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PASSAGE THROUGH A POTENTIAL BARRIER AND MULTIPLE WELLS

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To the memory of Vladimir Savel'evich Buslaev

Abstract. The semiclassical limit as the Planck constant $\hbar$ tends to 0 is considered for bound states of a one-dimensional quantum particle in multiple potential wells separated by barriers. It is shown that, for each eigenvalue of the Schrödinger operator, the Bohr–Sommerfeld quantization condition is satisfied for at least one potential well. The proof of this result relies on a study of real wave functions in a neighborhood of a potential barrier. It is shown that, at least from one side, the barrier fixes the phase of the wave functions in the same way as a potential barrier of infinite width. On the other hand, it turns out that for each well there exists an eigenvalue in a small neighborhood of every point satisfying the Bohr–Sommerfeld condition.

§1. Introduction

1.1. Our goal is to study the semiclassical limit as $\hbar \to 0$ of eigenvalues $\lambda = \lambda(\hbar)$ of the one-dimensional Schrödinger equation

$$-\hbar^2\psi''(x;\lambda,\hbar) + v(x)\psi(x;\lambda,\hbar) = \lambda(\hbar)\psi(x;\lambda,\hbar), \quad v = \bar{v}, \quad \psi = \bar{\psi} \in L^2(\mathbb{R}), \tag{1.1}$$

for the case of several potential wells $X_1(\lambda), \dots, X_L(\lambda)$ where $v(x) < \lambda$ separated by barriers $B_1(\lambda), \dots, B_{L-1}(\lambda)$ where $v(x) > \lambda$. We suppose that the energy λ is noncritical; in particular, it is separated away from the bottoms of the wells and the tops of the barriers. We also assume that $v(x) \geq v_0$ for some $v_0 > \lambda$ and large $|x|$, that is, there are infinite barriers to the left of $X_1(\lambda)$ and to the right of $X_L(\lambda)$. Of course, the spectrum of the Schrödinger operator $H(\hbar) = -\hbar^2 d^2/dx^2 + v(x)$ below the point v_0 is discrete. It is a common wisdom that the limit of its eigenvalues $\lambda(\hbar)$ as $\hbar \to 0$ is described by some version of the Bohr–Sommerfeld quantization condition. However, in the case of multiple wells, we have not found a precise formulation and a proof of this statement in the literature. So we are aiming at filling this gap. Although quite elementary, some of the results obtained seem to be rather unexpected.

To explain them at a heuristic level, let us first recall briefly the thoroughly studied case of one potential well $X = X(\lambda) = (x_-, x_+)$ where the $x_\pm = x_\pm(\lambda)$ are the (only) solutions of the equation $v(x) = \lambda$. Put

$$\Phi_\pm(x;\lambda) = \pm \int_x^{x_\pm(\lambda)} (\lambda - v(y))^{1/2}\, dy, \quad x \in (x_-(\lambda), x_+(\lambda)). \tag{1.2}$$

From the Green–Liouville approximation (see, for example, the book [21, Chapter 6]) it follows that for $x \in X$ (inside the well) an arbitrary real solution of equation (1.1) has

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the asymptotics

$$\psi(x;\hbar) = A_+(\hbar)(\lambda - v(x))^{-1/4}\big(\sin\big(\hbar^{-1}\Phi_+(x) + \varphi_+(\hbar)\big) + O(\hbar)\big) \tag{1.3}$$

and

$$\psi(x;\hbar) = A_-(\hbar)(\lambda - v(x))^{-1/4}\big(\sin\big(\hbar^{-1}\Phi_-(x) + \varphi_-(\hbar)\big) + O(\hbar)\big) \tag{1.4}$$

as $\hbar \to 0$. Here the amplitudes $A_\pm(\hbar) = A_\pm(\lambda,\hbar)$ are elements of $\mathbb{R}_+$ and the phases $\varphi_\pm(\hbar) = \varphi_\pm(\lambda,\hbar)$ belong to $\mathbb{R}/(2\pi\mathbb{Z})$. We emphasize that the phases are always defined up to terms of order $O(\hbar)$. H. Jeffreys [13] and H. Kramers [15] (see also the book [17]) observed that if $\psi \in L^2(\mathbb{R}_\pm)$, then necessarily $\varphi_\pm(\hbar) = \pi/4 \pmod{\pi}$. Their arguments are based on contouring the turning points $x_\pm$ in the complex plane.

Comparing relations (1.3) and (1.4) where $\varphi_\pm(\hbar) = \pi/4 \pmod{\pi}$, we see that if λ is an eigenvalue of the operator $H(\hbar)$, then necessarily

$$\Phi(\lambda) := \int_{x_-(\lambda)}^{x_+(\lambda)} (\lambda - v(y))^{1/2}\, dy = \pi(n + 1/2)\hbar + O(\hbar^2), \quad \hbar \to 0, \tag{1.5}$$

for some integer $n = n(\lambda,\hbar)$. Formula (1.5) is known as the Bohr–Sommerfeld quantization condition. It shows that all eigenvalues of the operator $H(\hbar)$ in a fixed (not depending on $\hbar$) neighborhood of a noncritical energy λ cannot lie away of the $O(\hbar^2)$ neighborhoods of the points $\Phi^{-1}(\pi(n + 1/2)\hbar)$. It can be additionally shown that there is exactly one eigenvalue of $H(\hbar)$ in each of these neighborhoods.

From the point of view of differential equations, these results were discussed in [25]. Analytically, the paper [25] was based on a detailed study of the asymptotics of the eigenfunctions $\psi(x;\hbar)$ of $H(\hbar)$ as $\hbar \to 0$. As is well known (see [21, Chapter 11]), their behavior in neighborhoods of the turning points x_+ and x_- can be described in terms of the Airy functions. It is also possible (see, e.g., [24, Chapter VIII], or [7, Chapter IV]) to justify the method of Jeffreys–Kramers, but this requires the very restrictive assumption that the potential $v(x)$ is an analytic function.

1.2. In the case of multiple wells $X_1(\lambda),\dots,X_L(\lambda)$, one can write L quantization conditions:

$$\Phi_\ell(\lambda) := \int_{X_\ell(\lambda)} (\lambda - v(y))^{1/2}\, dy = \pi(n + 1/2)\hbar + O(\hbar^2), \quad \hbar \to 0, \quad \ell = 1,\dots,L, \tag{1.6}$$

where $n = n_\ell(\lambda,\hbar)$ are some integers. Again, we consider all eigenvalues of the Schrödinger operator $H(\hbar) = -\hbar^2 d^2/dx^2 + v(x)$ in the vicinity of some noncritical energy λ (so we avoid the bottoms of wells and the tops of barriers) and show that at least one of the quantization conditions (1.6) is satisfied for each eigenvalue.

The proof of this result relies on the study of *real* solutions $\psi(x;\hbar)$ of equation (1.1) for an arbitrary noncritical λ in a neighborhood of a potential barrier between some points (b_1,b_2); thus, $v(b_j) = \lambda$, $v(x) > \lambda$ for $x \in (b_1,b_2)$, and $v(x) < \lambda$ for $x \notin (b_1,b_2)$. Of course, b_1 and b_2 depend on λ. Set

$$\Theta_j(x,\lambda) = (-1)^j \int_{b_j(\lambda)}^{x} (\lambda - v(y))^{1/2}\, dy, \quad j = 1,2. \tag{1.7}$$

The Green–Liouville approximation shows that the solutions $\psi(x;\hbar)$ are oscillating functions away from the barrier:

$$\psi(x;\hbar) = A_1(\hbar)(\lambda - v(x))^{-1/4}\big(\sin\big(\hbar^{-1}\Theta_1(x,\lambda) + \theta_1(\hbar)\big) + O(\hbar)\big) \tag{1.8}$$

for $x < b_1$, and

$$\psi(x;\hbar) = A_2(\hbar)(\lambda - v(x))^{-1/4}\big(\sin\big(\hbar^{-1}\Theta_2(x,\lambda) + \theta_2(\hbar)\big) + O(\hbar)\big) \tag{1.9}$$

for $x > b_2$, where the amplitudes $A_j(\hbar) = A_j(\lambda, \hbar)$ are positive, and the phases $\theta_j(\hbar) = \theta_j(\lambda, \hbar)$ belong to $\mathbb{R}/(2\pi\mathbb{Z})$. The striking result is that $\theta_j(\hbar) = \pi/4 \pmod \pi$ for at least one $j = 1, 2$. So the phase $\theta_j(\hbar)$ is fixed by a finite barrier exactly in the same way as by an infinitely wide (and probably infinitely high) potential barrier (cf. formulas (1.3) and (1.4) for $\varphi_\pm(\hbar) = \pi/4 \pmod \pi$). We use the term *fixing condition* for this fact. We emphasize that we consider real solutions of the Schrödinger equation. Thus, our problem differs from the famous problem of tunneling of a wave through a potential barrier where the solutions considered are necessarily complex.

In the case of L wells $X_1, \ldots, X_L$ separated by $L-1$ barriers, the stated result yields at least $L-1$ fixing conditions. Additionally, if λ is an eigenvalue of the operator $H(\hbar)$, then in accordance with formulas (1.3) and (1.4) with $\varphi_\pm(\hbar) = \pi/4 \pmod \pi$ the fixing conditions hold at the left point of X_1 and at the right point of X_L. Thus, we have $L+1$ fixing conditions for L wells, and hence there exists a well X_ℓ for which two fixing conditions are satisfied. The quantization condition (1.5) for this well can be obtained essentially in the same way as for the one-well problem.

Furthermore, we show that, for each n, there is at most one solution λ of equation (1.6). Unfortunately, our proof of this fact requires an additional assumption. In general, this assumption is rather implicit, but it is automatically satisfied in the case of two symmetric wells.

Finally, constructing appropriate trial functions, we check that, for all $\ell = 1, \ldots, L$ and $n \in \mathbb{Z}$ such that $\Phi_\ell^{-1}(\pi(n+1/2)\hbar)$ belongs to a neighborhood of λ_0, there is at least one eigenvalue of $H(\hbar)$ in an $O(\hbar^2)$-neighborhood of each point $\Phi_\ell^{-1}(\pi(n+1/2)\hbar)$. This yields a one-to-one correspondence between the eigenvalues of $H(\hbar)$ in a neighborhood of λ_0 and the points $\Phi_\ell^{-1}(\pi(n+1/2)\hbar)$.

1.3. This paper can be viewed as a continuation of [25], where the case of one potential well was studied in detail. It is organized as follows. In §2, we collect various results on the asymptotics as $\hbar \to 0$ of solutions $\psi(x; \hbar)$ of equation (1.1). It is a common wisdom that this asymptotics is described by the Green–Liouville approximation away from the turning points x where $\lambda = v(x)$. In neighborhoods of the turning points, the asymptotics of $\psi(x; \hbar)$ is more complicated and is given in terms of Airy functions. The corresponding results were obtained by Langer in [18, 19] and thoroughly exposed, for example, by Olver in his book [21]. We essentially follow the approach of [21]. The main difference concerns estimates of remainders. It is convenient to treat separately the classically allowed (where $v(x) < \lambda$) and forbidden (where $v(x) > \lambda$) regions, which seems to be intuitively clearer. The results on solutions exponentially decaying in the classically forbidden region are borrowed from [25]; they are stated as Theorem 2.2. The results on solutions exponentially growing in the classically forbidden region are stated as Theorem 2.7. Its proof is postponed to §3.

The case of a one potential well is considered in §4. Here our results are rather standard, but in contrast to the usual presentations, we do not suppose that $\psi \in L^2(\mathbb{R})$ and our arguments are of local nature.

The behavior of real solutions $\psi(x; \hbar)$ of equation (1.1) in a neighborhood of a potential barrier is studied in §5. The main result where the fixing conditions are established is stated as Theorem 5.5. In the Appendix, it is compared with the tunneling of a wave (described by a complex solution of equation (1.1)) through a barrier.

Theorem 5.5 allows us to study the quantization conditions for eigenvalues in the case of multiple potential wells. This is done in §6; see Theorems 6.2, 6.3, and 6.4. Here we establish one-to-one correspondence between the eigenvalues of the Schrödinger operator $H(\hbar) = -\hbar^2 d^2/dx^2 + v(x)$ in a neighborhood of a noncritical energy and the solutions of equations (1.6). The results of such type imply the semiclassical Weyl formula for the distribution of eigenvalues of the operator $H(\hbar)$ as $\hbar \to 0$ with a strong estimate of the remainder. It turns out (see Propositions 6.6 and 6.7) that this remainder never exceeds L.

