes and the number of quasimodes)**.** *If a self-adjoint operator A in a Hilbert space Γ has n orthonormal quasimodes*

$$\langle u_i, u_j \rangle = \delta_{ij}, \qquad \|(A-\lambda)u_i\| \le \varepsilon, \quad i,j = 1,2,\dots,n,$$

then there are at least n orthogonal eigenfunctions ψ_k of A with eigenvalues in an ε-neighborhood of λ:

$$(A-\lambda_k)\psi_k = 0, \qquad |\lambda - \lambda_k| \le \varepsilon, \quad k = 1,2,\dots,n.$$

Theorem 5 (expansion of a quasimode)**.** *Let Γ be a Hilbert space, and let an operator A be self-adjoint. Let a quasimode $u \in \Gamma$ such that $\|u\| = 1$ and $\|(A-\lambda)u\| \le \varepsilon$ be given. If the interval $(\lambda-\varepsilon, \lambda+\varepsilon)$ contains only one point of the spectrum of A,*

$$A\psi = \mu\psi, \qquad |\lambda - \mu| < \varepsilon,$$

then the quasimode u has the expansion

$$u = \langle u, \psi \rangle \psi + \widetilde{u}, \qquad \|\tilde{u}\| \le \frac{\varepsilon}{d},$$

where d is the distance from λ to the spectrum of A with the point μ taken into account.

Remark 1. It is meaningful to use Theorem 5 in the case where it is known that $d \gg \varepsilon$. This theorem can suggest the form of the exact eigenfunction.

The following theorem is practically identical to a theorem proved in [9]; only the statement and the proof are somewhat different.

Theorem 6. *Let a self-adjoint operator A be given in a Hilbert space Γ. Let the following conditions be satisfied*:

1. *The set of n orthonormal quasimodes of the operator A is given,*

$$\langle u_i, u_j \rangle = \delta_{ij}, \qquad \|(A-\lambda)u_i\| \le \varepsilon, \quad i,j = 1,2,\dots,n.$$

2. *Let d be the distance from λ to the spectrum of A with the n closest points not taken into account* (*the number of points is counted with the multiplicity taken into account*)*. The estimate*

$$d > \sqrt{2n}\varepsilon$$

   holds.

3. *The eigenvalues μ_i and the corresponding eigenvectors z_i, $i = \overline{1,n}$, of the matrix with the elements*

$$V_{ij} = \langle (A-\lambda)u_i, u_j \rangle, \quad i,j = 1,2,\dots,n,$$

   are determined. The eigenvectors z_i are chosen orthonormal.

Then there exist $y_i \in \Gamma$ *such that*

$$y_i = v_i + w_i, \quad i = 1, 2, \dots, n,$$

$$v_i = \sum_{j=1}^{n} z_i^j u_j, \qquad \|w_i\| \le \frac{\sqrt{2n}\varepsilon}{d - \sqrt{2n}\varepsilon},$$

$$\|(A - \lambda - \mu_i) y_i\| \le \frac{4n\varepsilon^2}{d - \sqrt{2n}\varepsilon}.$$

Remark 2. If $d \gg \varepsilon$, then condition 2 is satisfied automatically, and calculating the eigenvalues of the matrix V permits obtaining the spectrum of A up to $O(\varepsilon^2/d)$.

Proof of Theorem 6. It follows from the first condition of this theorem that the interval contains at least n points of the spectrum of the operator A, and it follows from the second condition of this theorem that their number does not exceed n. We let ψ_i denote the eigenfunctions of A corresponding to the eigenvalues λ_i in this interval. Then d is the distance from the point λ to the spectrum of A without the points λ_i, $i = 1, \dots, n$, taken into account.

Let E be the operator of orthonormal projection on the linear span of the vectors u_i, $i = 1, \dots, n$, and let $E' = I - E$. We need to determine the operators

$$V = (A - \lambda)E + E(A - \lambda) - E(A - \lambda), \qquad A_0 = A - V.$$

We show that V is a finite-dimensional operator. Let $u_1, \dots, u_n, \dots, u_{\mathrm{r}}$ be an orthonormal basis in the space formed by the set of vectors $u_1, \dots, u_n$, $(A - \lambda)u_1, \dots, (A - \lambda)u_n$. Let a function $\phi \in \Gamma$ be orthogonal to all u_i, $i = \overline{1, r}$. Then

$$\|E(A - \lambda)\phi\|^2 = \langle E(A - \lambda)\phi, E(A - \lambda)\phi \rangle = \langle (A - \lambda)E(A - \lambda)\phi, \phi \rangle = 0$$

because the function ϕ is orthogonal to the image of $(A - \lambda)E$. The dimension of the operator $E(A - \lambda)$ therefore does not exceed $r \le 2n$. The other terms in the definition of V are obviously finite-dimensional.

