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# Comparison Theorems for the Gap of Schrödinger Operators

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## 1. THE BASIC THEOREM

There are two cases where it is well known that Schrödinger operators have non-degenerate eigenvalues: The lowest eigenvalue in general dimension and all one-dimensional eigenvalues. One can ask about making this quantitative, i.e., obtain explicit lower bounds on the distance to the nearest eigenvalues. Obviously, one cannot hope to do this without any restrictions on $V$ since, for example, if $\chi$ is the characteristic function of $(-1, 1)$, one can show that, for $l$ large, $-d^2/dx^2 - \chi(x) - \chi(x-l)$ has at least two eigenvalues and $E_1 - E_0 \to 0$ as $l \to \infty$ (see, e.g., Harrell [7]). Thus, we ask the following: Can one obtain lower bounds on eigenvalue splittings only in terms of geometric properties of the set with $V(x) < E$ ($E$ at or near the eigenvalues in question) and the size of $V$ on this set? We will do precisely this for the two lowest eigenvalues in general dimension in this paper, and we have proven results on any one-dimensional eigenvalue in [11].

This is not the first paper to try to estimate the gap $E_1 - E_0$ for $-\Delta + V$; see, e.g., [8, 16, 9, 19]. Here we will present a very elementary device which is also quite powerful. It depends on the fact that many Schrödinger operators can be realized as Dirichlet forms. This subject has been studied

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by many authors, e.g., [2, 5, 6, 3]. Here we quote some results of Davies and Simon [3, Proposition 4.4 and Theorem C.1]. The class $K_\nu$ is discussed in [3, 15].

THEOREM 1.1. *Let $H = -\Delta + V$, $V_- \in K_\nu$, $V_+ \in K_\nu^{\mathrm{loc}}$ and let $H\psi_0 = E_0\psi_0$ for a positive $L^2$ function, $\psi_0$. Let $A$ be the operator on $L^2(\mathbb{R}^\nu, \psi_0^2\, d^\nu x)$ with $D(A) = \{f \mid f\psi_0 \in D(H)\}$ and $Af = \psi_0^{-1}(H - E_0)(f\psi_0)$. Then*

$$Q(A) = \{f \in L^2(\mathbb{R}^\nu, \psi_0^2\, d^\nu x) \mid \nabla f \in L^2(\mathbb{R}^\nu, \psi_0^2\, d^\nu x)\} \tag{1.1}$$

*and*

$$(f, Af) = \int (\nabla f)^2\, \psi_0^2\, d^\nu x. \tag{1.2}$$

THEOREM 1.2. *Let $H_0$ be the Dirichlet Laplacian for a bounded region $U \subseteq R^n$, and let $H_0\psi_0 = E_0\psi_0$ for a positive $L^2$ function $\psi_0$. Suppose that $\psi_0(x) \to 0$ as $x \to \partial U$. Let $A$ be the operator on $L^2(U, \psi_0^2\, d^\nu x)$ with $D(A) = \{f \mid f\psi_0 \in D(H)\}$ and $Af = \psi_0^{-1}(H_0 - E_0)(f\psi_0)$. Then $Q(A) = \{f \in L^2(U, \psi_0^2\, d^\nu x) \mid \nabla f \in L^2(\mathbb{R}^\nu, \psi_0^2\, d^\nu x)\}$ and*

$$(f, Af) = \int (\nabla f)^2\, \psi_0^2\, d^\nu x.$$

*Remarks.* 1. $\nabla f$ is intended in a distributional sense.

2. There are geometric conditions on $U$ which imply that $\psi_0(x) \to 0$ as $x \to \partial U$; see Corollary C.4 of [3].

3. Theorem 1.2 and its proof in [3] extend to $H = H_0 + V$ with $V \in K_\nu$.

4. Similar theorems hold with periodic and Neumann boundary conditions (where, for periodic boundary conditions, we must think of the operator on a torus) with $\nabla f$ a distribution on the torus (including possible singularities at the boundary of the cube stitched to a torus).

Since $A$ is unitarily equivalent to $H - E_0$, we obtain a variational principle for the gap:

COROLLARY 1.3. $E_1 - E_0 = \inf\{\int (\nabla f)^2\, \psi_0^2\, d^\nu x / \int f^2\, \psi_0^2\, d^\nu x \mid \int f\psi_0^2 = 0\}$.