1.4. The quantization conditions for one-dimensional multiple wells is of course one of the basic problems in quantum mechanics. Therefore, it is rather surprising that it was thoroughly considered mainly for the case of two symmetric wells, and in the majority of the papers (see, e.g., [9, 10, 14, 20]) on this subject only the exponential splitting due to the tunneling through the barrier of two close eigenvalues was studied. A similar problem was also considered in the multidimensional case (see, e.g., [12, 23]). In several papers mentioned above, a special attention was paid to eigenvalues lying at the bottoms of potential wells. There are also numerous papers (see, e.g., [8, 5]) where the Bohr–Sommerfeld quantization condition was discussed near the tops of potential barriers. All these problems are fairly far from the present paper.

The closest to the present paper is apparently the paper [11] by Helffer and Robert, where the quantization conditions were studied for two symmetric potential wells. The paper [11] is written in a very general context of multidimensional pseudodifferential operators and, analytically, it relies on the semiclassical functional calculus combined with some results of the microlocal analysis (see the books [6, 22]). We emphasize that, for symmetric wells, there is only one quantization condition. It was stated in Theorem 3.9 of [11] (probably, there is a misprint in the formula in that theorem, the correct formula being given in Remark 3.13).

Finally we note that semiclassical methods were successfully applied to substantially more difficult one-dimensional problems. For example, we mention the series of papers [2, 3, 4] by Buslaev with collaborators, who developed the semiclassical theory on a periodic background.

We emphasize that multidimensional problems are out of the scope of this paper, which relies exclusively on the methods of ordinary differential equations.

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1.5. We introduce some standard notation. We denote by C and c various positive constants whose precise values are of no importance. The parameter $\hbar$ (the Planck constant) is always assumed to be sufficiently small. The phases in various asymptotic formulas such as (1.3), (1.4) or (1.8), (1.9) are defined up to terms of order $O(\hbar)$ as $\hbar \to 0$. All asymptotic relations are assumed to be differentiable with respect to x and λ with natural estimates of remainders in the differentiated formulas.

We work in a neighborhood of some noncritical energy λ_0 (it means that $v'(x) \neq 0$ if $v(x) = \lambda_0$). Various assumptions imposed at λ_0 are automatically satisfied for all λ in some neighborhood (Λ_1, Λ_2) of λ_0. We suppose of course that (Λ_1, Λ_2) is separated from all critical values of $v(x)$. If it cannot lead to confusion, the dependence of various objects on λ is often neglected in the notation. The derivatives in λ are usually denoted by dots.

The conditions on $v(x)$ at infinity are not very important; for example, $v(x)$ may tend to $+\infty$ or may have finite limits as $x \to \pm\infty$. However, we assume that

$$\liminf_{x\to\pm\infty} v(x) > \lambda_0 \tag{1.10}$$

so that there are infinite barriers to the left of the well X_1 and to the right of the well X_L.

§2. Semiclassical solutions of the Schrödinger equation

In this section we construct solutions of equation (1.1) that oscillate inside a potential well and (super)exponentially decay or grow inside a potential barrier. This standard construction will of course be given in terms of the Airy functions.

2.1. We recall the definition of the Airy functions and their necessary properties (see, e.g., the book [21, Chapter 11.1] for the details). Consider the equation

$$-\theta''(t) + t\theta(t) = 0 \tag{2.1}$$

and denote by $\mathrm{Ai}(t)$ its solution with the asymptotics

$$\mathrm{Ai}(t) = 2^{-1}\pi^{-1/2}t^{-1/4}\exp(-2t^{3/2}/3)(1 + O(t^{-3/2})), \quad t \to +\infty. \tag{2.2}$$

Then

$$\mathrm{Ai}(t) = \pi^{-1/2}|t|^{-1/4}\sin(2|t|^{3/2}/3 + \pi/4) + O(|t|^{-7/4}), \quad t \to -\infty. \tag{2.3}$$

The solution $\mathrm{Bi}(t)$ of equation (2.1) is defined by its asymptotics as $t \to -\infty$, which differs from (2.3) only by the phase shift:

$$\mathrm{Bi}(t) = \pi^{-1/2}|t|^{-1/4}\cos(2|t|^{3/2}/3 + \pi/4) + O(|t|^{-7/4}), \quad t \to -\infty. \tag{2.4}$$

It grows exponentially at $+\infty$:

$$\mathrm{Bi}(t) = \pi^{-1/2}t^{-1/4}\exp(2t^{3/2}/3)(1 + O(t^{-3/2})), \quad t \to +\infty. \tag{2.5}$$

Note that $\mathrm{Ai}(t) > 0$ and $\mathrm{Bi}(t) > 0$ for all $t \geq 0$.

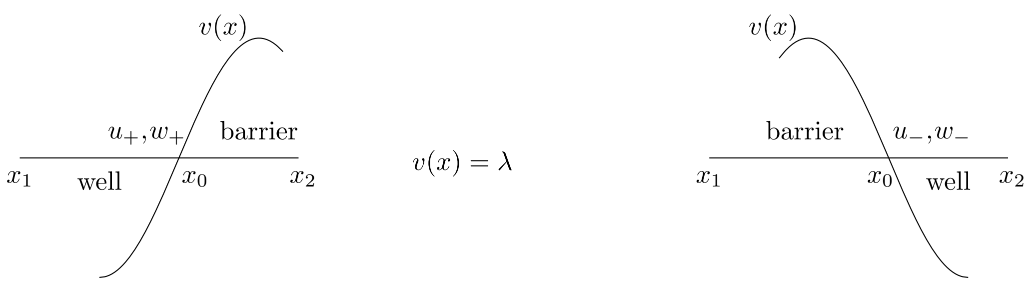
We also use the fact that all asymptotics (2.2), (2.3) and (2.4), (2.5) can be differentiated in t. In this case the remainders $O(|t|^{-3/2})$ in (2.2), (2.5) remain unchanged, and $O(|t|^{-7/4})$ in (2.3), (2.4) is replaced by $O(|t|^{-5/4})$. In particular, for the Wronskian we have

$$\{\mathrm{Ai}(t), \mathrm{Bi}(t)\} := \mathrm{Ai}'(t)\,\mathrm{Bi}(t) - \mathrm{Ai}(t)\,\mathrm{Bi}'(t) = -\pi^{-1}.$$

2.2. For a point $x_0 \in \mathbb{R}$ and the signs "$+$" or "$-$", we make the following assumption.

Assumption 2.1. The function v is of class C^2 on some interval (x_1, x_2) containing x_0, and $\pm(v(x) - v(x_0)) < 0$ for $x \in (x_1, x_0)$ and $\pm(v(x) - v(x_0)) > 0$ for $x \in (x_0, x_2)$. Moreover, the function v belongs to the class C^3 in some neighborhood of the point x_0 and $\pm v'(x_0) > 0$.

Let $\lambda = v(x_0)$ in equation (1.1). If Assumption 2.1 is fulfilled with the sign "$+$", then (x_1, x_0) is a potential well and (x_0, x_2) is a potential barrier. On the contrary, if it holds true with the sign "$-$", then (x_1, x_0) is a potential barrier and (x_0, x_2) is a potential well. In both cases x_0 is a turning point. Note that Assumption 2.1 is automatically satisfied for all x_0' in some neighborhood of x_0.



Case "$+$" Case "$-$"

Our goal in this section is to describe the asymptotics as $\hbar \to 0$ of the solutions $u_\pm(x; x_0, \hbar)$ of equation (1.1) that exponentially decay and of solutions $w_\pm(x; x_0, \hbar)$ that exponentially grow inside the barrier. Both these solutions are oscillating inside the well.

To state the results, we need the following auxiliary functions:

$$
\begin{aligned}
\xi_+(x; x_0) &= \Big(\frac{3}{2}\int_{x_0}^{x} (v(y) - v(x_0))^{1/2}\, dy\Big)^{2/3}, \quad x \in (x_0, x_2),\\
\xi_+(x; x_0) &= -\Big(\frac{3}{2}\int_{x}^{x_0} (v(x_0) - v(y))^{1/2}\, dy\Big)^{2/3}, \quad x \in (x_1, x_0),
\end{aligned} \tag{2.6}
$$

and

$$
\begin{aligned}
\xi_-(x; x_0) &= \Big(\frac{3}{2}\int_{x}^{x_0} (v(y) - v(x_0))^{1/2}\, dy\Big)^{2/3}, \quad x \in (x_1, x_0),\\
\xi_-(x; x_0) &= -\Big(\frac{3}{2}\int_{x_0}^{x} (v(x_0) - v(y))^{1/2}\, dy\Big)^{2/3}, \quad x \in (x_0, x_2).
\end{aligned}
$$

Since the point x_0 is fixed, in this section we set for brevity

$$\xi_\pm(x) = \xi_\pm(x; x_0) \quad \text{and} \quad u_\pm(x; \hbar) = u_\pm(x; x_0, \hbar), \quad w_\pm(x; \hbar) = w_\pm(x; x_0, \hbar).$$

It is easy to show (see Lemma 3.1 in Chapter 11 of [21] for the details) that $\xi_\pm \in C^3(x_1, x_2)$, $\pm\xi_\pm'(x) > 0$ and

$$\xi_\pm'(x)^2 \xi_\pm(x) = v(x) - v(x_0). \tag{2.7}$$

It follows that

$$\xi_\pm'(x_0) = \pm|v'(x_0)|^{1/3}. \tag{2.8}$$

Now we are in a position to construct the solutions $u_\pm(x; \hbar)$ of equation (1.1). The following assertion is well known (see, e.g., Theorem 2.5 in [25]).

Theorem 2.2. *Let Assumption* 2.1 *be fulfilled with the sign* "$\pm$". *Then equation* (1.1) *with* $\lambda = v(x_0)$ *has a solution* $u_\pm(x; \hbar) = u_\pm(x; x_0, \hbar)$ *such that*:

(i) *if* $x \in [x_0, x_2)$ *for* u_+ *and* $x \in (x_1, x_0]$ *for* u_-, *then*

$$u_\pm(x; \hbar) = \pi^{1/2}\hbar^{-1/6}|\xi_\pm'(x)|^{-1/2}\operatorname{Ai}(\hbar^{-2/3}\xi_\pm(x))\big(1 + O(\hbar)\big); \tag{2.9}$$

(ii) *if* $x \in (x_1, x_0]$ *for* u_+ *and* $x \in [x_0, x_2)$ *for* u_-, *then*

$$u_\pm(x; \hbar) = \pi^{1/2}\hbar^{-1/6}|\xi_\pm'(x)|^{-1/2}\operatorname{Ai}(\hbar^{-2/3}\xi_\pm(x)) + O\big(\hbar(1 + \hbar^{-2/3}|x - x_0|)^{-1/4}\big). \tag{2.10}$$

These estimates are uniform on the compact subintervals of (x_1, x_2).

We emphasize that formulas (2.9) and (2.10) differ by the estimates of the remainders only. Away from the point x_0, we can replace the Airy function $\operatorname{Ai}(t)$ by its asymptotics (2.2) or (2.3). Indeed, by (2.8) we have

$$|\xi_\pm(x)| \geq c|x - x_0|, \quad c > 0, \tag{2.11}$$

whence

$$\hbar^{-2/3}\xi_+(x) \to \pm\infty \ \text{ if } \ \hbar^{-2/3}(x - x_0) \to \pm\infty$$

and

$$\hbar^{-2/3}\xi_-(x) \to \pm\infty \ \text{ if } \ \hbar^{-2/3}(x - x_0) \to \mp\infty.$$

This leads to the following result.

Corollary 2.3. *The functions* $u_\pm$ *have the following asymptotic behavior as* $\hbar \to 0$:

(i) *if $x > x_0$ for u_+ and $x < x_0$ for u_-, then*

$$u_\pm(x;\hbar) = 2^{-1}\big(v(x)-v(x_0)\big)^{-1/4}\exp\left(\mp\hbar^{-1}\int_{x_0}^{x}\big(v(y)-v(x_0)\big)^{1/2}\,dy\right)\big(1+O(\hbar)\big); \tag{2.12}$$

(ii) *if $x < x_0$ for u_+ and $x > x_0$ for u_-, then*

$$u_\pm(x;\hbar) = \big(v(x_0)-v(x)\big)^{-1/4}\sin\left(\pm\hbar^{-1}\int_{x}^{x_0}\big(v(x_0)-v(y)\big)^{1/2}\,dy+\pi/4\right)+O(\hbar). \tag{2.13}$$

These estimates are uniform in x on the compact subintervals of (x_1, x_0) and (x_0, x_2).

