A GENERALIZED VIRIAL THEOREM AND THE BALANCE OF KINETIC AND POTENTIAL ENERGIES IN THE SEMICLASSICAL LIMIT

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To the memory of Pierre Duclos

ABSTRACT. We obtain two-sided bounds on kinetic and potential energies of a bound state of a quantum particle in the semiclassical limit, as the Planck constant $\hbar \to 0$. Proofs of these results rely on the generalized virial theorem obtained in the paper as well as on a decay of eigenfunctions in the classically forbidden region.

1. INTRODUCTION

1.1. Let us consider an eigenfunction $\psi_\hbar(x)$ of the Schrödinger operator

$$H_\hbar = -\hbar^2 \Delta + v(x), \quad v(x) = \overline{v(x)}, \tag{1.1}$$

in the space $L_2(\mathbb{R}^d)$, that is

$$-\hbar^2 \Delta \psi_\hbar(x) + v(x)\psi_\hbar(x) = \lambda_\hbar \psi_\hbar(x), \quad \psi_\hbar \in L_2(\mathbb{R}^d). \tag{1.2}$$

We always suppose that the function $v(x)$ is semibounded from below, and hence we can set

$$\min_{x \in \mathbb{R}^d} v(x) = 0.$$

We typically assume that the potential $v(x)$ contains wells and study $\psi_\hbar(x)$ for $\lambda_\hbar$ close to some non-critical value $\lambda_0 > 0$ (that is $\nabla v(x) \neq 0$ for all x such that $v(x) = \lambda_0$). In particular, $\lambda_\hbar$ is separated from bottoms of potential wells. The eigenfunctions $\psi_\hbar(x)$ are supposed to be real and normalized, that is

$$\int_{\mathbb{R}^d} \psi_\hbar^2(x) dx = 1.$$

Our goal is to study the behavior of the kinetic

$$K(\psi_\hbar) = \hbar^2 \int_{\mathbb{R}^d} |\nabla \psi_\hbar(x)|^2 dx$$

and potential

$$U(\psi_\hbar) = \int_{\mathbb{R}^d} v(x)\psi_\hbar^2(x) dx$$

energies as $\hbar \to 0$ if the total energy

$$\lambda_\hbar = K(\psi_\hbar) + U(\psi_\hbar) \tag{1.3}$$

is close to λ_0.

1.2. To be more precise, we discuss the following

Problem 1.1. Is it true that

$$K(\psi_\hbar) \geq c > 0 \tag{1.4}$$

for all $\lambda_\hbar$ in a neighborhood of a non-critical point $\lambda_0 > 0$ uniformly in $\hbar$?

In view of equation (1.3) this problem can be equivalently reformulated in terms of the potential energy $U(\psi_\hbar)$ as the inequality

$$U(\psi_\hbar) \leq \lambda_\hbar - c. \tag{1.5}$$

Note that, for small $\hbar$, the eigenfunctions $\psi_\hbar$ are essentially localized (see [5, 8, 2]) in the classically allowed region where $v(x) \leq \lambda_\hbar + \varepsilon$ (for an arbitrary $\varepsilon > 0$). Therefore, inequality (1.5), roughly speaking, means that the eigenfunctions $\psi_\hbar$ are not too strongly localized in a neighborhood of the set $v(x) = \lambda_\hbar$.

Let us discuss Problem 1.1 in a heuristic way. The first level of the discussion is very superficial. Actually, as $\hbar \to 0$, one might expect that the term $-\hbar^2\Delta$ disappears so that in the limit we obtain the operator of multiplication by the function $v(x)$. This operator has a continuous spectrum and its "eigenfunctions" are Dirac functions of the variable $v(x)-\lambda$. Such functions "live" in a neighborhood of the set $v(x) = \lambda$ which might eventually interfere with the positive answer to Problem 1.1.

The second level is, on the contrary, quite deep and stipulates that, for small $\hbar$, the behavior of a quantum particle with Hamiltonian (1.1) is close to the behavior of the corresponding classical particle, and hence the classical equations of motion can be used. In this context we mention book [1] relying on the method of Maslov canonical operator and papers [4, 3] relying on methods of microlocal analysis.

We avoid this deep level using only the virial theorem and the fact that a quantum particle of energy $\lambda_\hbar$ should be essentially localized as $\hbar \to 0$ in the classically allowed region.