It is this variational principle first exploited by Kac and Thompson [10] and more recently by one of us [16] that we will use here. We will call a general operator $H$, so that $H - E_0$ is unitarily equivalent to an operator with $Q(A)$ given by (1.1) and $A$ given by (1.2), an operator related to a Dirichlet form. Our basic comparison result is:

THEOREM 1.4. *Let $H$, $\tilde{H}$ be two operators related to Dirichlet forms with lowest eigenvalues $E_0, E_1$ (resp. $\tilde{E}_0, \tilde{E}_1$) and lowest eigenfunction $\psi_0$ (resp. $\tilde{\psi}_0$). Let $a(x) = \psi_0 \tilde{\psi}_0^{-1}$ and*

$$a_+ = \max_x a(x); \qquad a_- = \min_x a(x).$$

*Then*

$$\left[\frac{a_-}{a_+}\right]^2 (E_1 - E_0) \leqslant \tilde{E}_1 - \tilde{E}_0 \leqslant \left[\frac{a_+}{a_-}\right]^2 (E_1 - E_0).$$

*Remark.* In all cases of interest, $a(x)$ is continuous, which is why we write max for $a_\pm$ rather than sup.

*Proof.* Let $b(x) = \psi_1 \psi_0^{-1}$, where $\psi_1$ is the eigenfunction of $H$ associated to $E_1$. Then we can find $\alpha$ so

$$\int [\alpha + b(x)] \tilde{\psi}_0^2 \, d^\nu x = 0.$$

Let $c(x) = \alpha + b(x)$,

$$\begin{aligned}
\tilde{E}_1 - \tilde{E}_0 &\leqslant \int (\nabla c)^2 \tilde{\psi}_0^2 \, d^\nu x \Big/ \int c^2 \tilde{\psi}_0^2 \, d^\nu x \\
&= \int (\nabla c)^2 (\tilde{\psi}_0 \psi_0^{-1})^2 \psi_0^2 \, d^\nu x \Big/ \int c^2 (\tilde{\psi}_0 \psi_0^{-1})^2 \psi_0^2 \, d^\nu x \\
&\leqslant (a_+/a_-)^2 \int (\nabla c)^2 \psi_0^2 \, d^\nu x \Big/ \int c^2 \psi_0^2 \, d^\nu x \\
&= (a_+/a_-)^2 \, [(E_1 - E_0)/(\alpha^2 + 1)] \\
&\leqslant (a_+/a_-)^2 (E_1 - E_0).
\end{aligned}$$

Let $\tilde{a}(x) = a(x)^{-1}$ so $\tilde{a}_+ = a_-^{-1}$, $\tilde{a}_- = a_+^{-1}$. Reversing the roles of $H$ and $\tilde{H}$ in the above arguments

$$E_1 - E_0 \leqslant (\tilde{a}_+/\tilde{a}_-)^2 (\tilde{E}_1 - \tilde{E}_0) = (a_+/a_-)^2 (\tilde{E}_1 - \tilde{E}_0),$$

which is the other desired inequality. ∎

Despite the simplicity of this argument, it is quite useful. In the next section, we use the theorem and its strategy to find new bounds on the lowest band in a solid. In Section 3, we prove bounds on a special situation which we use elsewhere [11]; actually, it was this application that motivated the present note. In Section 4, we prove bounds that answer the question raised in the first paragraph of this section.

The methods and results of this paper carry over to the case of finite difference Hamiltonians on a lattice $\mathbb{Z}^\nu$. Let $h_0$ denote the finite difference Laplacian, i.e.,

$$h_0 u(n) = -\sum_{|\alpha|=1} [u(n+\alpha) - u(n)],$$

and set $h = h_0 + V$, $V$ multiplication by the function (sequence) $V(n)$. If $\Omega$ denotes the ground state of $h$ and $E_0$ the ground state energy, then the corresponding Dirichlet form is given by

$$\langle u, Au \rangle = \sum_{n \in \mathbb{Z}^\nu} \left[ \sum_{i=1}^{\nu} \right] \Omega(n)\, \Omega(n+\delta_i) |u(n+\delta_i) - u(n)|^2$$

with $A = \Omega^{-1}(h - E_0)\, \Omega$.

## 2. The Ground State Band in a Solid

Let $H = -(2m)^{-1} \Delta + V(x)$, where $V(x)$ is periodic on $\mathbb{R}^\nu$, i.e.,

$$V(x+a) = V(x)$$

for $a$ in some lattice, $L$, i.e., a discrete subgroup of $\mathbb{R}^\nu$ spanning $\mathbb{R}^\nu$ as a real vector space. Let $L^*$ be the dual lattice, i.e., $K \in L^*$ if and only if $K \cdot a \in 2\pi\mathbb{Z}$ for all $a \in L$. Let $B$ be the Brillouin zone, i.e.,

$$B = \{ k \in \mathbb{R}^\nu \mid |k| < \operatorname{dist}(k, L^* \setminus \{0\}) \}.$$

It is well known (see, e.g., [13, Sect. XIII.16]) that

$$L^2(R^\nu, d^\nu x) \simeq \int_B^\oplus \mathscr{H}_k\, d^\nu k; \qquad H = \int_B^\oplus H(k)\, d^\nu k, \tag{2.1}$$

where the $H(k)$ are operators we will describe later. They have discrete spectra and their eigenvalues $\varepsilon_0(k) \leqslant \varepsilon_1(k) \leqslant \cdots$ are called *band functions.* We want to prove the following in this section:

THEOREM 2.1. *Let $\psi_0$ be the positive periodic solution of $H\psi_0 = \varepsilon_0(0)\, \psi_0$. Then*

$$(a_-/a_+)^2 (2m)^{-1} k^2 \leqslant \varepsilon_0(k) - \varepsilon_0(0) \leqslant (2m)^{-1} k^2, \tag{2.2}$$

*where $a_\pm = {\max \atop \min} [\psi_0(x)]$.*

It often happens that for reasons of symmetry $(\partial^2\varepsilon_0/\partial k_\alpha\, \partial k_\beta)(0)$ is a multiple of the identity matrix, in which case the "effective mass" is defined by

$$\varepsilon_0(k) = \varepsilon_0(k) + (2m_{\text{eff}})^{-1}\, k^2 + O(k^3).$$

(Actually, the physical effective mass is associated with the curvature of bands higher than $\varepsilon_0$.)

COROLLARY 2.2. $m \leqslant m_{\text{eff}} \leqslant (a_+/a_-)^2\, m$.

We also note that (2.2) implies that $\varepsilon_0(k)$ isn't flat (constant). For general $\varepsilon_l$, this is a result of Thomas [18] proven by rather different means.

*Proof of Theorem* 2.1. We need to describe (2.1) in more detail [13, 17]. Define the Wigner–Seitz cell by

$$C = \{x \in \mathbb{R}^\nu \mid |x| < \operatorname{dist}(x, L \setminus \{0\})\}.$$

Then $\mathcal{H}_k = \{\psi \in L^2_{\text{loc}}(\mathbb{R}^\nu) \mid \psi(x+a) = e^{ik\cdot a}\psi(x);\ \text{all}\ \ a \in L\}$ with inner product

$$(\psi, \varphi)_k = \int_C \overline{\psi(x)}\, \varphi(x)\, d^\nu x$$

and

$$H(k)\,\psi = [-(2m)^{-1}\, \Delta + V(x)]\,\psi,$$

where $H(k)$ (suppose $V$ is locally $L^{\nu/2}$ if $\nu \geqslant 5$, $L^2$ if $\nu = 1, 2, 3$, $L^p$, $p \geqslant 2$ if $\nu = 4$) has a domain $\{\psi \in \mathcal{H}_k \mid \Delta\psi \in \mathcal{H}_k\}$. Let $\psi_0$ be the positive periodic solution of $H\psi_0 = \varepsilon_0(0)\,\psi_0$ (i.e., $\psi_0$ is the lowest eigenfunction of $H(0)$) and define

$$\tilde{\mathcal{H}}_k = \mathcal{H}_k$$

but with the inner product

$$\langle f, g\rangle_{\tilde{k}} = \int_C \bar{f}(x)\, g(x)\, \psi_0^2(x)$$

and the operator $A(k)$ on $\tilde{\mathcal{H}}_k$ by $D(A(k)) = \{f \mid f\psi_0 \in D(H(k))\}$ and

$$A(k)\, f = \psi_0^{-1}(H(k) - \varepsilon_0(0))[f\psi_0].$$

Then, as usual, one can easily show that

$$Q(A(k)) = \{f \mid \nabla f \in \mathcal{H}_k\}$$

and

$$(f, A(k) f) = (2m)^{-1}(\|\nabla f\|_{\bar{k}})^2. \tag{2.3}$$

Taking $f = e^{ik \cdot x} \in \mathscr{H}_k$, we see that

$$\varepsilon_0(k) - \varepsilon_0(0) = \inf\{(f, A(k) f) \mid \|f\|_{\bar{k}} = 1\} \leqslant (2m)^{-1} k^2.$$

On the other hand, if $f$ is the lowest eigenfunction of $A(k)$, we can use $f$ as a trial function for $A_0(k)$ (the $A(k)$ associated to $V = 0$), so

$$\begin{aligned}
(2m)^{-1} k^2 &\leqslant \int_C (\nabla f)^2 \, d^\nu x \Big/ \int_C f^2 \, d^\nu x \\
&\leqslant a_-^{-2} \int_C (\nabla f)^2 \psi_0^2 \, d^\nu x / a_+^{-2} \int_C f^2 \psi_0^2 \, d^\nu x \\
&= (a_+/a_-)^2 \, [\varepsilon_0(k) - \varepsilon_0(0)],
\end{aligned}$$

yielding the other bound. ∎

We will describe this application in detail for the discrete case, expanding on the remark in the Introduction.