Remark 2.4. Formulas (2.12) and (2.13) allow x to approach to x_0 as $\hbar \to 0$, but not too rapidly. To be precise, it suffices to require that x lie away of a $O(\hbar^{2/3})$-neighborhood of the point x_0. In this case the remainders in (2.12) and (2.13) should be replaced by $O(\hbar|x-x_0|^{-3/2})$ and $O(\hbar|x-x_0|^{-7/4})$, respectively.

On the other hand, using estimates (2.11) and $|\operatorname{Ai}(t)| \leq C(1+|t|)^{-1/4}$, we obtain estimates, uniform in $\hbar$, for the functions $u_\pm(x;\hbar)$ in neighborhoods of the turning points.

Corollary 2.5. *For all $x \in (x_1, x_2)$, we have*

$$|u_\pm(x;\hbar)| \leq C(\hbar^{2/3} + |x-x_0|)^{-1/4}$$

with a constant C independent of $\hbar$.

Note that all asymptotic relations (2.9), (2.10), (2.12), and (2.13) can be differentiated in x. In particular, we have the asymptotics

$$u'_\pm(x;\hbar) = \mp\pi^{-1/2}\hbar^{-1}\big(v(x_0)-v(x)\big)^{1/4}\cos\left(\pm\hbar^{-1}\int_{x}^{x_0}\big(v(x_0)-v(y)\big)^{1/2}\,dy+\pi/4\right)+O(1)$$

as $\hbar \to 0$ for u_+ if $x < x_0$ and for u_- if $x > x_0$.

All these relations can also be differentiated with respect to x_0. For example, we have (recall that $\lambda = v(x_0)$)

$$\begin{aligned}
&\partial u_\pm(x; x_0, \hbar)/\partial x_0 \\
&\quad = \pm 2^{-1}\pi^{-1/2}\hbar^{-1}\big(v(x_0)-v(x)\big)^{-1/4}\int_{x}^{x_0}\big(v(x_0)-v(y)\big)^{-1/2}\,dy \\
&\qquad \times v'(x_0)\cos\left(\pm\hbar^{-1}\int_{x}^{x_0}\big(v(x_0)-v(y)\big)^{1/2}\,dy+\pi/4\right)+O(1)
\end{aligned}$$

as $\hbar \to 0$ for u_+ if $x < x_0$ and for u_- if $x > x_0$.

We also need to look at the behavior of the solutions $u_\pm(x;\hbar)$ as $x \to \pm\infty$. For that, we need some weak condition on the behavior of the function $v(x)$ at infinity. The following result is a particular case of Theorem 2.5 in [25].

Theorem 2.6. *Under the assumptions of Theorem 2.2, suppose that condition (1.10) is satisfied with $\lambda_0 = v(x_0)$ and that, for some $\rho_0 > 1$, the function*

$$\big(|v(x)-\lambda_0|^{-3}v'(x)^2 + |v(x)-\lambda_0|^{-2}|v''(x)|\big)\left|\int_{x_0}^{x}|v(y)-\lambda_0|^{1/2}\,dy\right|^{\rho_0} \tag{2.14}$$

is bounded as $x \to \pm\infty$. Then

$$u_\pm(\hbar) \in L^2(\mathbb{R}_\pm).$$

The function (2.14) is bounded in all reasonable cases. For example, if $v(x) \to v_0 > v(x_0)$, it suffices to require that

$$v'(x)^2 + |v''(x)| = O(|x|^{-\rho_0}), \quad \rho_0 > 1, \quad |x| \to \infty.$$

This is also true if $v(x)$ behaves at infinity as $|x|^\alpha$ or $e^{\alpha|x|}$ where $\alpha > 0$; in these cases $\rho_0 = 2$.

2.3. Next we consider the solutions of equation (1.1) that are exponentially growing as $\hbar \to 0$ inside the barrier. The following assertion complements Theorem 2.2. Its proof will be given in the next section.

Theorem 2.7. *Let Assumption* 2.1 *be fulfilled with the sign "$\pm$". Then equation* (1.1) *where $\lambda = v(x_0)$ has a solution $w_\pm(x;\hbar) = w_\pm(x;x_0,\hbar)$ such that*:

(i) *if $x \in [x_0, x_2)$ for w_+ and $x \in (x_1, x_0]$ for w_-, then*

$$w_\pm(x;\hbar) = \pi^{1/2}\hbar^{-1/6}|\xi_\pm'(x)|^{-1/2}\,\mathrm{Bi}(\hbar^{-2/3}\xi_\pm(x))\big(1+O(\hbar)\big); \tag{2.15}$$

(ii) *if $x \in (x_1, x_0]$ for w_+ and $x \in [x_0, x_2)$ for w_-, then*

$$w_\pm(x;\hbar) = \pi^{1/2}\hbar^{-1/6}|\xi_\pm'(x)|^{-1/2}\,\mathrm{Bi}(\hbar^{-2/3}\xi_\pm(x)) + O\big(\hbar(1+\hbar^{-2/3}|x-x_0|)^{-1/4}\big). \tag{2.16}$$

These estimates are uniform on the compact subintervals of (x_1, x_2).

Obviously, formulas (2.15) and (2.16) differ by the remainders only. Using estimate (2.11) away from the points x_0, we can replace the Airy function $\mathrm{Bi}(t)$ by its asymptotics (2.4) or (2.5). This leads to the following result (cf. Corollary 2.3).

Corollary 2.8. *The functions $w_\pm$ have the following asymptotic behavior as $\hbar \to 0$*:

(i) *if $x > x_0$ for w_+ and $x < x_0$ for w_-, then*

$$w_\pm(x;\hbar) = \big(v(x)-v(x_0)\big)^{-1/4}\exp\Big(\pm\hbar^{-1}\int_{x_0}^{x}\big(v(y)-v(x_0)\big)^{1/2}dy\Big)\big(1+O(\hbar)\big); \tag{2.17}$$

(ii) *if $x < x_0$ for w_+ and $x > x_0$ for w_-, then*

$$w_\pm(x;\hbar) = \big(v(x_0)-v(x)\big)^{-1/4}\cos\Big(\pm\hbar^{-1}\int_{x}^{x_0}\big(v(x_0)-v(y)\big)^{1/2}dy+\pi/4\Big)+O(\hbar). \tag{2.18}$$

These estimates are uniform in x on the compact subintervals of (x_1, x_0) and (x_0, x_2).

Remark 2.9.

(i) Like in Theorem 2.2, the estimate of the remainders in (2.16) can be improved.
(ii) Formulas (2.17) and (2.18) allow x to approach x_0 as $\hbar \to 0$, but not too rapidly. To be precise, it suffices to require that x lie away of a $O(\hbar^{2/3})$-neighborhood of the point x_0. In this case the remainders in (2.17) and (2.18) should be replaced by $O(\hbar|x-x_0|^{-3/2})$ and $O(\hbar^{7/6}|x-x_0|^{-7/4})$, respectively.
(iii) Corollary 2.5 remains true for the functions $w_\pm$.
(iv) All asymptotic formulas (2.15), (2.16) and (2.17), (2.18) admit differentiation in x (and in x_0). For derivatives, the remainders $O(\hbar)$ should be replaced by $O(1)$.

Of course, the solutions u_+, w_+ and u_-, w_- of equation (1.1) are linearly independent. The two pairs of formulas (2.12), (2.17) or (2.13), (2.18) allow one to calculate their Wronskians:

$$\{u_\pm(\hbar), w_\pm(\hbar)\} := u_\pm'(x,\hbar)w_\pm(x,\hbar) - u_\pm(x,\hbar)w_\pm'(x,\hbar) = \mp\hbar^{-1}(1+O(\hbar)). \tag{2.19}$$

2.4. An arbitrary *real* solution ψ of equation (1.1) on the interval (x_1, x_2) is a linear combination of the solutions u_+, w_+ and u_-, w_-, that is,

$$\psi(x,\hbar) = \alpha_\pm(\hbar)u_\pm(x,\hbar) + \beta_\pm(\hbar)w_\pm(x,\hbar).$$

It is convenient to put $A_\pm(\hbar) = \sqrt{\alpha_\pm(\hbar)^2 + \beta_\pm(\hbar)^2}$ and

$$\alpha_\pm(\hbar) = A_\pm(\hbar)\cos\vartheta_\pm(\hbar), \quad \beta_\pm(\hbar) = A_\pm(\hbar)\sin\vartheta_\pm(\hbar);$$

the phases $\vartheta_\pm(\hbar)$ are of course defined up to terms $2\pi n$, where $n \in \mathbb{Z}$. If Assumption 2.1 holds true with the sign "$+$", then from formulas (2.13), (2.18) it follows that ψ has the asymptotic behavior

$$\psi(x;\hbar) = A_+(\hbar)\big(\lambda - v(x)\big)^{-1/4}\left(\sin\left(\hbar^{-1}\int_x^{x_0}(\lambda - v(y))^{1/2}\,dy + \frac{\pi}{4} + \vartheta_+(\hbar)\right) + O(\hbar)\right) \tag{2.20}$$

for $x \in (x_1, x_0)$. Similarly, if Assumption 2.1 is fulfilled with the sign "$-$", then ψ has the asymptotic behavior

$$\psi(x;\hbar) = A_-(\hbar)\big(\lambda - v(x)\big)^{-1/4}\left(\sin\left(\hbar^{-1}\int_{x_0}^{x}(\lambda - v(y))^{1/2}\,dy + \frac{\pi}{4} + \vartheta_-(\hbar)\right) + O(\hbar)\right) \tag{2.21}$$

for $x \in (x_0, x_2)$. Of course, relations (2.20) and (2.21) are uniform in x on the compact subintervals of (x_1, x_0) and (x_0, x_2), respectively.

§3. Proof of Theorem 2.7

3.1. We shall prove Theorem 2.7 for the sign "$+$" and omit this index. Let the function $\xi(x) = \xi_+(x; x_0)$ be defined by formulas (2.6), and let $\xi_j = \xi(x_j)$ for $j = 1, 2$. Since $\xi'(x) > 0$, the variable x can be regarded as a function of ξ for $\xi \in (\xi_1, \xi_2)$.

We make the change of variables $x \mapsto \xi$ in equation (1.1) for $w(x;\hbar)$ and set

$$w(x;\hbar) = \pi^{1/2}\hbar^{-1/6}\xi'(x)^{-1/2} f(\hbar^{-2/3}\xi(x);\hbar). \tag{3.1}$$

Then, using identity (2.7), we obtain

$$-f''(\hbar^{-2/3}\xi;\hbar) + \hbar^{-2/3}\xi f(\hbar^{-2/3}\xi;\hbar) = \hbar^{4/3} r(\xi) f(\hbar^{-2/3}\xi;\hbar), \tag{3.2}$$

where

$$r(\xi) = p(x(\xi)) \tag{3.3}$$

and

$$p(x) = (\xi'(x)^{-1/2})''\xi'(x)^{-3/2} \tag{3.4}$$

is a continuous function of $x \in (x_1, x_2)$. Setting $t = \hbar^{-2/3}\xi$ in (3.2), we get the following intermediary result.

Lemma 3.1. *Let $t = \hbar^{-2/3}\xi(x)$, and let the functions $w(x;\hbar)$ and $f(t;\hbar)$ be related by formula* (3.1)*. Then equation* (1.1) *for $w(x;\hbar)$ and $x \in (x_1, x_2)$ is equivalent to the equation*

$$-f''(t;\hbar) + tf(t;\hbar) = R(t;\hbar) f(t;\hbar) \tag{3.5}$$

for $f(t;\hbar)$ and $t \in (\xi_1\hbar^{-2/3}, \xi_2\hbar^{-2/3})$. Here

$$R(t;\hbar) = \hbar^{4/3} r(\hbar^{2/3}t)$$

and the function $r(\xi)$ is defined by (3.3) *and* (3.4)*.*

Since $r(\xi)$ is a bounded function, we have the estimate

$$|R(t;\hbar)| \le C\hbar^{4/3} \tag{3.6}$$

where for all $\eta_1 > \xi_1$ and $\eta_2 < \xi_2$, the constant $C = C(\eta_1, \eta_2)$ does not depend on $t \in (\eta_1\hbar^{-2/3}, \eta_2\hbar^{-2/3})$.