1.3. Problem 1.1 arose by the proof of the limiting absorption principle for the Hamiltonian K of a quantum particle moving in a magnetic field of an infinite straight current (see [9]). This problem reduces to a study of eigenvalues $\lambda_\hbar$ close to a point $\lambda_0 > 0$ for a potential

$$v(x) = v_0 \ln^2 |x|, \quad v_0 > 0, \quad x \in \mathbb{R}^2.$$

The limiting absorption principle for the operator K requires the estimate

$$d\lambda_\hbar/d\hbar \geq c\hbar^{-1}, \quad c > 0.$$

It looks somewhat exotic but in view of the formula (see, e.g., [6])

$$d\lambda_\hbar/d\hbar = 2\hbar \int_{\mathbb{R}^d} |\nabla\psi_\hbar(x)|^2 dx,$$

it is equivalent to estimate (1.4).

1.4. We also discuss a problem dual to Problem 1.1.

Problem 1.2. Is it true that

$$K(\psi_\hbar) \leq \lambda_\hbar - c, \quad c > 0,$$

for all λ in a neighborhood of a non-critical point $\lambda_0 > 0$ uniformly in $\hbar$?

This fact is equivalent to the estimate $U(\psi_\hbar) \geq c > 0$ which means that, in the semiclassical limit, the eigenfunctions $\psi_\hbar$ are not too strongly localized at the bottom of the potential well.

2. A GENERALIZED VIRIAL THEOREM

2.1. Below the operator $H_\hbar$ is always defined by formula (1.1). The following result generalizes the classical virial theorem.

Theorem 2.1. *Suppose that $v \in C^1(\mathbb{R}^d)$. Let $a = \bar{a} \in C^4(\mathbb{R}^d)$, and let its four derivatives be bounded. Then eigenfunctions $\psi_\hbar$ of the operator $H_\hbar$ satisfy an identity*

$$\int_{\mathbb{R}^d} \left(4\hbar^2 \sum_{j,k=1}^d a_{jk} \partial_k \psi_\hbar \partial_j \psi_\hbar - \hbar^2 (\Delta^2 a) \psi_\hbar^2 - 2 \langle \nabla a, \nabla v \rangle \psi_\hbar^2 \right) dx = 0, \qquad (2.1)$$

where $a_{jk} = \partial^2 a / \partial x_j \partial x_k$.

Proof. Let

$$A = \sum_{j=1}^d \big(a_j(x) \partial_j + \partial_j a_j(x) \big), \quad a_j = \partial a / \partial x_j,$$

be a general self-adjoint first order differential operator. Then the commutators

$$[-\Delta, A] = -4 \sum_{j,k=1}^d \partial_j a_{jk} \partial_k - \Delta^2 a$$

and

$$[v, A] = -2 \langle \nabla a, \nabla v \rangle.$$

It remains to use that, for a function $\psi_\hbar$ satisfying equation (1.2), the identity

$$([H_\hbar, A] \psi_\hbar, \psi_\hbar) = 0$$

holds. $\qquad \square$

Note that since eigenfunctions corresponding to isolated eigenvalues decay exponentially, identity (2.1) requires practically no assumptions on the behavior of the function $a(x)$ as $|x| \to \infty$. However we consider only bounded functions $a(x)$.

If $a(x) = x^2$, then identity (2.1) reduces to the usual (see, e.g., [7]) form

$$2\hbar^2 \int_{\mathbb{R}^d} |\nabla \psi_\hbar(x)|^2 dx = \int_{\mathbb{R}^d} r v_r(x) \psi_\hbar^2(x) dx, \quad r = |x|, \qquad (2.2)$$

of the virial theorem. Combining equations (1.3) and (2.2) we see that

$$\int_{\mathbb{R}^d} \big(2^{-1} r v_r(x) + v(x) \big) \psi_\hbar^2(x) dx = \lambda_\hbar, \qquad (2.3)$$

where the eigenfunctions $\psi_\hbar$ are real and normalized.

2.2. As is well known, for homogeneous potentials, the kinetic $K(\psi_\hbar)$ and potential $U(\psi_\hbar)$ energies are related to the total energy by exact equalities.

Proposition 2.2. *Suppose that*

$$v(tx) = t^\alpha v(x), \quad t > 0, \quad \alpha > 0. \qquad (2.4)$$

Then

$$K(\psi_\hbar) = \alpha(\alpha + 2)^{-1} \lambda_\hbar \quad \text{and} \quad U(\psi_\hbar) = 2(\alpha + 2)^{-1} \lambda_\hbar. \qquad (2.5)$$

Indeed, it suffices to use that $rv_r(x) = \alpha v(x)$ in (2.3).