Lemma 2.3. *Let*

$$(h_0 u)(n) = -\sum_{|\alpha| = 1} [u(n+\alpha) - u(n)]$$

*on* $l^2(\mathbb{Z}^\nu)$. *Let* $V$ *be a periodic multiplication operator, and let* $\Omega_0$ *be the positive periodic ground state of* $H = H_0 + V$ *with* $H\Omega_0 = E_0 \Omega_0$. *Then for* $u \in \mathscr{H}_k$,

$$(\Omega_0 u, (H - E_0)(\Omega_0 u)) = \sum_{n \in \mathbb{Z}^\nu} \sum_{i=1}^{\nu} \Omega_0(n)\, \Omega_0(n + \delta_i)\, |u_{n+\delta_i} - u_n|^2. \tag{2.4}$$

*Proof.* Without loss, take $u$ real-valued. For simplicity we take $k = 0$; the proof is similar for general $k$, and we write $n + \delta_i$ models the periods of $V$. Let $D_i$ and $\nabla_i$ be defined by

$$(D_i f)(n) = f(n + \delta_i)$$
$$\nabla_i = (D_i - 1)$$

so $h_0 = -\sum (D_i + D_i^* - 2)$

A straightforward calculation shows that

$$[D_i, g] = (\nabla_i g) D_i$$

so

$$[[D_i, u], u] = (\nabla_i u)^2 D_i$$

and

$$\langle \Omega_0, [[D_i, u], u] \Omega_0 \rangle = \sum_{n \in \mathbb{Z}^\nu} |(\nabla_i u)(n)|^2 \Omega_0(n) \Omega_0(n + \delta_i).$$

Because of the sum over $n$, we get the same formula for $D_i^*$. Thus

$$\langle \Omega_0, [[H_0, u] u] \Omega_0 \rangle = -2(\text{rhs of } (2.4)).$$

But $[[(H - E_0), u], u] = [[H_0, u] u]$, so expanding the double commutator and using $(H - E_0) \Omega_0 = 0$, we obtain (2.4). ▮

THEOREM 2.4. *In the above case, let $\varepsilon_0(k)$ be the band function for the ground state band of $H$. Then*

$$(a_- / a_+)^2 E_0(k) \leqslant \varepsilon_0(k) - \varepsilon_0(0) \leqslant E_0(k),$$

*where* $E_0(k) = 2\nu - \sum_{i=1}^{\nu} \cos k_i$ *is the free ground state band and* $a_\pm = {}^{\max}_{\min} \Omega_0$.

*Proof.* Given the lemma and $[e^{ik(\delta_i + n)} - e^{ikn}]^2 = 2 - 2 \cos k_i$, the proof is identical to that of Theorem 2.1. ▮

## 3. Bound on Some Neumann Laplacians

In our study [12] of Lifshitz tails for random plus periodic potentials, we require lower bounds on the gaps of some Neumann Laplacians whose dependence on the region's diameter is qualitatively similar to that for free Laplacians. Our comparison theorem is ideal for this. We state the general $\nu$-result here. In [12], we give a more general result in one dimension.

THEOREM 3.1. *Let $V(x)$ obey $V(x + a) = V(x)$ for all $a \in \mathbb{Z}^\nu$ and $V(\pm x_1, \pm x_2, ..., \pm x_\nu) = V(x)$. Let $E_j^{(L)}$ $(L = 1, 2, ...)$ denote te $(j+1)$st eigenvalue of $-\Delta + V$ in the box $B_L = \{x \mid 0 \leqslant x_i \leqslant L\}$ with Neumann boundary conditions. Then, for some $\alpha > 0$,*

$$E_1^{(L)} - E_0^{(L)} \geqslant \alpha L^{-2}.$$

*Remark.* If $f(x)$ is spherically symmetric and $|f(x)| \leqslant c(1 + |x|)^{-\nu - \varepsilon}$, *then* $V(x) = \sum_{a \in \mathbb{Z}^\nu} f(x - a)$ obeys all the hypotheses of the theorem.

*Proof.* Let $\psi_0$ be the positive periodic solution of $(-\Delta + V)\psi_0 = E_0\psi_0$ with $E_0$ the ground state energy of $-\Delta + V$ (on $\mathbb{R}^\nu$). Then $\psi_0(\pm x_1, ..., \pm x_\nu) = \psi_0(x)$, by the hypothesis on $V$ and the uniqueness of this periodic solution. Thus, $\psi_0$ obeys Neumann boundary conditions on the boundary of $B_L$, so $E_0^{(L)} = E_0$ and $\eta_L = \psi_0 | B_L$ is the ground state. In particular, $[\min(\eta_L)/\max(\eta_L)]^2 = \tilde{\alpha}$ is independent of $L$ (by the periodicity of $\psi_0$). Applying Theorem 1.4 with $\tilde{V} = 0$ (Neumann b.c.), we see that

$$E_1 - E_0 \geqslant \tilde{\alpha}(\tilde{E}_1 - \tilde{E}_0) = \tilde{\alpha}(\pi/L)^2$$

as desired. ∎

## 4. Tunneling Bounds

In this section we want to describe how to obtain explicit lower bounds on the gap depending only on the geometry of the set, $C$, where $V(x) < E_1$ and the maximum value of $|V(x) - E|$ on the convex hull of $C$ and $E$ in the gap.

