OPTIMAL BOUNDS ON THE FUNDAMENTAL SPECTRAL GAP WITH SINGLE-WELL POTENTIALS

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Abstract. We characterize the potential-energy functions $V(x)$ that minimize the gap $\Gamma$ between the two lowest Sturm-Liouville eigenvalues for

$$H(p,V)u := -\frac{d}{dx} \left( p(x) \frac{du}{dx} \right) + V(x)u = \lambda u, \quad x \in [0, \pi],$$

where separated self-adjoint boundary conditions are imposed at end points, and $V$ is subject to various assumptions, especially convexity or having a “single-well” form. In the classic case where $p = 1$ we recover with different arguments the result of Lavine that $\Gamma$ is uniquely minimized among convex $V$ by the constant, and in the case of single-well potentials, with no restrictions on the position of the minimum, we obtain a new, sharp bound, that $\Gamma > 2.04575\ldots$.

1. Introduction

In this article, we consider a Sturm-Liouville operator on a finite interval, scaled without loss of generality to have length $\pi$,

$$H(p,V)u := -\frac{d}{dx} \left( p(x) \frac{du}{dx} \right) + V(x)u = \lambda u, \quad x \in [0, \pi],$$

where $p(x)$ is a bounded $C^1$ function that is uniformly positive on $(0, \pi)$ and various assumptions are made on the potential energy $V(x)$, for instance that $V(x) = V_0 \pm V_1$, where $V_1$ is either convex or of “single-well” form and $V_0$ is fixed. We shall always make assumptions so that $H$ is self-adjoint with purely discrete spectrum. According to [12], §8.4, this is guaranteed without further conditions when $V(x) \geq C > -\infty$ is in the limit-point case, while if $V(x) \geq C > -\infty$ is in the limit-circle case, we may impose any separated homogeneous boundary conditions.

Date: July 21, 2018.
1991 Mathematics Subject Classification. 34B27, 35J60, 35B05.
Key words and phrases. Fundamental gap spectral, Schrödinger operator, single-well potentials, Dirichlet boundary conditions.
of the form
\[ u(0) \cos \alpha - (pu')(0) \sin \alpha = 0; \]
\[ u(\pi) \cos \beta - (pu')(\pi) \sin \beta = 0, \] (2)
where \(0 \leq \alpha, \beta < \pi\) (In particular this encompasses the possibility of either Dirichlet or Neumann boundary conditions. See [14], §4.6 for further discussion of the boundary conditions for Sturm-Liouville problems.) If \(V(x)\) is not bounded from below, further conditions are required. A sufficient but far from necessary condition that is good for our purposes is that
\[ V(x) \geq C - \frac{1}{4x} - \frac{1}{4(\pi - x)} \] (3)
for some \(C > -\infty\). Again, in the limit-circle case, we may fix any of the boundary conditions \([2]\) to make \(H\) self-adjoint.

We denote the eigenvalues \(\{\lambda_n\}, n = 1, 2, \ldots\), and arrange them in nondecreasing order:
\[ \lambda_1 \leq \lambda_2 \leq \lambda_3 \ldots \lambda_m \leq \cdots \]
The function \(V\) is called a single-well function if \(V\) is non-increasing on \([0,a]\) and non-decreasing on \([a,\pi]\) for some \(a \in [0,\pi]\). The point \(a\) is called a transition point. We do not assume that \(a\) is unique.