This result remains true for some $\alpha < 0$; however to define $H_\hbar$ as a self-adjoint operator, we have to require that $|\alpha|$ be not too large.

2.3. The case of homogeneous potentials is of course exceptional. In general, one cannot expect (if $d > 1$) to have even a semiclassical asymptotics of the kinetic (or potential) energy. Let us consider a simple

Example 2.3. Set

$$v(x) = |x_1|^{\alpha_1} + |x_2|^{\alpha_2}, \quad x = (x_1, x_2) \in \mathbb{R}^2, \quad \alpha_j > 0, \quad j = 1, 2. \tag{2.6}$$

For every $\lambda > 0$ and every

$$u \in (2(\alpha_1 + 2)^{-1}\lambda, 2(\alpha_2 + 2)^{-1}\lambda),$$

there exist sequences of eigenvalues $\lambda_\hbar$ and eigenfunctions $\psi_\hbar$ of the operator $H_\hbar$ such that $\lambda_\hbar \to \lambda$ and $U(\psi_\hbar) \to u$ as $\hbar \to 0$.

Indeed, let $a_n^{(j)}$, $n = 1, 2\ldots$, be eigenvalues of the one-dimensional operators $-D_j^2 + |x_j|^{\alpha_j}$, $j = 1, 2$. Eigenvalues $\lambda_\hbar$ of operator (1.1) with potential (2.6) are given by the formula

$$\lambda_\hbar = \lambda_\hbar^{(1)} + \lambda_\hbar^{(2)} \tag{2.7}$$

where $\lambda_\hbar^{(j)} = \hbar^{\gamma_j} a_{n_j}^{(j)}$, $j = 1, 2$, $\gamma_j = 2\alpha_j(\alpha_j + 2)^{-1}$ and $n_j = 1, 2\ldots$ are arbitrary. Normalized eigenfunctions $\psi_\hbar$ are scaled products of normalized eigenfunctions $\varphi_{n_j}^{(j)}$ of these two one-dimensional operators, that is

$$\psi_\hbar(x) = \hbar^{-(\beta_1 + \beta_2)/2} \varphi_{n_1}^{(1)}(\hbar^{-\beta_1} x_1) \varphi_{n_2}^{(2)}(\hbar^{-\beta_2} x_2), \quad \beta_j = 2(\alpha_j + 2)^{-1}.$$

For this eigenfunction, the potential energy equals

$$U(\psi_\hbar) = \hbar^{\gamma_1} \int_{\mathbb{R}} |x_1|^{\alpha_1} \varphi_{n_1}^{(1)}(x_1)^2 dx_1 + \hbar^{\gamma_2} \int_{\mathbb{R}} |x_2|^{\alpha_2} \varphi_{n_2}^{(2)}(x_2)^2 dx_2$$

so that in view of the second formula (2.5)

$$U(\psi_\hbar) = \beta_1 \hbar^{\gamma_1} a_{n_1}^{(1)} + \beta_2 \hbar^{\gamma_2} a_{n_2}^{(2)}. \tag{2.8}$$

Let us now take into account that

$$a_n^{(j)} = c_j n^{\gamma_j}(1 + o(1)), \quad c_j > 0, \quad n \to \infty.$$

Pick some numbers $\mu_j > 0$ and set $n_j = [(\mu_j c_j^{-1})^{1/\gamma_j} \hbar^{-1}]$ where $[b]$ is the integer part of a number b. Then

$$\lambda_\hbar^{(j)} = \hbar^{\gamma_j} a_{n_j}^{(j)} \to \mu_j \tag{2.9}$$

as $\hbar \to 0$. Moreover, it follows from (2.8) that

$$\lim_{\hbar \to 0} U(\psi_\hbar) = 2(\alpha_1 + 2)^{-1}\mu_1 + 2(\alpha_2 + 2)^{-1}\mu_2. \tag{2.10}$$

If $\mu_1 + \mu_2 = \lambda$, then according to (2.7) and (2.9) $\lambda_\hbar \to \lambda$. However the limit (2.10) may take arbitrary values between $2(\alpha_1 + 2)^{-1}\lambda$ and $2(\alpha_2 + 2)^{-1}\lambda$.