As a warm-up, we consider a periodic potential $V(x)$ obeying

$$V(x + aL) = V(x) \qquad \text{for all } a \in \mathbb{Z}^\nu. \tag{4.1}$$

We let $\tau_\nu$ denote the volume of the unit ball in $\nu$-dimensions. Let $G(x)$ be the integral kernel of $(-\Delta + 1)^{-1}$ and let $C_\nu = \int |(\nabla G)(x)| \, d^\nu x$.

THEOREM 4.1. *Set $m = \frac{1}{2}$ in Theorem 2.1. Then, if $\lambda L \geqslant (2C_\nu)^{-1}$,*

$$\left[\frac{a_-}{a_+}\right] \geqslant \frac{1}{2}\tau_\nu (4C_\nu)^{-\nu} (\pi\lambda L\sqrt{\nu})^{-\nu/2} \exp(-\tfrac{1}{2}\lambda\sqrt{\nu}\, L),$$

*where $\lambda = \max_x |V(x) - E_0|^{1/2}$.*

*Remarks.* 1. This yields a bound on the band size $O(e^{-\lambda\sqrt{\nu}L})$ for $\lambda$ large. The analysis of [7] shows that no lower bound of the form $O(e^{-(1-\varepsilon)L})$ can hold.

2. If $\lambda L < (C_\nu\sqrt{\nu})^{-1}$, the proof below shows that $[a_-/a_+] \geqslant 1 - (C_\nu\sqrt{\nu}\, L\lambda)$. Moreover, the proof shows that $\lambda$ can be replaced by any number larger than $\max|V(x) - E_0|^{1/2}$.

We turn to the proof of Theorem 4.1. For later use, we single out the following lemma:

LEMMA 4.2. *Let $V$ be a bounded potential (not necessarily periodic), and let $E$ be an eigenvalue of $-\Delta + V$ with eigenfunction $\psi$. Then*

$$\|\nabla\psi\|_\infty \leqslant 2C_\nu\, \mu\, \|\psi\|_\infty$$

*if* $|V(x) - E|^{1/2} < \mu$.

*Proof* (*Lemma*). From

$$(-\Delta + \mu^2)\,\psi = (E - V(x) + \mu^2)\,\psi$$

we see that

$$\nabla\psi(x) = \int \nabla_x G^{(\mu)}(x, y)(E - V(y) + \mu^2)\,\psi(y)\,dy,$$

where $G^{(\mu)}$ is the kernel of $(-\Delta + \mu^2)^{-1}$. Hence

$$|\nabla\psi(x)| \leqslant 2\mu^2 \int |\nabla G^{(\mu)}(x)|\,dx\,\|\psi\|_\infty$$
$$\leqslant 2c_\nu\,\mu\,\|\psi\|_\infty$$

by scaling. ∎

*Proof* (*Theorem*). Normalize $\psi_0$ so that $\|\psi_0\|_\infty = \psi_0(x_0) = 1$. By the lemma, if $|x - x_0| \leqslant 1/4C_\nu\lambda$ then $\psi_0(x) \geqslant \frac{1}{2}$. By hypothesis, $(4C_\nu\,\lambda)^{-1} < L/2$, so the sphere of radius $(4C_\nu\,\lambda)^{-1}$ about $x_0$ and its translates are all disjoint. For any $y$ and $T$,

$$\psi_0(y) \geqslant (e^{-T(H-E_0)}\psi_0)(y)$$
$$\geqslant e^{-\lambda^2 T} \int_C e^{-TH_0}(y, x)\,\psi_0(x), \tag{4.2}$$

where $H_0$ is the Laplacian on $C = \{x \mid |x_i| < L/2\}$ with periodic B.C. Since some translate of $x_0$ is within $\frac{1}{2} L\sqrt{\nu}$ of $y$, we have that

$$e^{-TH_0}(y, x) \geqslant (4\pi T)^{-\nu/2} \exp(-(\tfrac{1}{2} L\sqrt{\nu})^2/4T) \tag{4.3}$$

by the method of images. Looking at the contribution of (4.2) from the set of $x$ with $|x - x_0| < (4C_\nu\lambda)^{-1}$ (where $\psi_0 \geqslant \frac{1}{2}$), choosing $T = L\sqrt{\nu}/4\lambda$, and using (4.3), we obtain the required bound on $a_-$. ∎

Now we turn to the announced tunneling result. We consider a Schrödinger operator $H = -\Delta + V$ with $V$ bounded. We assume that $H$ has at least two eigenvalues below its essential spectrum. We denote by $E_0$ and $E_1$ the lowest eigenvalue and the second, respectively. It is well known that

$E_0$ is non-degenerate (see, e.g., Reed and Simon [13]). In certain tunneling situations the difference $E_1 - E_0$ is exponentially small (see, e.g., [16]). We will apply Theorem 1.2 to prove that in any case $E_1 - E_0$ is not smaller than an exponential. The exponent we obtain is not too far from the typical "tunneling exponent" and one might hope that the difference $E_1 - E_0$ can never be smaller than in the tunneling case. This was proven to be true in [11] for the one-dimensional case, where we used ODE techniques.