3.2. Let us reduce the differential equation (3.5) to a Volterra integral equation. Set

$$K(t,s;\hbar)=\pi\big(\operatorname{Ai}(t)\operatorname{Bi}(s)-\operatorname{Ai}(s)\operatorname{Bi}(t)\big)R(s;\hbar)$$

and consider the equation

$$f(t;\hbar)=\operatorname{Bi}(t)+\int_0^t K(t,s;\hbar)f(s;\hbar)\,ds. \tag{3.7}$$

Differentiating twice, we see that its solution satisfies also the differential equation (3.5). We shall study equation (3.7) separately for $t\le 0$ and $t\ge 0$.

If $t\le 0$, we use the inequality

$$|\operatorname{Ai}(t)|+|\operatorname{Bi}(t)|\le C(1+|t|)^{-1/4},$$

in accordance with (2.2) and (2.5). Hence, by (3.6), we have the estimate

$$|K(t,s;\hbar)|\le C\hbar^{4/3}(1+|s|)^{-1/2},\quad t\le s\le 0. \tag{3.8}$$

We consider equation (3.7) on the interval $(\eta_1\hbar^{-2/3},0)$ in the space $\mathbf{B}(\hbar)$ of functions f with the norm

$$\|f\|=\sup_{t\in(\eta_1\hbar^{-2/3},0)}(1+|t|)^{1/4}|f(t)|.$$

In this space, we introduce an auxiliary operator $\mathbf{K}(\hbar)$ by the formula

$$(\mathbf{K}(\hbar)f)(t)=\int_0^t K(t,s;\hbar)f(s)\,ds.$$

By (3.8), we have

$$|(\mathbf{K}(\hbar)f)(t)|\le C\hbar^{4/3}(1+|t|)^{1/4}\|f\|\le C_1\hbar(1+|t|)^{-1/4}\|f\|$$

if $t\in(\eta_1\hbar^{-2/3},0)$, so that $\|\mathbf{K}(\hbar)\|=O(\hbar)$. It follows that equation (3.7) has a unique solution $f(t;\hbar)$ and

$$|f(t;\hbar)-\operatorname{Bi}(t)|\le C\hbar(1+|t|)^{-1/4}\quad\text{if}\quad t\in(\eta_1\hbar^{-2/3},0). \tag{3.9}$$

By (2.11), this yields representation (2.16) for the function (3.1).

For $t\ge 0$, we make the multiplicative change of variables

$$f(t;\hbar)=\pi^{1/2}\hbar^{-1/6}\operatorname{Bi}(t)g(t;\hbar). \tag{3.10}$$

Then equation (3.7) reads as

$$g(t;\hbar)=1+\int_0^t L(t,s;\hbar)g(s;\hbar)\,ds \tag{3.11}$$

where

$$L(t,s;\hbar)=\pi\Big(\frac{\operatorname{Ai}(t)}{\operatorname{Bi}(t)}\operatorname{Bi}(s)^2-\operatorname{Ai}(s)\operatorname{Bi}(s)\Big)R(s;\hbar),\quad 0\le s\le t.$$

From (2.2) and (2.5) it follows that

$$|\operatorname{Ai}(s)\operatorname{Bi}(s)|\le C(1+s)^{-1/2}.$$

Since $\operatorname{Bi}(t)$ is a monotone increasing function of $t>0$, this yields the estimate (cf. (3.8))

$$|L(t,s;\hbar)|\le C\hbar^{4/3}(1+s)^{-1/2},\quad 0\le s\le t.$$

Thus, much as in the case of $t\le 0$, we get the bound (cf. (3.9))

$$|g(t;\hbar)-1|\le C\hbar^{4/3}(1+t)^{1/2}\le C_1\hbar\quad\text{if}\quad t\in(0,\eta_2\hbar^{-2/3}).$$

Using (3.10), we see that function (3.1) satisfies estimate (2.15). Differentiating the integral equations (3.7) and (3.11) with respect to t, we obtain asymptotic relations for $g'(t;\hbar)$ and then for $w'(x;\hbar)$. This concludes the proof of Theorem 2.7.

§4. One potential well

4.1. Here we consider one potential well (x_-, x_+) bounded by the turning points $x_- = x_-(\lambda)$ and $x_+ = x_+(\lambda)$. To be precise, we assume the following.

Assumption 4.1. The function v is of class C^2 on some interval $(x_1, x_2) \subset \mathbb{R}$. The equation $v(x) = \lambda_0$ has two solutions $x_+ = x_+(\lambda_0), x_- = x_-(\lambda_0)$ in (x_1, x_2), $x_- < x_+$ and $v(x) < \lambda_0$ for $x \in (x_-, x_+)$, $v(x) > \lambda_0$ for $x \notin [x_-, x_+]$. Moreover, the function v belongs to the class C^3 in some neighborhood of the points x_-, x_+ and $v'(x_-) < 0$, $v'(x_+) > 0$.

Set

$$\Phi(\lambda) = \int_{x_-(\lambda)}^{x_+(\lambda)} (\lambda - v(x))^{1/2}\, dx. \tag{4.1}$$

It is easy to check that $\Phi \in C^1(\Lambda_1, \Lambda_2)$. Moreover, differentiating formula (4.1) and using the equation $\lambda - v(x_\pm(\lambda)) = 0$, we obtain

$$\dot\Phi(\lambda) = 2^{-1} \int_{x_-(\lambda)}^{x_+(\lambda)} (\lambda - v(x))^{-1/2}\, dx > 0. \tag{4.2}$$

Thus, Φ is a one-to-one mapping of a neighborhood (Λ_1, Λ_2) of λ_0 onto a neighborhood $(\Phi(\Lambda_1), \Phi(\Lambda_2))$ of the point $\mu_0 = \Phi(\lambda_0)$.

Note that a classical particle of the energy λ and the mass $m = 1/2$ oscillates between the points $x_-(\lambda)$ and $x_+(\lambda)$ (see the book [16, §11 and §44]). The function $\Phi(\lambda)$ is known as the abbreviated action (with the coefficient 1/2) of this motion, and the function $\dot\Phi(\lambda)$ is the half-period of the oscillations.

We are interested in the asymptotic behavior as $\hbar \to 0$ of an arbitrary *real* solution $\psi(x; \hbar)$ of equation (1.1) on the interval (x_-, x_+). Recall that the functions $u_\pm(x; x_\pm, \hbar)$ and $w_\pm(x; x_\pm, \hbar)$ were constructed in Theorems 2.2 and 2.7, respectively. Since, by (2.19), the functions $u_+(x; x_+, \hbar)$, $w_+(x; x_+, \hbar)$ as well as $u_-(x; x_-, \hbar)$, $w_-(x; x_-, \hbar)$ are linearly independent, we have

$$\begin{aligned} \psi(x, \hbar) &= \alpha_+(\hbar) u_+(x; x_+, \hbar) + \beta_+(\hbar) w_+(x; x_+, \hbar) \\ &= \alpha_-(\hbar) u_-(x; x_-, \hbar) + \beta_-(\hbar) w_-(x; x_-, \hbar) \end{aligned} \tag{4.3}$$

for some $\alpha_\pm(\hbar), \beta_\pm(\hbar) \in \mathbb{R}$. We put $A_\pm(\hbar) = \sqrt{\alpha_\pm(\hbar)^2 + \beta_\pm(\hbar)^2}$ and

$$\alpha_\pm(\hbar) = A_\pm(\hbar) \cos\phi_\pm(\hbar), \quad \beta_\pm(\hbar) = A_\pm(\hbar) \sin\phi_\pm(\hbar), \quad \phi_\pm(\hbar) \in \mathbb{R}/(2\pi\mathbb{Z}). \tag{4.4}$$

Let functions $\Phi_\pm(x; \lambda)$ be defined by formula (1.2), and let $\lambda = v(x_\pm)$. From (2.13) and (2.18) with $x_0 = x_+$ and $x_0 = x_-$ it follows that the asymptotic behavior of $\psi(x; \hbar)$ for $x \in (x_-, x_+)$ is given by formulas (1.3) and (1.4), where

$$\varphi_\pm(\hbar) = \phi_\pm(\hbar) + \pi/4.$$

Of course formulas (1.3) and (1.4) are uniform in x on the compact subintervals of (x_-, x_+) and can be differentiated in x; in the asymptotic formulas for the derivatives, the remainders $O(\hbar)$ should be replaced by $O(1)$.

The phases $\varphi_+(\hbar)$, $\varphi_-(\hbar)$ in formulas (1.3) and (1.4) are linked by some relations that we shall derive now.

The arguments below are essentially the same as those used for the derivation of the Bohr–Sommerfeld quantization condition (see, e.g., Subsection 4.1 in [25]).

First, we calculate various Wronskians. The next assertion follows from the asymptotic formulas (2.13) and (2.18) for $u_\pm(x; x_\pm(\lambda), \hbar)$ and $w_\pm(x; x_\pm(\lambda), \hbar)$. These formulas can be differentiated both in x and λ. We also use the fact that

$$\Phi(\lambda) = \Phi_+(x; \lambda) + \Phi_-(x; \lambda). \tag{4.5}$$

Lemma 4.2. *Under Assumption* 4.1*, and let the function* Φ *be defined by formula* (4.1)*. Then, as* $\hbar \to 0$*,*

$$\begin{aligned} \{u_-(x_-,\hbar), u_+(x_+,\hbar)\} &= \hbar^{-1}\cos(\hbar^{-1}\Phi) + O(1), \\ \{u_-(x_-,\hbar), w_+(x_+,\hbar)\} &= -\hbar^{-1}\sin(\hbar^{-1}\Phi) + O(1), \\ \{w_-(x_-,\hbar), u_+(x_+,\hbar)\} &= -\hbar^{-1}\sin(\hbar^{-1}\Phi) + O(1), \end{aligned} \tag{4.6}$$

and

$$\{w_-(x_-,\hbar), w_+(x_+,\hbar)\} = -\hbar^{-1}\cos(\hbar^{-1}\Phi) + O(1).$$

All these formulas can be differentiated in λ*; in this case the remainders* $O(1)$ *should be replaced by* $O(\hbar^{-1})$*.*

For brevity, we set $u_\pm(\hbar) = u_\pm(x_\pm,\hbar)$, $w_\pm(\hbar) = w_\pm(x_\pm,\hbar)$. By (4.4), we have

$$\begin{aligned} &(A_+(\hbar)A_-(\hbar))^{-1}\{\alpha_+(\hbar)u_+(\hbar) + \beta_+(\hbar)w_+(\hbar), \alpha_-(\hbar)u_-(\hbar) + \beta_-(\hbar)w_-(\hbar)\} \\ &\quad = \cos\phi_+(\hbar)\cos\phi_-(\hbar)\{u_+(\hbar), u_-(\hbar)\} + \sin\phi_+(\hbar)\sin\phi_-(\hbar)\{w_+(\hbar), w_-(\hbar)\} \\ &\qquad + \cos\phi_+(\hbar)\sin\phi_-(\hbar)\{u_+(\hbar), w_-(\hbar)\} + \sin\phi_+(\hbar)\cos\phi_-(\hbar)\{w_+(\hbar), u_-(\hbar)\}. \end{aligned} \tag{4.7}$$

Put

$$\varphi(\lambda,\hbar) = \varphi_+(\lambda,\hbar) + \varphi_-(\lambda,\hbar) = \phi_+(\lambda,\hbar) + \phi_-(\lambda,\hbar) + \pi/2. \tag{4.8}$$

In accordance with Lemma 4.2, expression (4.7) equals

$$\begin{aligned} &\hbar^{-1}\big(-\cos\phi_+(\hbar)\cos\phi_-(\hbar) + \sin\phi_+(\hbar)\sin\phi_-(\hbar)\big)\cos(\hbar^{-1}\Phi) \\ &\qquad + \hbar^{-1}\big(\cos\phi_+(\hbar)\sin\phi_-(\hbar) + \sin\phi_+(\hbar)\cos\phi_-(\hbar)\big)\sin(\hbar^{-1}\Phi) + O(1) \\ &\quad = \hbar^{-1}\big(-\sin\varphi(\hbar)\cos(\hbar^{-1}\Phi) - \cos\varphi(\hbar)\sin(\hbar^{-1}\Phi)\big) + O(1) \\ &\quad = -\hbar^{-1}\sin(\hbar^{-1}\Phi + \varphi(\hbar)) + O(1). \end{aligned}$$

On the other hand, identity (4.3) shows that expression (4.7) is zero. This yields the equation

$$\sin(\hbar^{-1}\Phi(\lambda) + \varphi(\lambda,\hbar)) = O(\hbar), \tag{4.9}$$

whence

$$\Phi(\lambda) = \big(\pi n - \varphi(\lambda,\hbar)\big)\hbar + O(\hbar^2) \tag{4.10}$$

with some integer $n = n(\lambda,\hbar)$.