The functional \(\Gamma(V)\) defined as
\[ \Gamma(V) = \lambda_2(V) - \lambda_1(V) \]
is called the fundamental gap, of interest in quantum mechanics as the excitation energy to raise a particle out of its ground state. There are both physical and mathematical reasons to study \(\Gamma(V)\). Most frequently in the literature, \(p \equiv 1\), that is, the equation is in Liouville normal form, sometimes referred to as Schrödinger form. (Given that any equation of the form \([1]\) can be put into this form (cf. [4], §10.9 or [14], §9.1), we observe that this transformation alters the spectral problem, because the required transformation depends on the eigenparameter. Hence the inclusion of the function \(p\) in the leading term is a true generalization.) Although \(\lambda_1\) is always simple, so that \(\Gamma > 0\), there is no positive lower bound on \(\Gamma\) without assumptions on \(V\), as exemplified by double-well potentials such as \(V = M\chi_{[\frac{\pi}{4}, \frac{3\pi}{4}]}\) where \(M\) is arbitrarily large, e.g., [2]. In [11] Ashbaugh and Benguria found that the optimal lower bound for \(\Gamma\) for symmetric single-well potentials and Dirichlet boundary conditions is achieved if and only if \(V\) is constant on \((0, \pi)\). In [3] Ashbaugh, Harrell and Svirsky studied the optimization of \(\Gamma(V)\) under \(L^p\) constraints (even in \(n\) dimensions) by first proving
existence of optimizers and then carrying out a variational analysis, a strategy that we shall also employ here. An advance was made by Lavine in 1994 \cite{9}, who considered the class of convex potentials on \([0, \pi]\) and proved that with either Dirichlet or Neumann boundary conditions, \(\Gamma\) attains its minimum if and only if \(V\) is constant. Later, in 2002, Horváth \cite{10} returned with Lavine’s methods to the problem of single-well potentials, without symmetry assumptions, but assuming a transition point at \(\frac{\pi}{2}\), and showed that the gap for the Dirichlet problem is minimized when the potential is constant. In 2015 Yu and Yang \cite{13} extended Horváth’s result by allowing other transition points (under a technical condition) and both Dirichlet and Neumann conditions. In this article, we provide lower bounds for the gap between the first two eigenvalues of the problems \((\text{II})\) with general single-well potential \(V(x)\) with a transition point \(a \in [0, \pi]\), without any restriction on \(a\), and also for the case where the potential is convex. We are furthermore able to analyze the case where \(V = V_0 + V_1\), where \(V_0\) is fixed and \(V_1\) is assumed either single-well or convex. In contrast to the earlier studies of single-well potentials, which restrict the transition point in one way or other, the minimizing potentials we find are not in general constant, although if extra conditions are imposed locating the transition point sufficiently far from 0 or \(\pi\), our methods can lead to constant potentials. Although we do not pursue this idea here in detail, this remark is a way of understanding the results in \cite{1, 10, 13}.

2. Classes of Potentials

We define here several classes of functions that will play a role below.

**Definition 2.1.** For \(0 \leq M \leq \infty\), let
\[
S_M := \{f(x) : 0 \leq f(x) \leq M: \text{there exists } a \in [0, \pi] \text{ such that } f(x) \text{ is nonincreasing for } x \leq a \text{ and nondecreasing for } x \geq a\}.
\]
We identify functions in \(S_M\) when they are equal a.e.
\[
C_M := \{f(x) : 0 \leq f(x) \leq M: f(x) \text{ is convex on } [0, \pi]\}.
\]

Each of these sets has a useful compactness property when \(M\) is bounded:

**Proposition 2.1.** Let \(A\) denote any of the sets in Definition 2.1 with \(M < \infty\). For any sequence \(f_n \in A\) there exist a subsequence \(f_{n_k}\) and a function \(f_*\) such that \(f_{n_k}(x) \to f_*(x)\) a.e. If \(f_*(x)\) is continuous on an interval \([b, c] \subset [0, \pi]\), then the convergence is uniform on that interval.

**Proof.** Suppose first that \(A = S_M\). Let \((f_n, a_n)\) be a sequence of functions in \(S_M\) with \(a_n\) the corresponding values as in Definition 2.1. By the Bolzano-Weierstrass theorem, there exists a first subsequence \((a_{n_l})\)
of \((a_n)\) such that \(a_{n_l} \to a_*\). There may be more than one point of accumulation \(a_*\) but by taking the least of them and passing to a further subsequence, if necessary, we can obtain a sequence \(f_{n_l}\) that is non-increasing on \([0, a_\ast]\) and non-decreasing on \([a_\ast, \pi]\). We can now invoke a theorem of Helly [7, §X.9] by which, for any sequence of uniformly bounded monotonic functions on a fixed, finite interval, there exists \(f_* \in S_M\) such that for a further subsequence, \(f_{n_l}(x) \searrow f_\ast(x)\) for all \(x\) (uniformly on any compact interval \(I\) on which \(f_*\) is continuous).

Suppose now that \(A = C_M\). Then the Blaschke Selection Theorem implies that for every \(f_n(x) \in C_M\), there exists a uniformly convergent subsequence \((f_{n_l})\) of \((f_n)\), such that

\[f_{n_l} \to f_\ast, \quad \text{with } f_* \in C_M.\]

(In the case of convex functions, continuity is automatic on any strict subinterval of \([0, \pi]\).) □

**Theorem 2.1.** Let \(A\) be any of the function classes of Definition 2.1 and suppose that \(V_1 \in A\). Consider the eigenvalue problem (1) where \(V = V_0 + V_1\), where one part is fixed, \(V_0(x) \geq C > -\infty\), and standard boundary conditions of the type (2) are imposed at either end point 0 or \(\pi\) if it is in the limit-circle case. (Due to the boundedness of \(V_1\) this depends only on \(V_0\).) Then the eigenvalues \(\lambda_k\) of (1) are continuous with respect to the topology of pointwise convergence for \(V \in A\), and there is a potential \(V_{\min,*} \in A\) that minimizes \(\Gamma(p, V)\) for \(V = V_0 + V_1\) with \(V_1 \in A\).