Let us denote by $\psi_0, \psi_1$ the ground state and the first excited state of $H$. We normalize $\psi_0, \psi_1$ such that $\psi_0 \geqslant 0$, $\|\psi_0\|_\infty = 1$, $\|\psi_1\|_\infty = 1$. Moreover, by shifting space we may assume that $\psi_0(0) = 1$. Let us denote by $x_1$ a point where $|\psi_1(x_1)| = 1$ and by $x_0$ a point where $\psi_1(x_0) = 0$. Note that $\psi_1$ must have zeros. By normalization we may assume that $\psi_1(x_1) = 1$. We set $f(x) = \psi_0(x)^{-1}\,\psi_1(x)$.

Let us denote $B_\varepsilon = \{x \in \mathbb{R}^\nu \mid V(x) > E_1 + \varepsilon^2\}$. $B_\varepsilon$ is a bounded set for $\varepsilon$ small enough. We fix such an $\varepsilon > 0$. Let us denote by $C = C_\varepsilon$ the smallest closed ball containing $B_\varepsilon$ and by $R$ its radius.

PROPOSITION 4.3. *The maxima of $\psi_0$ and $\psi_1$ and at least one zero of $\psi_1$ are contained in $C$.*

*Proof.* Outside $C$ we have $V(x) - E_1 \geqslant \varepsilon^2 > 0$ so

$$\Delta\psi_0 = (V(x) - E_0)\,\psi_0 > 0 \qquad \text{for } x \notin C.$$

Thus $\psi_0$ is a subharmonic function outside $C$, and hence $\psi_0$ assumes its maximum over $C^c$ on the boundary. Moreover, since $\Delta\psi_1 = (V(x) - E_1)\,\psi_1$, we have for $(\psi_1)_+ = \max(\psi_1, 0)$, $(\psi_1)_- = \max(-\psi_1, 0)$ (see, e.g., Lemma 2.9 in [1]):

$$\Delta(\psi_1)_+ \geqslant (V(x) - E_1)(\psi_1)_+$$

and

$$\Delta(\psi_1)_- \geqslant (V(x) - E_1)(\psi_1)_-.$$

It follows that $\psi_1$ assumes both its maxima and its minima inside $C$. Since $C$ is convex, $\psi_1$ has also a zero in $C$. ∎

By the above proposition, we have that $x_1, 0 \in \mathbb{R}^d$ belong to $C$(or even to $B_\varepsilon$ for any $\varepsilon > 0$). We may furthermore assume that $x_0 \in C$.

We will make use of this proposition in estimating $\psi_0$ and $|\nabla f|$ from below. From Theorem 1.2 we have

$$E_1 - E_0 = \frac{\int |\nabla f|^2\,\psi_0^2\,dx}{\int \psi_1^2\,dx} \geqslant \frac{(\int_C |\nabla f|\,dx)^2}{\int \psi_0^2\,dx \int \psi_1^2\,dx} \inf_{x \in C} \psi_0(x)^4. \tag{4.4}$$

We estimate the various pieces of the right-hand side of (4.4) in the following propositions:

Let us start with a lower bound on $\psi_0$. We set

$$\lambda_0 = \sup_{x \in \mathbb{R}^d} \sup_{E \in [E_0, E_1]} |V(x) - E|^{1/2}. \tag{4.5}$$

PROPOSITION 4.4. *For any* $\lambda \geqslant \lambda_0$ *we have*

$$\psi_0(x) \geqslant M_0(|x| + a)^{-\nu/2} e^{-\sqrt{2}\,\lambda |x|}, \tag{4.6}$$

*where* $a = (4C_\nu \lambda)^{-1}$ and $M_0 = \frac{1}{2}(\tau_\nu/(2\pi)^{\nu/2})\; a^\nu 2^{\nu/2} \lambda^{\nu/2} e^{-2^{-3/2} C_\nu^{-1}}$. *We set* $M_0(|x|) = M_0 \cdot (|x| + a)^{-\nu/2}$.

*Proof.* Let $\mathbb{E}_x$ denote the expectation with respect to a $\nu$-dimensional Brownian motion starting at $x$. By $\mathbb{P}_x$ we denote the corresponding probability measure. Then, by the Feynman–Kac formula,

$$\psi_0(x) = (e^{-t(H - E_0)} \psi_0)(x) = \mathbb{E}_x(e^{-\int_0^t (V(b(s)) - E_0)\, ds} \psi_0(b(t))),$$

where $b$ stands for a Brownian motion. (For standard facts on Brownian motion and the Feynman–Kac formula we refer to [4, 14].)