We prove that $\|V\| \le \sqrt{2n}\varepsilon$. Obviously,

$$\|(A - \lambda)E\| \le \sqrt{n}\varepsilon.$$

We need to estimate the norm of $E(A - \lambda)$. Because $E(A - \lambda)$ is dual to $(A - \lambda)E$, we have

$$\|E(A - \lambda)\| \le \sqrt{n}\varepsilon.$$

Let $\phi \in \Gamma$ and $\|\phi\| = 1$. Then

$$\|V\phi\|^2 = \|E'(A - \lambda)E\phi + E(A - \lambda)\phi\|^2 \le 2n\varepsilon^2 + 2\langle E'(A - \lambda)E\phi, E(A - \lambda)\phi \rangle = 2n\varepsilon^2.$$

We show that λ is an isolated point of multiplicity n of the spectrum of A_0. The definition of A_0 and the fact that $Eu_i = u_i$, $i = \overline{1, n}$, imply

$$(A_0 - \lambda)u_i = (A - \lambda)u_i - Vu_i = 0, \quad i = 1, 2, \dots, n.$$

Because $\|V\| \le \sqrt{2n}\varepsilon$, any eigenfunction of A is a quasimode of A_0, and conversely. The operator A_0 therefore has precisely n spectral points on the interval $\bigl(\lambda - d + \sqrt{2n}\varepsilon, \lambda + d - \sqrt{2n}\varepsilon\bigr)$ with the multiplicity taken into account. Otherwise, there is a contradiction to condition 2 in this theorem. From Lemma 1, we obtain

$$\|(A_0-\lambda)^{-1}E'\| \le \bigl(d-\sqrt{2n}\varepsilon\bigr)^{-1}.$$

Hence, we represent the operator A as the sum of A_0 and a small finite-dimensional operator V. The spectrum and the eigenvectors A_0 near the point λ are known. The corrections to the eigenvectors and eigenvalues of A can be obtained using the perturbation theory in the case of the isolated degenerate eigenvalue λ.

Let v_i such that $Ev_i = v_i$ be the eigenfunctions of the operator EVE. There are n of such functions v_i because EVE is finite-dimensional of dimension n:

$$EVv_i = \mu_i v_i, \qquad \|v_i\| = 1, \qquad i = 1, 2, \dots, n.$$

Let $w_i = -(A_0-\lambda)^{-1}E'Vv_i$. It follows from the definitions of v_i and w_i that

$$\begin{aligned}
&A_0 v_i = A_0 E v_i = \lambda v_i,\\
&(V-\mu_i)v_i = (E'+E)(V-\mu_i)v_i = E'Vv_i, \qquad (A_0-\lambda)w_i = -E'Vv_i,\\
&|\mu_i| \le \|V\| \le \sqrt{2n}\varepsilon, \qquad \|V-\mu_i\| \le \|V\| + |\mu_i| \le 2\sqrt{2n}\varepsilon,\\
&\|w_i\| = \|(A_0-\lambda)^{-1}E'Vv_i\| \le \|(A_0-\lambda)^{-1}E'\|\,\|V\|\,\|v_i\| \le \frac{\sqrt{2n}\varepsilon}{d-\sqrt{2n}\varepsilon},\\
&\|(A-\lambda-\mu_i)(v_i+w_i)\| = \|(A_0-\lambda+V-\mu_i)(v_i+w_i)\| =\\
&\qquad\qquad = \|(V-\mu_i)w_i\| \le \|(V-\mu_i)\|\,\|w_i\| \le \frac{4n\varepsilon^2}{d-\sqrt{2n}\varepsilon}.
\end{aligned}$$

We have thus proved that $v_i + w_i$ are quasimodes with the eigenvalues $\lambda + \mu_i$, where $i = 1, 2, \dots, n$.

We can seek v_i and μ_i using the matrix elements of the operator V in the basis containing the vectors u_i, $i = 1, 2, \dots, n$. Then

$$V_{i,j} = \langle Vu_i, u_j\rangle = \langle (A-\lambda)Eu_i, u_j\rangle = \langle (A-\lambda)u_i, u_j\rangle.$$

The eigenvectors of this matrix are coefficients of the expansion of the vector v_i in the vectors u_j, and precisely μ_i, $i = 1, 2, \dots, n$, are the eigenvalues. The proof of the theorem is complete.

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