**Remarks 2.1.**
1. This can be regarded as a variant of Theorem II.1 of [3], where in addition we control for the single-well or convex assumption. We caution that the optimizers are not claimed to be unique.
2. We note that, likewise, a minimizing potential exists for the eigenvalue gap for (1) with \(V = V_0 - V_1\). Moreover, potentials \(V_{\max,*;\pm} \in A\) exist that maximize \(\Gamma(p, V)\) for \(V = V_0 \pm V_1\).

**Proof.** Let \((V_n, a_n)\) be a minimizing sequence for the functional

\[\Gamma(V) = \lambda_2(V) - \lambda_1(V).\]

We know by Proposition 2.1 that by passing to a subsequence, \(V_{n_l}(x) \to V_\ast(x)\) for all \(x\), with \(V_* \in A\). Because \(A \subset L^p[0, \pi]\) for each \(p\), \(1 \leq p \leq \infty\), and \(L^p\) convergence follows by the Lebesgue Dominated Convergence Theorem (for any given \(p < \infty\)), we can now follow the proof of of Theorem II.1 of [3] to establish continuity of \(\Gamma\) and finish the claim. □
Once existence has been established, one can characterize the optimizers in some of the listed cases by a variational analysis, using the Feynman-Hellman formula. (See [4], below.)

3. Characterization of optimizers

In this section we characterize the optimizers of some of the problems in Proposition 2.1 by introducing a set of perturbations $P(x)$ which would lead to a contradiction to $\Gamma'(0) = 0$ unless $V_\star$ has special properties.

3.1. The class of single-well potentials.

Theorem 3.1. For any $M > 0$, the potential $V_1 \in S_M$ that minimizes $\Gamma(V_0 + V_1)$, with $V_0$ as described in the Introduction, is $M$ times the indicator function of a strict subinterval interval containing either 0 or $\pi$. The minimal gap $\Gamma_\star(M)$ is a decreasing function of $M$, and in the classical case where $p = 1$, $V_0 = 0$, and Dirichlet conditions are imposed at 0 and $\pi$, we have the following characterization of the gap minimizers.

1. The potential energy functions that minimize the gap in the category $S_M$ are of the form $V_\star(x,M) := M\chi_{x-(M)}(x)$ and $V_\star(\pi - x,M)$, for a function $x-(M) < \frac{\pi}{2}$ uniquely defined by an explicit system of equations.

2. For the gap-minimizing operators,

\[ M + 1 < \lambda_2 < M + 4, \quad \text{and} \quad M - 2 < \lambda_1 < M + 1, \]

and for sufficiently large $M$, $\lambda_1 < M$. (Again, the exact values of $\lambda_{1,2}$ are determined by explicit transcendental equations.)

3. If $M > \frac{7}{2}$, $\frac{5}{2\sqrt{M}} \leq x-(M) \leq \frac{5}{\sqrt{M}}$.

4. $\lim_{M \to \infty} \Gamma_\star(M) = \frac{(\theta/\pi)^2}{2.04575}$, where $\theta$ is the first positive solution of $\theta = \tan \theta$. There is no single-well potential such that this infimum is attained.

For $V \in S_M$ let $H(p,V) = -\frac{d}{dx}p(x)\frac{d}{dx} + V(x)$, for which

\[ \sigma(H(p,V)) = \{\lambda_1 < \lambda_2 < \cdots\}, \]

with corresponding normalized $u_1, u_2, \ldots$, $u_1 > 0$ on $[0,\pi]$. We may choose a sign for $u_2$ such that for some $x_0$,

\[ u_2(x) > 0 \quad \text{on} \quad (0,x_0), \]

\[ u_2(x) < 0 \quad \text{on} \quad (x_0,\pi). \]

We will make heavy use of first-order perturbation theory to characterize the effect on the eigenvalues of a small change in potential energy.
$V(x)$. Thus, let $V \in S_M$, and $V(x, \kappa)$ be a one-parameter family of functions in $S_M$ such that $\frac{\partial V(x, \kappa)}{\partial \kappa}$ exists as a bounded, measurable function. Let $\lambda_n(\kappa)$ denote the n-th eigenvalue of the Schrödinger operator with potential $V(x, \kappa)$. If $\lambda_n(\kappa)$ is a simple eigenvalue, then the standard “Feynman-Hellman formula” of perturbation theory states that

$$\frac{d\lambda_n(\kappa)}{d\kappa} = \int_0^\pi \frac{\partial V(x, \kappa)}{\partial \kappa} u_n^2(x, \kappa) dx.$$  \hfill (4)

(See, for instance, [8], §II.2.) We are guaranteed that $\lambda_1$ is simple, but this is not necessarily true of $\lambda_2$ and hence also not automatic for $\Gamma = \lambda_2 - \lambda_1$. Nonetheless, according to degenerate perturbation theory, cf. [8] §VII.6, if $\lambda_2$ is $l$-fold degenerate at $\kappa = \kappa_0$, then there is a relabeling of the eigenvalues $\lambda_2 \ldots \lambda_{2+l-1}$ and of the basis of eigenvectors, so that $\hat{\lambda}_2 \ldots \hat{\lambda}_{2+l-1}$ are analytic functions in a neighborhood of $t_0$, and (4) remains valid with the specified basis of eigenvectors. (In the situation of this article, $l \leq 2$ and we shall always have $\kappa_0 = 0$.) We note for future purposes that $\lambda_2 = \min(\hat{\lambda}_2, \hat{\lambda}_3)$.