3. Estimates of the kinetic energy

3.1. In addition to the virial theorem, we need results on a decay of eigenfunctions in the classically forbidden region. We suppose that

$$\liminf_{|x|\to\infty} v(x) =: v_\infty > 0$$

and consider eigenvalues $\lambda_\hbar$ which belong to a neighborhood of some non-critical energy $\lambda_0 \in (0, v_\infty)$. Our construction works for $v \in C^1(\mathbb{R}^d)$, but in order to use the results on a decay of eigenfunctions we assume that $v \in C^\infty(\mathbb{R}^d)$. As always, eigenfunctions $\psi_\hbar$ of the operator $H_\hbar$ are real and normalized. Let the sets $F(\lambda)$ and $G(\lambda)$ be defined by the formulas

$$F(\lambda) = \{x \in \mathbb{R}^d : v(x) < \lambda\}, \quad G(\lambda) = \mathbb{R}^d \setminus F(\lambda).$$

Then (see [5], [8] as well as [2] and references therein) for all *fixed* $\varepsilon > 0$,

$$\int_{G(\lambda_\hbar+\varepsilon)} \left(\hbar^2|\nabla\psi_\hbar|^2 + \psi_\hbar^2(x)\right)dx \to 0 \tag{3.1}$$

as $\hbar \to 0$. Actually, eigenfunctions $\psi_\hbar$ decay exponentially as $\hbar \to 0$ in the classically forbidden region $G(\lambda_\hbar + \varepsilon)$, but we do not need this result.

Relation (3.1) can be supplemented by an estimate of the potential energy. Of course the next lemma is useful only in the case when $v(x)$ is not bounded at infinity.

Lemma 3.1. *For all $\varepsilon > 0$, we have*

$$\int_{G(\lambda_\hbar+\varepsilon)} v(x)\psi_\hbar^2(x)dx \to 0$$

as $\hbar \to 0$.

Proof. In view of (3.1) it suffices to check that, for some R,

$$\lim_{\hbar\to 0} \int_{|x|\geq R} v(x)\psi_\hbar^2(x)dx = 0. \tag{3.2}$$

Choose R such that $v(x) \geq \lambda_\hbar + \varepsilon$ for $|x| \geq R/2$. Let $\eta \in C^\infty(\mathbb{R}^d)$ be such that $\eta(x) \geq 0$, $\eta(x) = 0$ for $|x| \leq R/2$ and $\eta(x) = 1$ for $|x| \geq R$. Multiplying equation (1.2) by η and integrating by parts, we see that

$$\int_{\mathbb{R}^d} \eta\left(\hbar^2|\nabla\psi_\hbar|^2 + v\psi_\hbar^2\right)dx = \lambda_\hbar \int_{\mathbb{R}^d} \eta\psi_\hbar^2 dx - \hbar^2 \int_{\mathbb{R}^d} \langle\nabla\psi_\hbar, \nabla\eta\rangle\psi dx. \tag{3.3}$$

Let us consider the right-hand side. The first integral tends to zero as $\hbar \to 0$ because $\eta(x) = 0$ in the classically allowed region. Using the Schwarz inequality and relation (1.3), we estimate the second term by $\hbar\lambda_\hbar^{1/2} \max|\nabla\eta(x)|$. Therefore expression (3.3) tends to zero as $\hbar \to 0$ which proves (3.2). $\qquad\square$

3.2. Relations (2.1) and (3.1) can be combined. The simplest example is given in the next statement.

Proposition 3.2. *Let the function $rv_r(x)v(x)^{-1}$ be bounded as $|x| \to \infty$. Choose some $\lambda_0 > 0$. Suppose that, for some $\varepsilon_0 \in (0, 2\lambda_0)$, the potential $v(x)$ admits representation (2.4) in the region $F(\lambda_0 + \varepsilon_0)$. Then for $\lambda_\hbar \in (\lambda_0 - \varepsilon_0/2, \lambda_0 + \varepsilon_0/2)$, we have, as $\hbar \to 0$, the asymptotic relations*

$$K(\psi_\hbar) = \alpha(\alpha+2)^{-1}\lambda_\hbar + o(1) \quad \text{and} \quad U(\psi_\hbar) = 2(\alpha+2)^{-1}\lambda_\hbar + o(1). \tag{3.4}$$

Indeed, it follows from (2.3) and Lemma 3.1 that

$$\int_{F(\lambda_0+\varepsilon_0)} \big(2^{-1}rv_r(x) + v(x)\big)\psi_\hbar^2(x)dx = \lambda_\hbar + o(1).$$

By virtue of (2.4) the integral in the left-hand side equals

$$2^{-1}(\alpha + 2)\int_{F(\lambda_0+\varepsilon_0)} v(x)\psi_\hbar^2(x)dx.$$

Therefore using again Lemma 3.1, we obtain (3.4).