Putting relations (4.5), (4.8) and the quantization condition (4.10) together, we see that formula (1.3) can be rewritten as

$$\psi_+(x;\lambda,\hbar) = (-1)^n A_+(\hbar)(\lambda - v(x))^{-1/4}\big(\sin\big(\hbar^{-1}\Phi_-(x;\lambda) + \varphi_-(\hbar)\big) + O(\hbar)\big).$$

Comparing it with formula (1.4), we conclude that

$$A_-(\lambda,\hbar) = A_+(\lambda,\hbar)(1 + O(\hbar)) \tag{4.11}$$

and that the integer n in (4.10) is even.

We summarize the results obtained.

Theorem 4.3. *Under Assumption* 4.1*, the following is true.*

(i) *An arbitrary real solution* $\psi(x;\lambda,h)$ *of equation* (1.1) *has both asymptotics* (1.3) *and* (1.4)*, where the functions* $\Phi_\pm(x;\lambda)$ *are defined by formula* (1.2)*.*
(ii) *The functions* (4.1) *and* (4.8) *satisfy conditions* (4.9) *and* (4.10) *with some even integer* $n = n(\lambda,\hbar)$*.*
(iii) *The amplitudes* $A_+(\lambda,\hbar)$*,* $A_-(\lambda,\hbar)$ *in* (1.3)*,* (1.4) *are linked by relation* (4.11)*.*

4.2. If $\varphi(\lambda,\hbar) = \pi/2 \pmod \pi$, then formula (4.10) reduces to the Bohr–Sommerfeld quantization condition. In particular, this is true if the fixing conditions $\varphi_\pm(\lambda,\hbar) = \pi/4 \pmod \pi$ are satisfied at both points $x_\pm(\lambda)$. We state this result explicitly.

Theorem 4.4. *Under Assumption* 4.1*, suppose that a real solution $\psi(x;\lambda,h)$ of equation* (1.1) *has asymptotics* (1.3) *and* (1.4)*, where $\varphi_\pm(\lambda,\hbar) = \pi/4 \pmod \pi$. Then the function* (4.1) *satisfies the condition*

$$\cos(\hbar^{-1}\Phi(\lambda)) = O(\hbar), \tag{4.12}$$

whence

$$\Phi(\lambda) = \pi(n+1/2)\hbar + O(\hbar^2) \tag{4.13}$$

for some integer $n = n(\lambda,\hbar)$.

Remark 4.5. It is possible that $\varphi_\pm(\lambda,\hbar) = \pi/4 \pmod \pi$ only for $\hbar$ in some set $\Gamma \subset \mathbb{R}_+$ such that $0 \in \operatorname{clos}\Gamma$. Then conditions (4.12) and (4.13) are also satisfied for $h \in \Gamma$.

Of course, in Theorem 4.4 the number n may be an arbitrary integer. Indeed, if $\pi^{-1}(\varphi_+ - \varphi_-)$ is even (respectively, odd), then Theorem 4.3(ii) implies (4.13) with n even (respectively, odd).

Theorem 4.4 can be supplemented by the following assertion. To state it, we need an additional assumption on the remainder $O(\hbar^2)$ in (4.13).

Proposition 4.6. *Under Assumption* 4.1*, let λ and $\Phi^{-1}(\pi(n+1/2)\hbar)$ belong to a neighborhood of λ_0. Suppose that*

$$\epsilon(\lambda,\hbar) = O(\hbar^2), \quad \dot\epsilon(\lambda,\hbar) = o(1). \tag{4.14}$$

Then for every integer n, there may exist only one value of $\lambda = \lambda_n(\hbar)$ satisfying the condition

$$\Phi(\lambda) = \pi(n+1/2)\hbar + \epsilon(\lambda,\hbar). \tag{4.15}$$

Proof. Assuming that there are two different $\lambda'(\hbar)$, $\lambda''(\hbar)$ satisfying (4.15), we find a point $\nu(\hbar) \in (\lambda'(\hbar), \lambda''(\hbar))$ such that

$$\dot\Phi(\nu(\hbar)) = \dot\epsilon(\nu(\hbar),\hbar). \tag{4.16}$$

By (4.2), we have $\dot\Phi(\nu(\hbar)) \geq c > 0$, while by (4.14) the right-hand side tends to 0 as $\hbar \to 0$. So, relation (4.16) leads to a contradiction. □

The following result is converse to Theorem 4.4.

Proposition 4.7. *Under Assumption* 4.1*, suppose that the number $\pi(n+1/2)\hbar$ belongs to a neighborhood of $\Phi(\lambda_0)$. Then there exists a value of $\widetilde\lambda = \widetilde\lambda_n(\hbar)$ (that is, it depends on n and $\hbar$) of λ such that relations* (4.13) *and*

$$u_-(x;x_-(\widetilde\lambda),\hbar) = a(\widetilde\lambda,\hbar)u_+(x;x_+(\widetilde\lambda),\hbar) \tag{4.17}$$

hold true. Moreover, the coefficient a in (4.17) *satisfies*

$$a(\widetilde\lambda,\hbar) = (-1)^n + O(\hbar). \tag{4.18}$$

Proof. The first formula (4.6) shows that the Wronskian of the solutions $u_+(x;x_+(\lambda),\hbar)$ and $u_-(x;x_-(\lambda),\hbar)$ of equation (1.1) is given by the formula

$$\{u_-(x_-(\lambda),\hbar), u_+(x_+(\lambda),\hbar)\} = \hbar^{-1}\cos(\hbar^{-1}\Phi(\lambda)) + \varepsilon(\lambda,\hbar) \tag{4.19}$$

where $\epsilon(\lambda,\hbar)$ is a continuous function of $\lambda \in (\Lambda_1,\Lambda_2)$ and $\varepsilon(\lambda,\hbar) = O(1)$ as $\hbar \to 0$. The expression (4.19) is zero for some $\widetilde\lambda = \widetilde\lambda_n(\hbar)$ obeying condition (4.13), whence (4.17) follows. By Corollary 2.3(ii), the asymptotics of $u_+(x;x_+(\widetilde\lambda),\hbar)$ and $u_-(x;x_-(\widetilde\lambda),\hbar)$ as

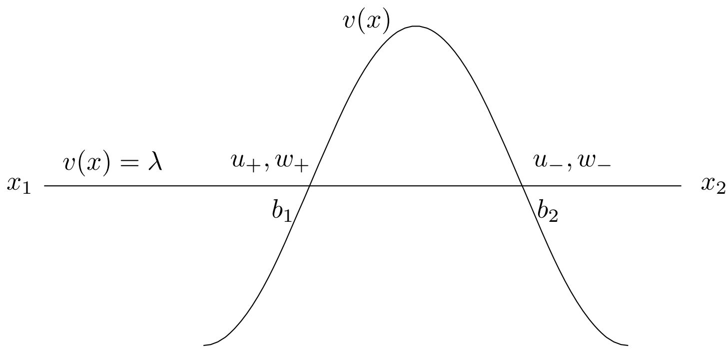
$\hbar \to 0$ are given by formulas (1.3), (1.4) with $A_\pm = 1$ and $\varphi_\pm = \pi/4$. Comparing these formulas, we obtain (4.18). $\square$

§5. Passage through a potential barrier. Fixing conditions

Here we show that, at least from one side, a potential barrier fixes the phase of a real solution of equation (1.1) in the same way as a barrier of infinite length.

5.1. We assume the following.

Assumption 5.1. The function v is of class C^2 on some interval $(x_1, x_2) \subset \mathbb{R}$. The equation $v(x) = \lambda_0$ has two solutions $b_1 = b_1(\lambda_0), b_2 = b_2(\lambda_0)$ in (x_1, x_2), $b_1 < b_2$ and $v(x) > \lambda$ for $x \in (b_1, b_2)$, $v(x) < \lambda$ for $x \notin [b_1, b_2]$. Moreover, the function v belongs to the class C^3 in some neighborhoods of the points b_1, b_2 and $v'(b_1) > 0$, $v'(b_2) < 0$.



Potential barrier between b_1 and b_2

Thus, we have a potential barrier between the points b_1 and b_2. The energy

$$\lambda = v(b_1) = v(b_2) \in (\Lambda_1, \Lambda_2)$$

is fixed. We are interested in the asymptotic behavior as $\hbar \to 0$ of an arbitrary *real* solution $\psi(x;\hbar)$ of equation (1.1) on the interval (x_1, x_2). Since by (2.19) the functions $u_+(x; b_1, \hbar)$, $w_+(x; b_1, \hbar)$ and $u_-(x; b_2, \hbar)$, $w_-(x; b_2, \hbar)$ (these functions were constructed in Theorems 2.2 and 2.7, respectively) are linearly independent, we have

$$\begin{aligned} \psi(x, \hbar) &= \alpha_1(\hbar) u_+(x; b_1, \hbar) + \beta_1(\hbar) w_+(x; b_1, \hbar) \\ &= \alpha_2(\hbar) u_-(x; b_2, \hbar) + \beta_2(\hbar) w_-(x; b_2, \hbar). \end{aligned} \tag{5.1}$$

We put $A_j(\hbar) = \sqrt{\alpha_j(\hbar)^2 + \beta_j(\hbar)^2}$ and

$$\begin{aligned} &\alpha_j(\hbar) = A_j(\hbar) \cos \vartheta_j(\hbar), \\ &\beta_j(\hbar) = A_j(\hbar) \sin \vartheta_j(\hbar), \\ &\theta_j(\hbar) \in \mathbb{R}/(2\pi\mathbb{Z}), \quad j = 1, 2. \end{aligned} \tag{5.2}$$

The phases $\vartheta_1(\hbar)$, $\vartheta_2(\hbar)$ (and the amplitudes $A_1(\hbar)$, $A_2(\hbar)$) in these formulas are linked by some relations that we are going to derive now. For that, we need to calculate various Wronskians.

Lemma 5.2. *Under Assumption* 5.1, *set*

$$\Omega(\lambda) = \int_{b_1(\lambda)}^{b_2(\lambda)} \sqrt{v(x) - \lambda}\, dx. \tag{5.3}$$

Then

$$\{u_+(b_1,\hbar),u_-(b_2,\hbar)\}=-2^{-1}\hbar^{-1}e^{-\hbar^{-1}\Omega}(1+O(\hbar)),\tag{5.4}$$

$$\{w_+(b_1,\hbar),w_-(b_2,\hbar)\}=2\hbar^{-1}e^{\hbar^{-1}\Omega}(1+O(\hbar))\tag{5.5}$$

and

$$\{u_\pm(b_1,\hbar),w_\mp(b_2,\hbar)\}=O\big(e^{-\hbar^{-1}(1-\varepsilon)\Omega}\big),\quad \forall\varepsilon>0.\tag{5.6}$$

Proof. We can calculate these Wronskians at an arbitrary point $x\in(b_1,b_2)$. We start with formulas (2.12) and (2.17), where $x_0=b_1$ or $x_0=b_2$ and $v(x_0)=\lambda$. These formulas can be differentiated with respect to x. Relation (5.4) follows from (2.12), and relation (5.5) follows from (2.17). Using (2.12) and (2.17) once again, we get

$$\{u_+(b_1,\hbar),w_-(b_2,\hbar)\}=\hbar^{-1}O\bigg(\exp\bigg(-\hbar^{-1}\int_{b_1}^{x}\sqrt{v(x)-\lambda}\,dx+\hbar^{-1}\int_{x}^{b_2}\sqrt{v(x)-\lambda}\,dx\bigg)\bigg).$$

Since x can be chosen arbitrarily close to b_2, this proves (5.6) for the upper sign. The lower sign is treated quite similarly. □

5.2. From (5.1) and (5.2) it follows that

$$\begin{aligned}&A_1(\hbar)\big(u_+(x;b_1,\hbar)\cos\vartheta_1(\hbar)+w_+(x;b_1,\hbar)\sin\vartheta_1(\hbar)\big)\\&\qquad=A_2(\hbar)\big(u_-(x;b_2,\hbar)\cos\vartheta_2(\hbar)+w_-(x;b_2,\hbar)\sin\vartheta_2(\hbar)\big).\end{aligned}\tag{5.7}$$

We take the Wronskian of the two sides of this equation with the function $u_+(x;b_1,\hbar)$:

$$\begin{aligned}&A_1(\hbar)\{u_+(b_1,\hbar),w_+(b_1,\hbar)\}\sin\vartheta_1(\hbar)\\&\qquad=A_2(\hbar)\big(\{u_+(b_1,\hbar),u_-(b_2,\hbar)\}\cos\vartheta_2(\hbar)+\{u_+(b_1,\hbar),w_-(b_2,\hbar)\}\sin\vartheta_2(\hbar)\big).\end{aligned}$$

Using relations (2.19), (5.4), and (5.6), we see that, for any $\varepsilon>0$,

$$A_1(\hbar)\sin\vartheta_1(\hbar)=A_2(\hbar)O\big(e^{-\hbar^{-1}(1-\varepsilon)\Omega}\big).\tag{5.8}$$

Quite similarly, taking the Wronskian of equation (5.7) with the function $u_-(x;b_2,\hbar)$, we find

$$A_2(\hbar)\sin\vartheta_2(\hbar)=A_1(\hbar)O\big(e^{-\hbar^{-1}(1-\varepsilon)\Omega}\big).\tag{5.9}$$

Multiplying equations (5.9) and (5.8) and neglecting the common factor $A_1(\hbar)A_2(\hbar)$, we obtain the following assertion.