The following lemma is a straightforward extension of a result in [1], which was central to [9].

**Lemma 3.2.** The equation $u_2^2(x) - u_1^2(x) = 0$ has at most two solutions in $(0, \pi)$.

**Proof.** Let $x_0$ be the unique zero of $u_2 = 0$ in $(0, \pi)$.

Suppose that there exist $\alpha_1, \alpha_2 \in (0, x)$ such that:

$$|u_2(\alpha_i)| = |u_1(\alpha_i)|; \quad i = 1, 2.$$

Define $v(x) = \frac{u_2(x)}{u_1(x)}$, so $v(\alpha_1) = v(\alpha_2) = 1$. By Rolle’s Theorem, there exists $\xi \in (\alpha_1, \alpha_2) \subset (0, x_0)$ such that

$$v'(\xi) = 0.$$  \hfill (5)

Defining the Wronskian $W(x) = u_1(x)p(x)u_2'(x) - u_2(x)p(x)u_1'(x)$, we get

$$W'(x) = (\lambda_2 - \lambda_1)u_1(x)u_2(x).$$

On the other hand, for all $x \in (0, x_0)$,

$$\left(\frac{u_2(x)}{u_1(x)}\right)' = -\frac{W(x)}{p(x)u_1^2(x)}$$

$$= \frac{1}{p(x)u_1^2(x)} \int_0^x (\lambda_1 - \lambda_2)u_1(s)u_2(s)ds < 0,$
which contradicts \([5]\). Hence there is at most one solution of the equation \(|u_2(x)| = |u_1(x)|\) in \((0, x_0)\), which implies that there is at most one zero of the equation

\[ u_2^2(x) - u_1^2(x) = 0 \]

for \(x \in (0, x_0)\). If we reflect the interval so that \(x \leftrightarrow \pi - x\) and repeat the argument, we can conclude that there is at most one zero of the equation \(|u_2(x)| = |u_1(x)|\) in \([x_0, \pi)\). Consequently, there are at most two zeroes of the equation

\[ u_2^2(x) - u_1^2(x) = 0 \]

in \((0, \pi)\). □

By Lemma 3.2 there exist \(x_0 : 0 \leq x_0 < x_0 < x_+ \leq \pi\), for which

\[ u_2^2(x) - u_1^2(x) = \begin{cases} > 0 & \text{if } x \in (0, x_0) \cup (x_+, \pi) \\ < 0 & \text{if } x \in (x_0, x_+) \end{cases} \]

(6)

**Proof of Theorem 3.1.** It has been established by compactness that \(S_M\) contains a function \(V_*\) such that \(V = V_0 + V_*\) minimizes \(\Gamma(V)\).

Let \(u_1\) and \(u_2\) be the first and second normalized eigenfunctions of the problem (1), respectively. By Lemma 3.2 there exists \(0 \leq x_- < x_+ \leq \pi\) satisfying (6) corresponding to \(V = V_0 + V_*\).

We consider first the case: \(x_- < a < x_+\). For suitable perturbations \(P\) we define

\[ V_*(x) = (1 - \kappa)V_* + \kappa P(x). \]

In the formula

\[ \Gamma'(k) = \int_0^\pi (u_2^2(x) - u_1^2(x)) (P(x) - V_*) \, dx \]

we choose

\[ P(x) = \begin{cases} V_*(x) & \text{on } [x_-, x_+]^c \\ \max (V_*(x_-), V_*(x_+)) & \text{on } [x_-, x_+]. \end{cases} \]

(7)

It can be seen that the functions \(V_*(\kappa) \in S_M\) for \(0 \leq \kappa \leq 1\), and that \(P(x) - V_*(x) \geq 0\) and is supported in \([x_-, x_+]\) (if not identically 0).