Estimates (1.4) on the kinetic energy or, equivalently, (1.5) on the potential energy can be obtained under much weaker assumptions on $v(x)$. In view of (3.1) the principal difficulty is to exclude that eigenfunctions $\psi_\hbar(x)$ are localized in neighborhoods of the surfaces $v(x) = \lambda_\hbar$.

3.3. Let us formulate the main result of this paper.

Theorem 3.3. *Let $\lambda_0 > 0$ be a non-critical energy, and let for some (sufficiently small) $\varepsilon_0 > 0$ and all $\lambda \in (\lambda_0 - \varepsilon_0, \lambda_0 + \varepsilon_0)$*

$$F(\lambda) = \bigcup_{n=1}^N F_n(\lambda), \quad F_n(\lambda) \cap F_m(\lambda) = \emptyset \quad \text{for} \quad n \neq m. \tag{3.5}$$

Suppose that for all $n = 1, \ldots, N$ and some points $x_n \in F_n(\lambda_0 - \varepsilon_0)$ an inequality

$$\langle x - x_n, \nabla v(x)\rangle \geq c_0 > 0, \quad x \in F_n(\lambda_0 + \varepsilon_0) \cap G(\lambda_0 - \varepsilon_0), \tag{3.6}$$

holds. Denote by $\psi_\hbar$ normalized eigenfunctions $\psi_\hbar$ of the operator $H_\hbar$ corresponding to eigenvalues $\lambda_\hbar$ in a neighborhood $(\lambda_0 - \varepsilon_0/2, \lambda_0 + \varepsilon_0/2)$ of the point λ_0. Then inequality (1.4) is true for sufficiently small $\hbar$.

The assumptions of this theorem are, actually, very mild. Roughly speaking, we suppose that the classically allowed region $F(\lambda)$ consists of a finite number of potential wells. Condition (3.6) means that $v(x)$ increases as x passes through the boundary of $F_n(\lambda)$. This is consistent with the fact that $F_n(\lambda)$ is a potential well of $v(x)$ for the energy λ. If $N = 1$, then setting $x_1 = 0$, we obtain that inequality (3.6) reduces to the condition $v_r(x) \geq c_0 > 0$.

We split the proof in a series of simple lemmas. Let us estimate the potential energy in two different ways. The first one is quite straightforward.

Lemma 3.4. *For all $\varepsilon > 0$ and all $\delta \in (0, \lambda_\hbar)$, we have*

$$\int_{F(\lambda_\hbar+\varepsilon)} v(x)\psi_\hbar^2(x)dx \leq \lambda_\hbar + \varepsilon - \delta\int_{F(\lambda_\hbar-\delta)} \psi_\hbar^2(x)dx.$$

Proof. Observe that

$$\int_{F(\lambda_\hbar-\delta)} v(x)\psi_\hbar^2(x)dx \leq (\lambda_\hbar - \delta)\int_{F(\lambda_\hbar-\delta)} \psi_\hbar^2(x)dx$$

and

$$\int_{F(\lambda_\hbar+\varepsilon)\cap G(\lambda_\hbar-\delta)} v(x)\psi_\hbar^2(x)dx \leq (\lambda_\hbar + \varepsilon)\int_{G(\lambda_\hbar-\delta)} \psi_\hbar^2(x)dx$$
$$= (\lambda_\hbar + \varepsilon)\Big(1 - \int_{F(\lambda_\hbar-\delta)} \psi_\hbar^2(x)dx\Big).$$

So it suffices to put these two estimates together. $\square$

Combining Lemmas 3.1 and 3.4, we see that for all $\varepsilon > 0$ and all $\delta \in (0, \lambda_\hbar)$,

$$U(\psi_\hbar) \leq \lambda_\hbar + \varepsilon - \delta \int_{F(\lambda_\hbar - \delta)} \psi_\hbar^2(x)dx + \sigma(\varepsilon, \hbar) \tag{3.7}$$

where $\sigma(\varepsilon, \hbar) \to 0$ as $\hbar \to 0$ if ε is *fixed*. The notation $\sigma(\varepsilon, \hbar)$ will also be used below.