This can be further estimated by

$$\psi_0(x) \geqslant e^{-t\lambda^2}\, \mathbb{E}_x(\psi_0(b(t))) = (*). \tag{4.7}$$

To estimate the last expectation, we recall that $\psi_0(0) = 1$ and that $|\nabla \psi_0| \leqslant 2C_\nu \lambda$ by Lemma 4.2. Thus we have $\psi_0(x) \geqslant \frac{1}{2}$ for $|x| \leqslant 1/(4C_\nu \lambda) = a$. Using this, we see

$$\begin{aligned}
(*) &\geqslant e^{-t\lambda^2} \frac{1}{2}\, \mathbb{P}_x(|b(t)| \leqslant a) \\
&= \frac{1}{2} e^{-t\lambda^2} \frac{1}{(2\pi t)^{\nu/2}} \int_{|y| \leqslant a} e^{-|x-y|^2/2t}\, dy \\
&\geqslant \frac{1}{2} \tau_\nu a^\nu \frac{1}{(2\pi t)^{\nu/2}} e^{-t\lambda^2 - (|x| + a)^2/2t}.
\end{aligned}$$

We choose $t = (|x| + a)/\sqrt{2}\,\lambda)$, the choice which minimizes the exponent, getting

$$\psi_0(x) \geqslant \frac{1}{2} \frac{\tau_\nu a^\nu}{(2\pi)^{\nu/2}} 2^{\nu/4} \lambda^{\nu/2} (|x| + a)^{-\nu/2} e^{-2^{-3/2} C_\nu^{-1}} e^{-\sqrt{2}|x|\lambda}. \quad \blacksquare$$

To get estimates on $\int \psi_0^2\, dx$, $\int \psi_1^2\, dx$ from above, we give an upper bound for $\psi_0(x)$, $\psi_1(x)$ for $x$ large enough. For this, we denote by $d(x)$ the distance of $x$ from the set $B$.

PROPOSITION 4.5. *If $x \notin B$, then*

$$|\psi_1(x)| \leqslant \left(1+\sqrt{\frac{2}{\pi d(x)}}\,2^{-7/4}(\lambda^2+\varepsilon^2)^{-7/4}\right)\exp\left(-\frac{\varepsilon^2}{\sqrt{2}\sqrt{\lambda^2+\varepsilon^2}}\,d(x)\right). \quad (4.8)$$

*The same estimate holds for $\psi_0$.*

*Proof.* We prove the assertion of the proposition for $\psi_1$. The proof can be taken over literally for $\psi_0$:

$$\begin{aligned} |\psi_1(x)| &= |e^{-t(H-E_1)}\psi_1(x)| \leqslant E_x(e^{-\int_0^t (V(b(s))-E_1)\,ds})\|\psi_1\|_\infty \\ &\leqslant e^{-t\varepsilon^2} P_x(b(s)\notin B \text{ all } 0\leqslant s\leqslant t) \\ &\quad + e^{t\lambda^2} P_x(b(s)\in B \text{ some } 0\leqslant s\leqslant t) \\ &\leqslant e^{-t\varepsilon^2} + e^{t\lambda^2} P_x(b(s)\in B \text{ some } 0\leqslant s\leqslant t). \end{aligned}$$

Let us denote by $b^{(1)}(s)$ the coordinate of $b$ along the line through $x$ normal to $B$. $b^{(1)}$ is a one-dimensional Brownian motion and

$$\begin{aligned} &P_x(b(s)\in B \text{ for some } 0\leqslant s\leqslant t) \\ &\quad\leqslant P_0^{(1)}(b^{(1)}(s)\geqslant d(x) \text{ for some } 0\leqslant s\leqslant t) \\ &\quad\leqslant 2P_0^{(1)}(b^{(1)}(t)\geqslant d(x)) \qquad \text{(see, e.g., Durrett [4])} \\ &\quad\leqslant \frac{2\sqrt{t}}{\sqrt{2\pi}\,d(x)}\,e^{-d(x)^2/2t} \end{aligned}$$

by standard estimates on the normal distribution.

Thus we obtain

$$|\psi_1(x)| \leqslant e^{-t\varepsilon^2} + \frac{2\sqrt{t}}{\sqrt{2\pi}\,d(x)}\,e^{-d(x)^2/2t+t\lambda^2}.$$

Choosing $t = d(x)/\sqrt{2}\sqrt{\lambda^2+\varepsilon^2}$ we get

$$|\psi_1(x)| \leqslant \left(1+\sqrt{\frac{2}{\pi d(x)}}\,2^{-1/4}(\lambda^2+\varepsilon^2)^{-1/4}\right) e^{-(\varepsilon^2/\sqrt{2}\sqrt{\lambda^2+\varepsilon^2})d(x)}. \quad \blacksquare$$

As a corollary we obtain the desired bound on the $L^2$ norms of $\psi_0$ and $\psi_1$. Let us denote by $\tau_\nu$ and $\omega_\nu$ the volume and the surface area of the unit ball, respectively.