If \(V_*\) is not constant on \([x_-, x_+]\), then this implies that \(\Gamma'(0) < 0\), which contradicts the minimality of \(V_*\). We conclude that \(V_* = \text{cst a.e.}\) in \((x_-, x_+)\).
Next for $0 \leq x \leq x_-$, we choose $P(x) = V_\star(x_\star)$, and otherwise set $P(x) = V_\star(x)$, with which

$$
\Gamma'(k) = \int_0^\pi \left( u_2^2(x) - u_1^2(x) \right) (P(x) - V_\star(x)) \, dx \\
= \int_0^{x_-} \left( u_2^2(x) - u_1^2(x) \right) (V_\star(x_-) - V_\star(x)) \, dx \leq 0,
$$

and $\Gamma'(k) < 0$ unless $V(x)$ is constant on $(x_-, x_+)$. For $[x_+, \pi]$ the same argument applies.

The second possibility is that $a < x_-$. We let

$$
P(x) = \begin{cases} 
V_\star(a) & \text{if } 0 \leq x < a \\
V_\star(x) & \text{otherwise},
\end{cases} \quad (8)
$$

so that

$$
\Gamma'(k) = \int_0^\pi \left( u_2^2(x) - u_1^2(x) \right) (P(x) - V_\star(x)) \, dx \\
= \int_0^a \left( u_2^2(x) - u_1^2(x) \right) (V_\star(a) - V_\star(x)) \, dx \leq 0,
$$

and $\Gamma'(k) < 0$ unless $V(x)$ is constant on $(0, x_-)$. Alternatively, let

$$
P(x) = \begin{cases} 
V_\star(x) & \text{if } x < x_+ \\
V_\star(x_+) & \text{otherwise},
\end{cases} \quad (9)
$$

with which

$$
\Gamma'(k) = \int_0^\pi \left( u_2^2(x) - u_1^2(x) \right) (P(x) - V_\star(x)) \, dx \\
= \int_{x_+}^\pi \left( u_2^2(x) - u_1^2(x) \right) (V_\star(x_+) - V_\star(x)) \, dx \leq 0.
$$

Thus $\Gamma'(k) < 0$ unless $V(x) = \text{cst}$ on $(x_+, \pi)$.

The statement that the minimal gap decreases monotonically with respect to $M$ is elementary, since the set over which the minimum is sought is larger for larger $M$.

We turn now to the characterization of the minimizers under the assumptions that $p = 1$, $V_0 = 0$ and Dirichlet boundary conditions are imposed at 0 and $\pi$. The first item is what has been proved above, where we assumed without loss of generality, that the step function equals 0 on the interval $[0, x_-)$. (The other possibility is covered by $x \leftrightarrow \pi - x$, $x_- \leftrightarrow \pi - x_+$.)

In the next claim the upper bounds on $\lambda_{1,2}$ are immediate from the fact that the first and second eigenvalues with $V$ set to 0 are 1 and
4, and that $V_\star \leq M$ a.e. To establish that $\lambda_2 > M + 1$, recall that, according to the argument given above, the support of the minimizing step function for $V \in S_M$ contains $x_0$, the unique interior zero of $u_2$. Now, on the support of $V_\star$, the eigenfunction $u_2$ is a multiple of $\sin(\sqrt{\lambda_2 - M(\pi - x)})$, which cannot have a zero in supp$(V_\star)$ unless $\lambda_2 - M > 1$. The estimate $\lambda_1 > M - 2$ is a consequence of the fact that the minimal value of $\Gamma$ is less than the gap for the case $V \equiv 0$, which equals 3.

For the upper bound on $x_-$, we use the Rayleigh-Ritz inequality to estimate $\lambda_1$, choosing for the test function a normalization constant times $\chi_{[0,x_-]} \sin\left(\frac{\pi x}{x_-}\right)$. A calculation of the Rayleigh quotient for this function yields that

$$\lambda_1 \leq \left(\frac{\pi}{x_-}\right)^2.$$  

When combined with the inequality $\lambda_1 > M - 2$, the claimed upper bound on $x_-$ follows. (It requires only $M > 2$ rather than $M > \frac{7}{2}$, to be used later.)

The lower bound on $x_-$ and the final estimate require a fine analysis of the transcendental equations solved by the eigenvalues. On the interval $[0, x_-)$, the eigenfunctions that satisfy Dirichlet conditions are multiples of $\sin(\sqrt{\lambda x})$ whereas on $(x_-, \pi]$ they are multiples of $\sin(\sqrt{\lambda - M(\pi - x)})$ (assuming for now that $\lambda > M$). Since the eigenfunctions must be $C^1$, by equating their logarithmic derivatives at $x_-$, the eigenvalues are determined by the transcendental equation

$$\sqrt{\lambda} \cot\left(\sqrt{\lambda} x_\star\right) = -\sqrt{\lambda - M} \cot\left(\sqrt{\lambda - M(\pi - x_\star)}\right).$$  

(10)

(This holds for any step-function potential, regardless of whether $x_-$ satisfies the condition to minimize the gap, $(u_2(x_-))^2 - (u_1(x_-))^2 = 0$.) If $\lambda < M$, then the same argument leads to

$$\sqrt{\lambda} \cot\left(\sqrt{\lambda} x_\star\right) = -\sqrt{M - \lambda} \coth\left(\sqrt{M - \lambda(\pi - x_-)}\right).$$