Theorem 5.3. *Under Assumption* 5.1, *an arbitrary real solution of equation* (1.1) *is given by formulas* (5.1) *and* (5.2), *where the phases satisfy the estimate*

$$\sin\vartheta_1(\hbar)\sin\vartheta_2(\hbar)=O(e^{-2\hbar^{-1}(1-\varepsilon)\Omega})\quad\textit{for all}\quad\varepsilon>0.\tag{5.10}$$

Corollary 5.4. *For every $\hbar$, at least one of the phases satisfies the condition*

$$\sin\vartheta_j(\hbar)=O(e^{-\hbar^{-1}(1-\varepsilon)\Omega}),\quad j=1,2,\quad\textit{for all}\quad\varepsilon>0.\tag{5.11}$$

Now we return to relations (5.1) and use the asymptotics (2.13) and (2.18) for the functions $u_\pm$ and $w_\pm$. We let the functions $\Theta_j(x,\lambda)$ be defined by formula (1.7), and put

$$\theta_j(\hbar)=\vartheta_j(\hbar)+\pi/4.\tag{5.12}$$

Since the phase shift $O(e^{-\hbar^{-1}(1-\varepsilon)\Omega})$ can be included in the error term $O(\hbar)$, estimate (5.11) yields the following result.

Theorem 5.5. *Under Assumption* 5.1*, an arbitrary real solution $\psi(x;h)$ of equation* (1.1) *admits the asymptotics* (1.8) *for $x \in (x_1, b_1)$ and the asymptotics* (1.9) *for $x \in (b_2, x_2)$, where $\theta_j(\hbar) = \pi/4 \pmod \pi$ at least for one $j = 1, 2$. Formulas* (1.8) *and* (1.9) *are uniform in x on the compact subintervals of (x_1, b_1) and (b_2, x_2) and can be differentiated with respect to x.*

Corollary 5.6. *If* (1.8) *is satisfied with $\theta_1(\hbar) = \theta_1 \neq \pi/4 \pmod \pi$, then* (1.9) *holds true with $\theta_2(\hbar) = \pi/4 \pmod \pi$. Similarly, if* (1.9) *is satisfied with $\theta_2(\hbar) = \theta_2 \neq \pi/4 \pmod \pi$, then* (1.8) *holds true with $\theta_1(\hbar) = \pi/4 \pmod \pi$.*

Theorem 5.5 shows that, at least from one side, a potential barrier fixes the phase of the real wave function in the same way as a potential barrier of infinite width does (cf. formulas (1.3) and (1.4), where $\varphi_\pm(\hbar) = \pi/4$). It is convenient to give a formal definition.

Definition 5.7. Under Assumption 5.1, let $\psi(x;h)$ be a real solution of equation (1.1) on the interval (x_1, x_2). The *fixing condition* is satisfied at the point $x = b_j$ with $j = 1$ or $j = 2$ if $\theta_j(\hbar) = \pi/4 \pmod \pi$ in formula (1.8) for $j = 1$ or in formula (1.9) for $j = 2$.

Remark 5.8. Estimate (5.10) is true for all $\hbar > 0$, while the sets of $\hbar$ where (5.11) is satisfied depend on $j = 1, 2$. This means that there exist sets $\Gamma_1, \Gamma_2 \subset \mathbb{R}_+$ such that $\Gamma_1 \cup \Gamma_2 = \mathbb{R}_+$ (possibly, $\Gamma_1 \cap \Gamma_2 \neq \varnothing$) and $\theta_j(\hbar) = \pi/4 \pmod \pi$ for $\hbar \in \Gamma_j$.

Remark 5.9. Estimate (5.10) is true for all $\lambda \in (\Lambda_1, \Lambda_2)$, while the sets Γ_j where (5.11) is satisfied may depend on λ. Note, however, that the derivative of the function (1.7) with respect to λ equals

$$\dot{\Theta}_j(x, \lambda) = (-1)^j 2^{-1} \int_{b_j(\lambda)}^{x} (\lambda - v(y))^{-1/2}\, dy,$$

whence it is a bounded function. It follows that

$$\hbar^{-1} |\Theta_j(x, \lambda') - \Theta_j(x, \lambda'')| \leq C \hbar^{-1} |\lambda' - \lambda''| = O(\hbar)$$

if $\lambda' - \lambda'' = O(\hbar^2)$. Since the phases $\theta_j(\hbar)$ in (1.8) and (1.9) are defined up to terms of order $O(\hbar)$, we see that if the fixing condition $\theta_j(\hbar) = \pi/4 \pmod \pi$ is satisfied for some j and λ, then so it does for the same j in a $O(\hbar^2)$-neighborhood of λ.

5.3. Now we consider the behavior of the modulus $|\psi(x;\hbar)|$ as $\hbar \to 0$ in a neighborhood of a potential barrier. Note that if the fixing condition (5.11) is only satisfied at one of the sides of the barrier, then the solution $\psi(x;\hbar)$ is localized on the same side. The following statement is a direct consequence of estimates (5.8) or (5.9). As usual, we use identity (5.12).

Theorem 5.10. *Under the assumptions of Theorem* 5.5*, the amplitudes and the phases in* (1.8) *and* (1.9) *satisfy the estimate*

$$\frac{A_k(\hbar)}{A_j(\hbar)} \leq C |\sin \vartheta_k(\hbar)|^{-1} e^{-\hbar^{-1}(1-\varepsilon)\Omega}, \quad j \neq k, \quad \textit{for all} \quad \varepsilon > 0.$$

In particular, if the fixing condition is not satisfied at the point b_k (that is, $|\sin \vartheta_k(\hbar)| \geq c > 0$), then

$$\frac{A_k(\hbar)}{A_j(\hbar)} \leq C e^{-\hbar^{-1}(1-\varepsilon)\Omega}, \quad j \neq k, \quad \textit{for all} \quad \varepsilon > 0.$$

Finally, we show that the solution $\psi(x, \hbar)$ decays exponentially inside the potential barrier.

Theorem 5.11. *Under the assumptions of Theorem* 5.5, *for arbitrary* $\varepsilon > 0$ *we have the estimate*

$$|\psi(x;\hbar)| \le CA_j(\hbar)e^{\varepsilon\hbar^{-1}\Omega(\lambda)}\big(e^{-\hbar^{-1}\int_{b_1}^{x}\sqrt{v(y)-\lambda}\,dy} + e^{-\hbar^{-1}\int_{x}^{b_2}\sqrt{v(y)-\lambda}\,dy}\big) \tag{5.13}$$

on all compact subintervals of (b_1, b_2) *with the same* j *as in* (5.11).

Proof. We start with formulas (5.1) and (5.2). Suppose, for example, that $j = 1$. The estimate

$$|u_+(x;b_1,\hbar)| \le Ce^{-\hbar^{-1}\int_{b_1}^{x}\sqrt{v(y)-\lambda}\,dy} \tag{5.14}$$

is a direct consequence of (2.12). Combining (2.17) and (5.11) we also see that

$$|w_+(x;b_1,\hbar)\sin\vartheta_1(\hbar)| \le Ce^{-\hbar^{-1}(1-\varepsilon)\Omega(\lambda)}e^{\hbar^{-1}\int_{b_1}^{x}\sqrt{v(y)-\lambda}\,dy}, \tag{5.15}$$

which gives the second term on the right-hand side of (5.13). Thus, being put together, estimates (5.14) and (5.15) yield (5.13). ☐

Of course, Theorem 5.11 is a particular case of Agmon's general estimates [1] (see also Chapter 6 in [6]) on an exponential decay of eigenfunctions in a classically forbidden region.

§6. Quantization conditions for multiple wells

6.1. Now we are in a position to deal with several potential wells. To be precise, we assume the following.

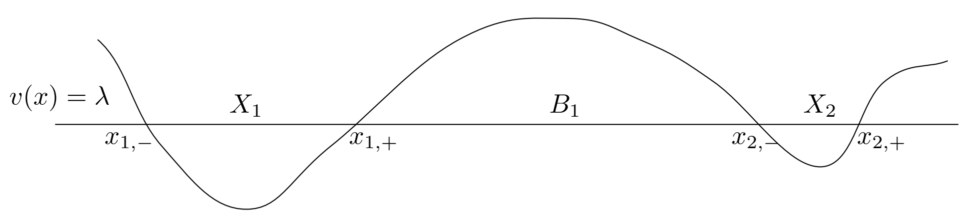
Assumption 6.1. The function v is of class $C^2(\mathbb{R})$ and for a point $\lambda_0 \in \mathbb{R}$, the equation $v(x) = \lambda_0$ has only finitely many solutions, $v'(x) \ne 0$ for all x, such that $v(x) = \lambda_0$ and $v \in C^3$ in some neighborhoods of these points. We also suppose that condition (1.10) is satisfied and that the function (2.14) is bounded for some $\rho_0 > 1$ as $|x| \to \infty$.

Let $x_{\ell,\pm} = x_{\ell,\pm}(\lambda)$, $\ell = 1,\dots,L$, be the solutions of the equation $v(x) = \lambda$. We enumerate them as follows:

$$x_{1,-} < x_{1,+} < x_{2,-} < x_{2,+} < \cdots < x_{L,-} < x_{L,+}.$$

This yields L wells $X_\ell(\lambda) = (x_{\ell,-}(\lambda), x_{\ell,+}(\lambda))$, $\ell = 1,\dots,L$, separated by $L-1$ potential barriers $B_\ell(\lambda) = (x_{\ell,+}(\lambda), x_{\ell+1,-}(\lambda))$, $\ell = 1,\dots,L-1$. We also have two infinite barriers $B_0(\lambda) = (-\infty, x_{1,-}(\lambda))$ and $B_L(\lambda) = (x_{L,+}(\lambda), \infty)$. Of course $\pm v'(x_{\ell,\pm}(\lambda)) > 0$ for all $\ell = 1,\dots,L$. For each well, we introduce the function (4.1):

$$\Phi_\ell(\lambda) = \int_{x_{\ell,-}(\lambda)}^{x_{\ell,+}(\lambda)} (\lambda - v(x))^{1/2}\,dx. \tag{6.1}$$



The case $L = 2$.

Theorem 6.2. *Let Assumption* 6.1 *be fulfilled for a point* λ_0. *Let an eigenvalue* $\lambda = \lambda(\hbar)$ *of the operator* $H(\hbar)$ *belong to a neighborhood* (Λ_1, Λ_2) *of* λ_0. *Then, at least for one* $\ell = \ell(\hbar) = 1, \dots, L$, *the estimate*

$$\cos(\hbar^{-1}\Phi_\ell(\lambda)) = O(\hbar) \tag{6.2}$$

is satisfied, and hence, the quantization condition

$$\Phi_\ell(\lambda) = \pi(n + 1/2)\hbar + O(\hbar^2) \tag{6.3}$$

holds true with some integer $n = n_\ell(\hbar)$.