We set, for short, $a = \varepsilon^2/(\sqrt{2}\sqrt{\lambda^2+\varepsilon^2})$, $b = 1+\sqrt{2/\pi}\,2^{-1/4}(\lambda^2+\varepsilon^2)^{-1/4}$.

We estimate

$$\int_{|x|\leqslant R+1} |\psi_1(x)|^2\,dx \leqslant \tau_\nu(R+1)^\nu$$

(recall that $\|\psi_1\|_\infty = 1$) and

$$\int_{|x|>R+1} |\psi_1(x)|^2\,dx \leqslant \int_{|x|>R+1} b^2 e^{-2a(|x|-R)}dx$$
$$\leqslant b^2 e^{2aR}\omega_\nu \int_{R+1}^{\infty} r^{\nu-1} e^{-2ar}dr$$
$$\leqslant b^2 e^{2aR}\omega_\nu C_a (R+1)^{\nu-1}\, e^{-2a(R+1)}$$

(we used $\int_{x_0}^{\infty} x^n e^{-\alpha x} \leqslant (C_\alpha)\, x_0^n e^{-\alpha x_0}$ for $x_0 > 1$). This gives the desired result.

Finally, we turn to a lower bound for $\int |\nabla f|\, dx$. To obtain such a bound, we will integrate $\nabla f$ along a tube, $\mathscr{T}$, of the following form: Take $y_0, y_1 \in \mathbb{R}^\nu$. Set $B_\varepsilon(y_0, y_1 - y_0) = \{x \in \mathbb{R}^\nu \mid |x - y_0| \leqslant \varepsilon;\ x \perp (y_1 - y_0)\}$ and $\mathscr{T} = \{x + t(y_1 - y_0) \mid x \in B_\varepsilon(y_0, y_1 - y_0)\ t \in [0, 1]\}$. Obviously

$$\int |\nabla f|\, dx \geqslant \int_{\mathscr{T}} |\nabla f|\, dx$$
$$\leqslant (\inf_{x \in B_\varepsilon(y_0, y_1 - y_0)} f(x) - \sup_{x \in B_\varepsilon(y_1, y_1 - y_0)} f(x))\, \tau_{\nu-1}\varepsilon^{\nu-1}.$$

Thus, we need estimates on $\inf f$ and $\sup f$ on suitably chosen regions.

Since $\psi_1(x_0) = 0$, we have $f(x_0) = 0$. Moreover, we know $\psi_1(x_1) = 1$ and $\psi_0(x_1) \leqslant 1$, so $f(x_1) \geqslant 1$.

To get estimates on $f$ near $x_0$ and $x_1$ we observe that

$$|\nabla f| \leqslant \frac{|\nabla\psi_1|}{\psi_0} + \frac{|\psi_1|\,|\nabla\psi_0|}{\psi_0^2}$$
$$\leqslant \frac{2C_\nu\lambda}{M_0(|x|)}\,(1 + M_0(|x|)^{-1}\, e^{+\sqrt{2}\lambda|x|})\, e^{+\sqrt{2}\lambda|x|},$$

where we used Lemma 4.2 and Proposition 4.4.

We have proven

LEMMA 4.6. *For $x \in B$ we have*

$$|\nabla f(x)| \leqslant \frac{2C_\nu\lambda}{M_0(2R)}\left(1 + \frac{e^{2\sqrt{2}\lambda R}}{M_0(2R)}\right) e^{\sqrt{2}\lambda 2R}. \tag{4.9}$$

Calling $a(R)$ the right-hand side of (4.9), we conclude that $f(x) < \frac{1}{4}$ for $|x - x_0| < 1/4a(R)$ and $f(x) > \frac{3}{4}$ for $|x - x_1| < 1/4a(R)$. Therefore, we find balls of radius at least $1/8a(R)$ inside $C$ where $f(x) < \frac{1}{4}$ resp. $f(x) > \frac{3}{4}$. Integrating along a tube connecting these balls, we obtain

$$\int |\nabla f| \, dx \geqslant \frac{1}{(8a(R))^{\nu-1}} \tau_{\nu-1} \cdot \frac{1}{2}.$$

Collecting the various estimates, we arrive at

THEOREM 4.7. *Suppose $V$ is a bounded potential $\lambda \geqslant \lambda_0$. Then*

$$E_1 - E_0 \geqslant C(R)\, e^{-8\sqrt{2\nu\lambda R}}.$$

*The factor $C(R)$ is bounded by a polynomial in $R$.*

We refrain from stating the explicit form of the factor $C(R)$ which is, of course, given in various pieces in the above calculations.

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