There remains the possibility that $\lambda_1 = M$, and indeed an eigenfunction with this eigenvalue is possible if the eigenfunction is a multiple of $\sin(\sqrt{M} x)$ for $x \leq x_-$ and linear on $[x_-, \pi]$. The condition for this function to be $C^1$ is that $x_-$ have the value for which $\sqrt{M} \cot(\sqrt{M} x_-) = -\frac{\cos(\sqrt{M} x_-)}{\pi - x_-}$, or, after simplification, $\sqrt{M}(\pi - x_-) = -\sin(\sqrt{M} x_-)$. For large $M$, however, an eigenfunction of this type is in contradiction with the upper bound on $x_-$. (A calculation using Mathematica shows that $M > \frac{7}{2}$ more than suffices to eliminate the possibility of eigenfunctions of this type.)
Since the transcendental equations for $\lambda$ contain a large parameter $M$, we find it convenient to rescale them. With the substitutions
\[
 r^2 := \lambda - M, \\
 y := \sqrt{M} x, \\
 \mu := M^{-\frac{1}{2}}
\]
and some simple algebra, (10) takes on the form
\[
 \tan (r(\pi - \mu y)) + \mu \left( r / \sqrt{1 + \mu^2 r^2} \right) \tan \left( \sqrt{1 + \mu^2 r^2} y \right) = 0,
\]
provided that $\lambda > M \Leftrightarrow r > 0$. In the case that $\lambda_1 < M$, a similar calculation with $s^2 := M - \lambda$ leads to
\[
 \tanh (s(\pi - \mu y)) + \mu \left( s / \sqrt{1 - \mu^2 s^2} \right) \tan \left( \sqrt{1 - \mu^2 s^2} y \right) = 0.
\]

We continue now with a narrow examination of the pair of transcendental equations (11) and (12) in the limit of small $\mu$. For fixed $\mu$ and $y$, $\tan (r(\pi - \mu y))$ increases monotonically between a succession of vertical asymptotes, while the second term in (11) is continuous and of small magnitude. It is easy to see by considering the vertical asymptotes of the first function in (11) that solutions for $r$ occur near the positive integers. To have an eigenvalue gap $< 3$ we will need a solution for $r$ in the interval containing $r = 1$ to correspond to a sign-changing eigenfunction, which means that the ground-state eigenvalue, which does not change sign, must correspond to a solution of (12) with $s > 0$, i.e., $\lambda_1 < M$. A necessary condition for this, needed to make the second term negative, is for $y > \frac{\pi}{2}$, which is equivalent to the claimed lower bound on $x_-$ in the theorem. At the same time, we must have $y \leq \frac{\pi}{2} + O(\mu)$ to have a solution, because of the factor $\mu$ in the second term. To obtain a precise asymptotic estimate, we therefore set $y = \frac{\pi}{2} + y_1 \mu + O(\mu^2)$ and expand (11) and (12) with Taylor’s formula, keeping only leading terms. The results are
\[
 \tan(\pi r) \left(1 + O(\mu)\right) = -\frac{\mu r}{\cot \left( \frac{\pi}{2} + y_1 \mu \right)} \left(1 + O(\mu^2)\right)
\]
\[
 = \frac{\mu r}{\tan(y_1 \mu)} \left(1 + O(\mu^2)\right)
\]
\[
 = \frac{r}{y_1} \left(1 + O(\mu^2)\right),
\]
and, similarly,
\[
 \tanh(\pi s) \left(1 + O(\mu)\right) = \frac{s}{y_1} \left(1 + O(\mu^2)\right).
\]
Since our task is to minimize $\Gamma = r^2 + s^2$ as a function of $y$ as $\mu \to 0$, we may neglect higher-order terms and instead minimize $r^2 + s^2$, defined by the solutions of

$$\tan(\pi r) = \frac{r}{y_1}$$  \hspace{1cm} (13)

and

$$\tanh(\pi s) = \frac{s}{y_1}.$$  \hspace{1cm} (14)

Eq. (14) has no solutions for $s \geq 0$ unless $y_1 \geq \frac{1}{\pi} \approx 0.31831$. A simple upper limit on $y_1$ is provided by the value corresponding to $s = \frac{3}{2}$ in (14), viz.