Proof. Theorem 5.5 implies that, for every $\lambda \in (\Lambda_1, \Lambda_2)$ and every $\hbar > 0$, each barrier $B_\ell(\lambda)$, $\ell = 1, \dots, L-1$, yields at least one fixing condition. Moreover, in accordance with Theorem 2.6, the two solutions $u_\pm$ of equation (1.1) belong to $L^2(\mathbb{R}_\pm)$. So, if λ is an eigenvalue of the operator $H(\hbar)$, then from formula (2.13) it follows that the fixing conditions are fulfilled at the points $x_{1,-}(\lambda)$ and $x_{L,+}(\lambda)$. Thus, for every $\hbar > 0$, we have at least $L+1$ fixing conditions for L wells, whence there exists a well $X_\ell(\lambda)$ (depending on $\hbar$) for which two fixing conditions are satisfied. Therefore it remains to refer to Theorem 4.4. □

Condition (4.2) on $\dot{\Phi}_\ell$ implies that Φ_ℓ is a one-to-one mapping of (Λ_1, Λ_2) onto a neighborhood of the point $\mu_{0,\ell} = \Phi_\ell(\lambda_0)$. We introduce the inverse mapping $\Psi_\ell = \Phi_\ell^{-1}$: $(\Phi_\ell(\Lambda_1), \Phi_\ell(\Lambda_2)) \to (\Lambda_1, \Lambda_2)$. Then condition (6.3) for $\lambda = \lambda_{n,\ell}(\hbar)$ is equivalent to the relation

$$\lambda_{n,\ell}(\hbar) = \Psi_\ell(\pi(n + 1/2)\hbar) + O(\hbar^2). \tag{6.4}$$

Therefore, Theorem 6.2 can be reformulated in the following way. Consider all intervals

$$I_{n,\ell}(\hbar) = \big(\Psi_\ell(\pi(n+1/2)\hbar) - O(\hbar^2), \Psi_\ell(\pi(n+1/2)\hbar) + O(\hbar^2)\big) \subset (\Lambda_1, \Lambda_2). \tag{6.5}$$

Since the lengths of these intervals are of order of $\hbar^2$, and the distances between the points $\Psi_\ell(\pi(n+1/2)\hbar)$ and $\Psi_\ell(\pi(m+1/2)\hbar)$ are of order of $\hbar$, we see that $I_{n,\ell}(\hbar) \cap I_{m,\ell}(\hbar) = \varnothing$ if $n \neq m$ and $\hbar$ is sufficiently small. However for different ℓ, the intersection of two intervals $I_{n,\ell}(\hbar)$ may be nontrivial. Theorem 6.2 means that all eigenvalues of the operator $H(\hbar)$ in the interval (Λ_1, Λ_2) belong to one of the intervals $I_{n,\ell}(\hbar)$, that is,

$$\operatorname{spec}_p H(\hbar) \cap (\Lambda_1, \Lambda_2) \subset \bigcup_{\ell=1}^{L} \bigcup_n I_{n,\ell}(\hbar) \tag{6.6}$$

if $\hbar$ is sufficiently small. This can also be equivalently stated as

$$\operatorname{dist}\Big\{ \operatorname{spec}_p H(\hbar) \cap (\Lambda_1, \Lambda_2), \bigcup_{\ell=1}^{L} \bigcup_n \Psi_\ell(\pi(n+1/2)\hbar) \Big\} = O(\hbar^2).$$

To prove the uniqueness of λ satisfying (6.3), we need an additional assumption on the remainder $O(\hbar^2)$ in (6.3). The following result is a direct consequence of Proposition 4.6.

Theorem 6.3. *Under Assumption* 6.1, *let* λ *and* $\Phi_\ell^{-1}(\pi(n+1/2)\hbar)$ *belong to a neighborhood of* λ_0. *Suppose that*

$$\cos(\hbar^{-1}\Phi_\ell(\lambda)) + \epsilon_\ell(\lambda, \hbar) = 0 \tag{6.7}$$

where

$$\epsilon_\ell(\lambda, \hbar) = O(\hbar), \quad \dot{\epsilon}_\ell(\lambda, \hbar) = o(\hbar^{-1}). \tag{6.8}$$

Then for every integer n, *there exists at most one value of* $\lambda = \lambda_{n,\ell}(\hbar)$ *satisfying* (6.3).

Being put together, Theorems 6.2 and 6.3 imply that, for a given ℓ, there is at most one eigenvalue in each of the intervals $I_{n,\ell}(\hbar)$ defined by (6.5).

Let us discuss the converse statement. As usual, we suppose that $\hbar$ is sufficiently small.

Theorem 6.4. *Let Assumption* 6.1 *be fulfilled for a point* λ_0. *Then, for every* $\ell = 1, \dots, L$ *and every* n *such that* $\Phi_\ell^{-1}(\pi(n+1/2)\hbar)$ *belongs to a neighborhood of* λ_0, *there exists an eigenvalue* $\lambda_{n,\ell}(\hbar)$ *of the operator* $H(\hbar)$ *satisfying relation* (6.4).

Proof. Pick some $\ell = 1, \dots, L$ and n. We need trial functions $f_\ell(x;\hbar) = f_{n,\ell}(x;\hbar)$ such that $f_\ell(\hbar) \in C_0^2(\mathbb{R})$ and

$$\|H(\hbar)f_\ell(\hbar) - \Psi_\ell(\pi(n+1/2)\hbar)f_\ell(\hbar)\| \le C\hbar^2\|f_\ell(\hbar)\|, \quad \text{for all} \quad \hbar > 0. \tag{6.9}$$

We start with Proposition 4.7. For every integer n, there exists $\widetilde{\lambda} =: \widetilde{\lambda}_{n,\ell}(\hbar)$ (so it depends on ℓ, n, and $\hbar$) obeing condition (6.3) and such that

$$u_-(x; x_{\ell,-}(\widetilde{\lambda}), \hbar) = a_\ell(\widetilde{\lambda}, \hbar)u_+(x; x_{\ell,+}(\widetilde{\lambda}), \hbar). \tag{6.10}$$

Moreover, the coefficient $a_\ell(\widetilde{\lambda}, \hbar)$ satisfies (4.18). We fix this value of $\widetilde{\lambda}$.

Let a cut-off function $\chi_\ell \in C_0^\infty(\mathbb{R})$ be such that $\chi_\ell(x) = 1$ in some neighborhood of the interval X_ℓ and $\chi_\ell(x) = 0$ outside of some larger neighborhood of that interval; in particular, $\chi_\ell(x) = 0$ on all other intervals X_k, $k \neq \ell$. Now we set

$$f_\ell(x;\hbar) = u_-(x; x_{\ell,-}(\widetilde{\lambda}), \hbar)\chi_\ell(x).$$

Since the function $u_+(x; x_{\ell,-}(\widetilde{\lambda}), \hbar)$ satisfies (1.1), we have

$$\begin{aligned} &-\hbar^{-2}f_\ell''(x;\hbar) + (v(x) - \widetilde{\lambda})f_\ell(x;\hbar) \\ &\quad = -\hbar^{-2}\big(2u_-'(x; x_{\ell,-}(\widetilde{\lambda}), \hbar)\chi_\ell'(x) + u_-(x; x_{\ell,-}(\widetilde{\lambda}), \hbar)\chi_\ell''(x)\big). \end{aligned} \tag{6.11}$$

Due to the functions χ_ℓ' and χ_ℓ'', this expression differs from zero only on compact subsets of the barriers $B_{\ell-1}$ and B_ℓ. Relation (2.12) shows that the expression (6.11) tends to zero exponentially as $\hbar \to 0$ on the left barrier $B_{\ell-1}$. Using (6.10), we can rewrite (6.11) as

$$-a_\ell(\widetilde{\lambda}, \hbar)\hbar^{-2}\big(2u_+'(x; x_{\ell,+}(\widetilde{\lambda}), \hbar)\chi_\ell'(x) + u_+(x; x_{\ell,+}(\widetilde{\lambda}), \hbar)\chi_\ell''(x)\big),$$

and therefore, in accordance with relation (4.18) for $a_\ell(\widetilde{\lambda}, \hbar)$, it also tends to zero exponentially as $\hbar \to 0$ on the right barrier B_ℓ. Thus, (6.11) implies that

$$\|H(\hbar)f_\ell(\hbar) - \widetilde{\lambda}(\hbar)f_\ell(\hbar)\| \le C\hbar^p\|f_\ell(\hbar)\| \quad \text{for all} \quad p > 0.$$

To conclude the proof of inequality (6.9), it remains to use the fact that

$$\widetilde{\lambda}(\hbar) - \Psi_\ell(\pi(n+1/2)\hbar) = O(\hbar^2),$$

by condition (6.3) on $\widetilde{\lambda}(\hbar)$. □

Remark 6.5. The support of the trial function $f_\ell(x;\hbar)$ lies in a small neighborhood of the interval X_ℓ. Therefore, for different ℓ, the supports of $f_\ell(x;\hbar)$ are disjoint.

6.2. Here we discuss some consequences of the results obtained. Let $N(\hbar)$ be the total number of eigenvalues of the operator $H(\hbar)$ in the interval (Λ_1, Λ_2). For each $\ell = 1, \dots, L$, we consider the intervals $I_{n,\ell}(\hbar)$ defined by formula (6.5). Since $I_{n,\ell}(\hbar) \cap I_{m,\ell}(\hbar) = \varnothing$ whenever $n \neq m$ and $\hbar$ is sufficiently small, the total number $\mathcal{N}_\ell(\hbar)$ of such intervals lying in (Λ_1, Λ_2) obeys the two-sided bound

$$(\Phi_\ell(\Lambda_2) - \Phi_\ell(\Lambda_1))(\pi\hbar)^{-1} - 1 \le \mathcal{N}_\ell(\hbar) \le (\Phi_\ell(\Lambda_2) - \Phi_\ell(\Lambda_1))(\pi\hbar)^{-1} + 1. \tag{6.12}$$

Proposition 6.6. *Let Assumption* 6.1 *be fulfilled for a point* λ_0. *Then*

$$N(\hbar) \geq \sum_{\ell=1}^{L} (\Phi_\ell(\Lambda_2) - \Phi_\ell(\Lambda_1))(\pi\hbar)^{-1} - L \tag{6.13}$$

for sufficiently small $\hbar$.

Proof. By Theorem 6.4, for every $\ell = 1, \ldots, L$ and n, there is an eigenvalue of the operator $H(\hbar)$ lying in each interval $I_{n,\ell}(\hbar)$. Although for different ℓ the intersection of the intervals $I_{n,\ell}(\hbar)$ may be nontrivial, the corresponding trial functions have disjoint supports (see Remark 6.5). It follows that

$$N(\hbar) \geq \sum_{\ell=1}^{L} \mathcal{N}_\ell(\hbar).$$

So, it suffices to use the left estimate in (6.12). ☐

We emphasize that the lower bound (6.13) does not require the results of §5 on passage through a potential barrier.

Proposition 6.7. *Let the assumptions of Theorem* 6.3 *be satisfied for all* $\ell = 1, \ldots, L$. *Then*

$$N(\hbar) \leq \sum_{\ell=1}^{L} (\Phi_\ell(\Lambda_2) - \Phi_\ell(\Lambda_1))(\pi\hbar)^{-1} + L \tag{6.14}$$

if $\hbar$ *is sufficiently small.*

Proof. Using the inclusion (6.6) and the fact that there is at most one eigenvalue in each of the intervals $I_{n,\ell}(\hbar)$, we see that

$$N(\hbar) \leq \sum_{\ell=1}^{L} \mathcal{N}_\ell(\hbar).$$

So, it suffices to use the right-hand estimate in (6.12). ☐

The definition (6.3) of the function Φ_ℓ implies

$$\sum_{\ell=1}^{L} (\Phi_\ell(\Lambda_2) - \Phi_\ell(\Lambda_1)) = 2^{-1} \iint_{\Lambda_1 < p^2 + v(x) < \Lambda_2} dp\, dx$$
$$= 2^{-1} \mathrm{meas}\big\{(x,p) \in \mathbb{R}^2 : \Lambda_1 < p^2 + v(x) < \Lambda_2\big\}.$$

Thus, estimates (6.13) and (6.14) yield the semiclassical Weyl formula with a strong estimate of the remainder. Unfortunately, the upper bound (6.14) requires the implicit assumption (6.8).