The second estimate relies on the virial theorem which we need in the following form.

Lemma 3.5. *Let $x_n \in F_n(\lambda_0 + \varepsilon_0)$ be arbitrary points. Then*

$$\sum_{n=1}^N \int_{F_n(\lambda_0 + \varepsilon_0)} \left(2\hbar^2 |\nabla \psi_\hbar(x)|^2 - \langle x - x_n, \nabla v(x)\rangle \psi_\hbar^2(x)\right)dx = o(1), \quad \hbar \to 0. \tag{3.8}$$

Proof. Let us use Theorem 2.1 for a suitable function $a(x)$ which we construct now. Choose functions $\varphi_n \in C_0^\infty(\mathbb{R}^d)$ such that $\varphi_n(x) = 1$ for $x \in F_n(\lambda_0 + \varepsilon_0)$ and $\varphi_n(x) = 0$ away from some neighborhoods of $F_n(\lambda_0 + \varepsilon_0)$ so that $\text{supp}\, \varphi_n \cap \text{supp}\, \varphi_m = \emptyset$ if $n \neq m$. We define the function $a(x)$ by the equality

$$a(x) = \sum_{n=1}^N |x - x_n|^2 \varphi_n(x). \tag{3.9}$$

Neglecting in (2.1) the classically forbidden region, we see that

$$\int_{F(\lambda_0 + \varepsilon_0)} \left(4\hbar^2 \sum_{j,k=1}^d a_{jk}\partial_k \psi_\hbar \partial_j \psi_\hbar - \hbar^2(\Delta^2 a)\psi_\hbar^2 - 2\langle \nabla a, \nabla v\rangle \psi_\hbar^2\right)dx = o(1) \tag{3.10}$$

as $\hbar \to 0$. If $x \in F_n(\lambda_0 + \varepsilon_0)$, then according to (3.9) we have $(\nabla a)(x) = 2(x - x_n)$, $a_{jj}(x) = 2$ and $a_{jk}(x) = 0$ if $j \neq k$. Thus, relation (3.8) follows from (3.10). $\qquad \square$

Lemma 3.6. *Let assumption (3.6) hold for some points $x_n \in F_n(\lambda_0 - \varepsilon_0)$, and set*

$$c_1 = \max_n \sup_{x \in F_n(\lambda_0 - \varepsilon_0)} (-\langle x - x_n, \nabla v(x)\rangle). \tag{3.11}$$

Then

$$2\hbar^2 \int_{\mathbb{R}^d} |\nabla \psi_\hbar(x)|^2 dx \geq c_0 - c_2 \int_{F(\lambda_0 - \varepsilon_0)} \psi_\hbar^2(x)dx + \sigma(\varepsilon_0, \hbar) \tag{3.12}$$

where $c_2 = c_0 + c_1$ and $\sigma(\varepsilon_0, \hbar) \to 0$ as $\hbar \to 0$.

Proof. According to (3.6) and (3.11), we have

$$\int_{F_n(\lambda_0 + \varepsilon_0)} \langle x - x_n, \nabla v(x)\rangle \psi_\hbar^2(x)dx \geq c_0 \int_{F_n(\lambda_0 + \varepsilon_0) \cap G(\lambda_0 - \varepsilon_0)} \psi_\hbar^2(x)dx$$
$$- c_1 \int_{F_n(\lambda_0 - \varepsilon_0)} \psi_\hbar^2(x)dx.$$

Summing these estimates over $n = 1, \cdots, N$ and using (3.8), we see that

$$2\hbar^2 \int_{F(\lambda_0 + \varepsilon_0)} |\nabla \psi_\hbar(x)|^2 dx \geq c_0 \int_{F(\lambda_0 + \varepsilon_0) \cap G(\lambda_0 - \varepsilon_0)} \psi_\hbar^2(x)dx$$
$$- c_1 \int_{F(\lambda_0 - \varepsilon_0)} \psi_\hbar^2(x)dx + o(1)$$

as $\hbar \to 0$. The first integral in the right-hand side equals 1 minus the integrals of $\psi_\hbar^2(x)$ over $F(\lambda_0 - \varepsilon_0)$ and $G(\lambda_0 + \varepsilon_0)$. The integral over $G(\lambda_0 + \varepsilon_0)$ tends to zero because $G(\lambda_0 + \varepsilon_0)$ lies in the classically forbidden region.   □