$$\frac{3}{2 \tanh (\frac{3\pi}{2})} \approx 1.50024.$$  

By differentiating (13) and (14), applying the identities that

$$\frac{d}{dz} \tan(z) = 1 + \tan(z)^2, \quad \frac{d}{dz} \tanh(z) = 1 - \tanh(z)^2,$$

and algebraically arranging terms, we obtain

$$\frac{d}{dy_1} (r^2 + s^2) = \frac{2}{\pi} \left( \frac{s^2}{s^2 - \eta} - \frac{r^2}{r^2 + \eta} \right)$$

with $\eta := y_1 (y_1 - \frac{1}{\pi}) \geq 0$. Hence a critical point of the function $r^2 + s^2$ must satisfy

$$\frac{s^2}{s^2 - \eta} - \frac{r^2}{r^2 + \eta} = 0,$$

which is equivalent to

$$\frac{s^2}{r^2} = \frac{s^2 - \eta}{r^2 + \eta}.$$  \hspace{1cm} (15)

It is evident that a critical point requires $\eta = 0 \Leftrightarrow y_1 = \frac{1}{\pi}$ (which furthermore implies $s = 0$). Since a calculation shows that $r(1.50024)^2 + s(1.50024)^2 \approx 4.8171$, which is larger than 3, and there are no critical points for smaller values of $y_1 > \frac{1}{\pi}$, the remaining possibility for the minimal gap is $y_1 = \frac{1}{\pi}$. Having determined the next-order correction to $y$, we conclude:

$$V_\star(M) = M \chi_{x_-(M)}(x)$$

with

$$x_- = \frac{\pi}{2\sqrt{M}} + \frac{1}{\pi M} + \cdots,$$

and

$$\Gamma(V_\star(M)) = \left( \frac{\theta}{\pi} \right)^2,$$
proving the lower bound claimed in the theorem. We finally note that as $\mu \to 0$ the gap-minimizing potential energy does not have a sensible limit.

3.2. The class of convex potentials. We show in this section how Lavine’s result can be obtained and extended by our methods.

**Proposition 3.1.** Consider $V = V_0 + V_1$ where $V_1 \in C$ or $C_M$. If $V_1 = V_*$ minimizes $\Gamma(V)$, then $V_*$ cannot be strictly convex on any interval.

**Proof.** Suppose that $V_*$ were convex on an interval $I$. By passing to a subinterval if necessary, we can arrange that $u_2^2 - u_1^2$ does not change sign on $I$. We can then choose $P(x) \in C^2$, supp $P(x) \subset I$ and $P(x)(u_2^2 - u_1^2) < 0$ on $I$. By (4) $\Gamma'(0) < 0$, which is a contradiction. □

**Proposition 3.2.** $V_* = mx + b$.

**Proof.** We begin by recalling that a convex function has right and left derivatives at every interior point of an interval, with only at most a countable number of points at which the right and left derivatives can differ. Restating this in the language of distributions, we may write

$$V_*'' = \sum \alpha_n \delta(x - x_n), \quad \alpha_n \geq 0.$$ 

We need to show that all $\alpha_n = 0$.

Suppose that there exists $x_n \leq x_-$ or $x_n \geq x_+$ with $\alpha_n > 0$. Then, assuming $x_n \leq x_-$, consider a perturbation $P(x) := (x - x_n)\chi_{[0,x_n]}(x)$, which preserves convexity. Then

$$\Gamma'(0) = \int_0^{x_n} (x - x_n)(u_2^2 - u_1^2)dx < 0,$$

contradicting the assumed minimality of $\Gamma(V_0 + V_*)$. The same argument works assuming $x_n \geq x_+$. If $x_- < x_n < x_+$, then we take

$$P(x) = \begin{cases} \frac{x - x_-}{x_n - x_-} & \text{if } x < x_n \\ \frac{x - x_-}{x_n - x_+} & \text{if } x \geq x_n. \end{cases} \quad (16)$$

For small $t$, $V_*(x) + tP(x)$ is convex, but again

$$\Gamma'(0) = \int_0^{x_n} (x - x_n)(u_2^2 - u_1^2)dx < 0,$$

so this possibility also contradicts the assumed minimality. □
When $V_0 = 0$ as in [9], a particular argument is needed to establish that $m = 0$, i.e., that the optimal potential is a constant. This is generally not the case when there is a background potential $V_0$, as can be seen from the trivial example where $V_0 = x$: In this example, $V_\ast$ must equal $-x + b$, because of the original result of [9].

Lastly, we turn to the question about what happens if there is no finite upper bound $M$. In prior work going back to Lavine it has been customary to assume without comment that $V(x)$ is continuous on the closed interval $[0, \pi]$, and therefore bounded. This leaves open the possibility that there are convex, resp. single-well potentials, which diverge to $+\infty$ as $x$ tends to 0 or $\pi$, which have lower fundamental gaps than the lim-inf of the minimal gaps for $M < \infty$. In our next result we show that this is not possible. For simplicity we restrict ourselves to Liouville normal form and Dirichlet boundary conditions.