6.3. Let us discuss the case of $L = 2$ in detail. For brevity, we set $u_- = u_-(x_{1,-})$, $u_+ = u_+(x_{2,+})$, $u_1 = u_+(x_{1,+})$, $w_1 = w_+(x_{1,+})$, and $u_2 = u_-(x_{2,-})$, $w_2 = w_-(x_{2,-})$. Let $\lambda = \lambda(\hbar)$ be an eigenvalue and $\psi(x) = \psi(x; \lambda, \hbar)$ a real eigenfunction of the operator $H(\hbar)$. Since $u_\pm \in L^2(\mathbb{R}_\pm)$ and the functions u_ℓ, w_ℓ are linearly independent, we have

$$\psi = A_\ell(\cos\phi_\ell\, u_\ell + \sin\phi_\ell\, w_\ell), \quad x \in (x_{\ell,-}, x_{\ell,+}), \quad \ell = 1, 2.$$

On the other hand, $\psi = A_\pm u_\pm$ because $u_\pm \in L^2(\mathbb{R}_\pm)$. It follows that

$$\gamma_1 := \tan\phi_1 = -\frac{\{u_-, u_1\}}{\{u_-, w_1\}}, \quad \gamma_2 := \tan\phi_2 = -\frac{\{u_+, u_2\}}{\{u_+, w_2\}}. \tag{6.15}$$

The condition

$$\{u_1 + \gamma_1 w_1, u_2 + \gamma_2 w_2\} = 0$$

yields the equation

$$\left(\gamma_1 + \frac{\{u_1, w_2\}}{\{w_1, w_2\}}\right)\left(\gamma_2 + \frac{\{w_1, u_2\}}{\{w_1, w_2\}}\right) = -\{u_1, u_2\} + \frac{\{u_1, w_2\}\{w_1, u_2\}}{\{w_1, w_2\}^2} =: \omega_0 \tag{6.16}$$

for γ_1 and γ_2.

By Lemma 5.2, we have

$$\omega_1 := \frac{\{u_1, w_2\}}{\{w_1, w_2\}} = O(e^{-\hbar^{-1}(2-\varepsilon)\Omega}), \quad \omega_2 := \frac{\{w_1, u_2\}}{\{w_1, w_2\}} = O(e^{-\hbar^{-1}(2-\varepsilon)\Omega}) \tag{6.17}$$

for all $\varepsilon > 0$, and

$$\omega_0 = 2^{-1}\hbar^{-1}e^{-\hbar^{-1}\Omega}(1 + O(\hbar)). \tag{6.18}$$

Moreover, these relations may be differentiated with respect to λ. From Lemma 4.2 it follows that the numbers (6.15) are given by the formula

$$\gamma_\ell(\hbar) = \frac{\cos(\hbar^{-1}\Phi_\ell) + \sigma_\ell(\hbar)}{\sin(\hbar^{-1}\Phi_\ell) + \eta_\ell(\hbar)}, \tag{6.19}$$

where the functions Φ_ℓ are defined by (6.1) and

$$\sigma_\ell(\hbar) = O(\hbar), \quad \eta_\ell(\hbar) = O(\hbar), \quad \dot\sigma_\ell(\hbar) = O(1), \quad \dot\eta_\ell(\hbar) = O(1) \tag{6.20}$$

as $\hbar \to 0$.

In view of (6.17), (6.18), equation (6.16) implies that

$$\min\left\{|\gamma_1(\hbar) + \omega_1(\hbar)|, |\gamma_2(\hbar) + \omega_2(\hbar)|\right\} \le \hbar^{-1/2}e^{-(2\hbar)^{-1}\Omega}. \tag{6.21}$$

Suppose, for example, that the first term on the left is smaller than the second. Then conditions (6.2) and (6.3) for $\ell = 1$ follow from estimates (6.17) and (6.21).

Now we shall discuss the second condition (6.8) for $\ell = 1$. For that, we need an explicit expression for the remainder $\epsilon_1(\hbar)$ in (6.7). Relations (6.16) and (6.19) show that equation (6.7) with $\ell = 1$ is satisfied with

$$\epsilon_1(\hbar) = \sigma_1(\hbar) + \left(\sin(\hbar^{-1}\Phi_1) + \eta_1(\hbar)\right)\left(\omega_1(\hbar) - \frac{\omega_0(\hbar)}{\gamma_2(\hbar) + \omega_2(\hbar)}\right),$$

where, of course, all terms depend on λ. We differentiate this equality with respect to λ. By (6.17), (6.18), and (6.20), for the proof of estimate (6.8), we only need to exclude the possibility that the denominator $\gamma_2(\hbar) + \omega_2(\hbar)$ tends to zero exponentially as $\hbar \to 0$. By (6.19), we have

$$\frac{1}{\gamma_2(\hbar) + \omega_2(\hbar)} = \frac{\sin(\hbar^{-1}\Phi_2) + \eta_2(\hbar)}{\cos(\hbar^{-1}\Phi_2) + \sigma_2(\hbar) + \omega_2(\hbar)(\sin(\hbar^{-1}\Phi_2) + \eta_2(\hbar))}.$$

This expression is $O(\hbar^{-1})$ provided $|\cos(\hbar^{-1}\Phi_2)| \ge c\,\hbar$ for a sufficiently large $c > 0$. Roughly speaking, this means that the quantization condition is not satisfied in the well X_2. Thus, Theorem 6.3 can be supplemented by the following assertion. Recall that the intervals $I_{n,\ell}(\hbar)$ were defined by relation (6.5).

Proposition 6.8. *Under Assumption* 6.1, *let* $L = 2$. *Then the operator* $H(\hbar)$ *has at most one eigenvalue in an interval* $I_{n,\ell}(\hbar)$ *provided*

$$|\cos(\hbar^{-1}\Phi_k(\lambda))| \ge c\,\hbar, \quad k \ne \ell, \quad \lambda \in I_{n,\ell}(\hbar),$$

for a sufficiently large $c > 0$.

So, the problems with estimate (6.8) may arise if the quantization conditions (6.2) are satisfied in both wells. However this estimate may still be true under both quantization conditions. As an example, consider the symmetric double well in the case where $L = 2$ and $v(-x) = v(x)$. Then $\Phi_1 = \Phi_2 =: \Phi$, $\gamma_1 = \gamma_2 =: \gamma$, $\sigma_1 = \sigma_2 =: \sigma$, $\eta_1 = \eta_2 =: \eta$ and $\omega_1 = \omega_2 =: \omega$. In this case from (6.16) it follows that

$$\gamma = -\omega \pm \sqrt{\omega_0}$$

which yields 2 equations (6.7) for Φ with

$$\epsilon_\ell(\hbar) = \sigma(\hbar) + \big(\sin(\hbar^{-1}\Phi) + \eta(\hbar)\big)\big(\omega + (-1)^\ell \sqrt{\omega_0}\big), \quad \ell = 1, 2. \tag{6.22}$$

These functions satisfy the estimates $\epsilon_\ell(\hbar) = O(\hbar)$ and $\dot\epsilon_\ell(\hbar) = O(1)$, so that conditions (6.8) are fulfilled for both ℓ. Thus, there is exactly one eigenvalue of $H(\hbar)$ in each interval $I_{n,\ell}(\hbar)$, $\ell = 1, 2$. Note also that since the second term on the right-hand side of (6.22) decays exponentially, the intervals $I_{n,1}(\hbar)$ and $I_{n,2}(\hbar)$ defined up to the length $O(\hbar^2)$ may be identified. Then one can say that there are exactly 2 eigenvalues in each interval $I_{n,1}(\hbar) = I_{n,2}(\hbar)$.

Appendix A. Tunneling of a particle through a potential barrier

Here we again consider a potential barrier and accept Assumption 5.1. In contrast to bound states, tunneling of a particle (wave) through a barrier is described by complex solutions of equation (1.1). They are again distinguished by their asymptotics away from the barrier. As in §5, the energy λ is fixed.

Consider the solutions

$$\begin{aligned} f_1(x;\hbar) &= i w_+(x; b_1, \hbar) + u_+(x; b_1, \hbar), \\ f_2(x;\hbar) &= w_-(x; b_2, \hbar) + i u_-(x; b_2, \hbar) \end{aligned} \tag{A.1}$$

of equation (1.1). In view of relations (2.13) and (2.18), they have the asymptotics

$$f_j(x;\hbar) = (\lambda - v(x))^{-1/4} \exp\left(i\hbar^{-1} \int_{b_j}^x (\lambda - v(y))^{1/2}\, dy + \frac{\pi i}{4}\right) + O(\hbar) \tag{A.2}$$

as $\hbar \to 0$ on the compact subsets of the interval (x_1, b_1) for $f_1(x;\hbar)$ and of the interval (b_2, x_2) for $f_2(x;\hbar)$. The function $f_1(x;\hbar)$ corresponds to the incident wave propagating from $x = -\infty$ in the direction of the barrier. Its part reflected by the barrier is described by the function $\overline{f_1(x;\hbar)}$, and the part transmitted through the barrier is described by the function $f_2(x;\hbar)$.

From formula (2.19), it follows that the Wronskian obeys the relation

$$\{f_1(\hbar), \overline{f_1(\hbar)}\} = -2i\{u_+(b_1,\hbar), w_+(b_1,\hbar)\} = 2i\hbar^{-1}(1 + O(\hbar)), \tag{A.3}$$

so that the functions $f_1(x;\hbar)$ and $\overline{f_1(x;\hbar)}$ are linearly independent, whence

$$f_2(x;\hbar) = A(\hbar) f_1(x;\hbar) + B(\hbar)\overline{f_1(x;\hbar)}, \tag{A.4}$$

where the complex numbers $A(\hbar)$ and $B(\hbar)$ are determined by the equations

$$\{f_1(\hbar), \overline{f_1(\hbar)}\}A(\hbar) = \{f_2(\hbar), \overline{f_1(\hbar)}\}, \quad \{f_1(\hbar), \overline{f_1(\hbar)}\}B(\hbar) = \{f_1(\hbar), f_2(\hbar)\}. \tag{A.5}$$

Recall that the function Ω is defined by formula (5.3). By Lemma 5.2, we have

$$\begin{aligned} \{f_2(\hbar), \overline{f_1(\hbar)}\} &= \{w_-(b_2,\hbar) + i u_-(b_2,\hbar), -i w_+(b_1,\hbar) + u_+(b_1,\hbar)\} \\ &= 2i\hbar^{-1} e^{\hbar^{-1}\Omega}(1 + O(\hbar)) \end{aligned} \tag{A.6}$$

and similarly,

$$\begin{aligned} \{f_2(\hbar), f_1(\hbar)\} &= \{w_-(b_2,\hbar) + i u_-(b_2,\hbar), i w_+(b_1,\hbar) + u_+(b_1,\hbar)\} \\ &= -2i\hbar^{-1} e^{\hbar^{-1}\Omega}(1 + O(\hbar)). \end{aligned} \tag{A.7}$$

Substituting (A.3), (A.6), and (A.7) in equations (A.5), we find asymptotic expressions for $A(\hbar)$ and $B(\hbar)$:

$$A(\hbar) = e^{\hbar^{-1}\Omega}(1 + O(\hbar)), \quad B(\hbar) = e^{\hbar^{-1}\Omega}(1 + O(\hbar)). \tag{A.8}$$

Dividing (A.4) by $A(\hbar)$, we see that

$$f_1(x;\hbar) + R(\hbar)\overline{f_1(x;\hbar)} = T(\hbar)f_2(x;\hbar) \tag{A.9}$$

where $R(\hbar) = A(\hbar)^{-1}B(\hbar)$ and $T(\hbar) = A(\hbar)^{-1}$ are known as the reflection and transmission coefficients for scattering of the wave $f_1(x;\hbar)$ by the potential barrier $v(x)$. Formulas (A.8) show that

$$R(\hbar) = 1 + O(\hbar) \quad \text{and} \quad T(\hbar) = e^{-\hbar^{-1}\Omega}\big(1 + O(\hbar)\big). \tag{A.10}$$

Thus, we have obtained the following result.

Theorem A.1. *Let the solutions $f_1(x;\hbar)$ and $f_2(x;\hbar)$ of equation* (1.1) *be defined by formula* (A.1)*. They have the asymptotics* (A.2) *as $\hbar \to 0$ and are linked by identity* (A.9)*. The asymptotics as $\hbar \to 0$ of the reflection coefficient $R(\hbar)$ and the transmission coefficient $T(\hbar)$ are given by formulas* (A.10)*.*

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