Using the energy conservation (1.3) and the obvious inclusion $F(\lambda_0 - \varepsilon_0) \subset F(\lambda_\hbar - \varepsilon_0/2)$, we deduce from (3.12) the estimate

$$U(\psi_\hbar) \leq \lambda_\hbar - 2^{-1}c_0 + 2^{-1}c_2 \int_{F(\lambda_\hbar - \varepsilon_0/2)} \psi_\hbar^2(x)dx + \sigma(\varepsilon_0, \hbar). \qquad (3.13)$$

If $c_2 \leq 0$, then (3.13) directly implies (1.5). So below we assume $c_2 > 0$.

Now we are in a position to conclude the *proof* of Theorem 3.3. Let us compare estimates (3.7) where we set $\delta = \varepsilon_0/2$ and (3.13). Roughly speaking, if the integral

$$X = \int_{F(\lambda_\hbar - \varepsilon_0/2)} \psi_\hbar^2(x)dx$$

is small, then we use (3.13). If it is big, we use (3.7). To be more precise, estimates (3.7) and (3.13) imply that

$$U(\psi_\hbar) \leq \lambda_\hbar + 2^{-1} \max_{0 \leq X \leq 1} \min\{2\varepsilon - \varepsilon_0 X, -c_0 + c_2 X\} + \sigma(\varepsilon, \varepsilon_0, \hbar),$$

where $\sigma(\varepsilon, \varepsilon_0, \hbar) \to 0$ as $\hbar \to 0$ for fixed ε and ε_0. Observe that

$$\max_{0 \leq X \leq 1} \min\{2\varepsilon - \varepsilon_0 X, -c_0 + c_2 X\} \leq 2\varepsilon - \varepsilon_0 c_0 (1 + c_2)^{-1}$$

(if $\varepsilon_0 \leq 1$). Since ε is arbitrary small, this yields estimates (1.5) and hence (1.4). In these estimates c is any number smaller than $2^{-1}\varepsilon_0 c_0 (1 + c_0 + c_1)^{-1}$.

3.4. Our lower bound on the potential energy (and hence an upper bound on the kinetic energy) is almost trivial.

Proposition 3.7. *Let, for some $\lambda_0 > 0$ and $\varepsilon_0 > 0$, representation (3.5) hold for $\lambda = \lambda_0 + \varepsilon_0$. Suppose that for all $n = 1, \ldots, N$ there exist points $x_n \in F_n(\lambda_0)$ such that the estimates*

$$\langle x - x_n, \nabla v(x) \rangle \leq c_0 v(x), \quad x \in F_n(\lambda_0), \qquad (3.14)$$

are satisfied with some constant $c_0 > 0$. Then

$$U(\psi_\hbar) \geq c\lambda_\hbar \qquad (3.15)$$

for all $\lambda_\hbar \in (\lambda_0 - \varepsilon_0/2, \lambda_0 + \varepsilon_0/2)$, an arbitrary $c < 2(c_0 + 2)^{-1}$ and sufficiently small $\hbar$.

Proof. Comparing relation (3.8) with assumption (3.14), we see that

$$2\hbar^2 \int_{F(\lambda_0 + \varepsilon_0)} |\nabla \psi_\hbar(x)|^2 dx \leq c_0 \int_{F(\lambda_0 + \varepsilon_0)} v(x)\psi_\hbar^2(x)dx + \sigma(\varepsilon_0, \hbar).$$

Then using relation (3.1) and Lemma 3.1, we obtain the estimate

$$2K(\psi_\hbar) \leq c_0 U(\psi_\hbar) + o(\hbar).$$

In view of the energy conservation (1.3), this yields (3.15).   □

Assumption (3.14) essentially means that, inside every well $F_n(\lambda_0)$, the function $v(x)$ may equal zero only at the point x_n. If, for example,

$$v(x) = v_n |x - x_n|^{\alpha_n}, \quad v_n > 0, \quad \alpha_n > 0, \quad x \in F_n(\lambda_0), \quad n = 1, \ldots, N,$$

then estimate (3.14) holds with $c_0 = \max\{\alpha_1, \ldots, \alpha_N\}$.

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