**Theorem 3.3.** Consider the eigenvalue problem

$$H(1, V)u = \lambda u,$$

with homogeneous Dirichlet boundary conditions at 0 and $\pi$, and $V(x) \geq 0$ either convex or of single-well form. Then for any $\epsilon > 0$ and $M > \lambda_2(V)$, there exists $V_{M, \epsilon} \in S_M$ or respectively $V_{M, \epsilon} \in C_M$, such that $\lambda_k(V) - \epsilon \leq \lambda_k(V_{M, \epsilon}) \leq \lambda_k(V)$ for $k = 1, 2$.

**Proof.** We consider the case where $\lim_{x \downarrow 0} V(x) = +\infty$; the case where there is a divergence as $x \uparrow \pi$ is the same after a simple change of variable. We also assume without loss of generality that $\min V = 0$ and that $u_{1,2} > 0$ on a neighborhood of 0. We begin by observing if $V \geq 0$ on $[0, \pi]$, then there exists a constant $C$ independent of $V$ such that the normalized eigenfunctions satisfy

$$\|u_k\|_{\infty} \leq C \lambda_k^{1/2}.$$

(In Example 2.1.8 of [6] this is shown with $C = e^{1/8\pi}$.)

Because $V$ diverges at 0, there is an interval $[0, \ell]$, $\ell > 0$ on which $V - \lambda_2 \geq 0$, and therefore $u_{1,2}$ are convex. In particular, for any $\ell_0 < \ell$, if $x < \ell_0$, then

$$\psi'(x) \leq \frac{\psi(\ell)}{\ell - x}.$$

This estimate holds for any $\tilde{V}$ such that $\tilde{V} > \lambda_2$ for $x < \ell_0 < \ell$, not only for the originally assumed $V$.

We first consider the case of single-well potentials and finish the argument. Fix some $M > \lambda_2(V)$ and consider the perturbation where

$$V(x) \to V(\kappa, x) := (1 - \kappa)V(x) + \kappa M.$$
when \( x \leq \ell_1 \) but leaving \( V \) unchanged for larger \( x \). This family of functions is of single-well form for all \( 0 \leq \kappa \leq 1 \) and is nonincreasing in \( \kappa \). Here \( \ell_1 < \ell/2 \) will be chosen later depending on \( \epsilon \). According to (4),

\[
\lambda_k'(\kappa) = -\int_0^{\ell_1} u_k^2(x) (V(x) - M) \, dx < 0,
\]

for all \( 0 \leq \kappa \leq 1 \). On the other hand,

\[
\lambda_k'(\kappa) = -\int_0^{\ell_1} u_k^2(x) (V(x) - M) \, dx \\
\geq -\int_0^{\ell_1} u_k^2(x) (V(x) - \lambda_k(\kappa)) \, dx \\
= -\int_0^{\ell_1} u_k(x) u_k''(x) \, dx \\
= -\int_0^{\ell_1} (u_k(x) u_k'(x))' \, dx + \int_0^{\ell_1} (u_k'(x))^2 \, dx \\
\geq -u_k(\ell_1) u_k'(\ell_1).
\]

(For notational simplicity we have not indicated explicitly the dependence of these eigenfunctions on \( \kappa \).) Appealing to the convexity of the eigenfunctions and knowing that their maximum is not attained in the interval \([0, \ell]\), we get

\[
\lambda_k' \geq -\left( C \lambda_2^{\frac{1}{4}} \right)^2 \frac{\ell_1}{\ell} \frac{\ell/2 - \ell_1}{\ell/2}.
\]

Finally, for any \( \epsilon > 0, \epsilon < 1 \), we can choose

\[
\ell_1 \leq \frac{\ell}{\left( C \lambda_2^{\frac{1}{4}} \right)^2 + 2} \epsilon
\]

to conclude that

\[
\lambda_k' \geq -\epsilon.
\]

The claim follows by defining \( V_M = V(1, x) \) and observing that

\[
\lambda_k(V_M) = \lambda_k(V) + \int_0^1 \lambda'(\kappa) \, d\kappa.
\]

A closely similar argument yields the same conclusion for convex potentials, except that the perturbation must now preserve convexity rather than the single-well property. A suitable family of perturbations is

\[
V(x) \to V(\kappa, x) := (1 - \kappa)V(x) + \kappa (V(\ell) + V'(\ell)(x - \ell))
\]
on a sufficiently small interval $[0, \ell]$ to guarantee that $V_{M, \epsilon} > M > \lambda_2(M)$. We omit the details, being quite similar to the case treated above.

In particular, when $V_0 = 0$, then Lavine's result that the constant potentials are the (only) minimizers of the fundamental gap holds without the assumption that $V(x)$ is continuous at $x = 0$ and $\pi$, at least with Dirichlet boundary conditions.

Acknowledgments. The authors wish to thank Joachim Stubbe and Timo Weidl for useful conversations and insights.

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