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A LOWER BOUND FOR THE GROUND STATE ENERGY OF A SCHRÖDINGER OPERATOR ON A LOOP

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Abstract. Consider a one-dimensional quantum mechanical particle described by the Schrödinger equation on a closed curve of length 2π. Assume that the potential is given by the square of the curve's curvature. We show that in this case the energy of the particle cannot be lower than 0.6085. We also prove that it is not lower than 1 (the conjectured optimal lower bound) for a certain class of closed curves that have an additional geometrical property.

1. Introduction

Let Γ be a smooth closed curve of length 2π in the plane with the curvature $\kappa(s)$ which is regarded as a function of the arc length. We consider the Schrödinger operator

$$H_\Gamma = -\Delta + \kappa^2(s) \quad \text{in} \quad L^2([0, 2\pi))$$

with periodic boundary conditions. Let λ_Γ be the lowest eigenvalue of H_Γ. It has been conjectured that $\lambda_\Gamma \geq 1$ for any Γ. The class F of the conjectured minimizers of λ_Γ contains the circle and certain point-symmetric oval loops. For all curves in F the equality $\lambda_\Gamma = 1$ holds, but so far it has not been shown that this is actually the smallest possible value of λ_Γ. In their paper [1] Benguria and Loss established a connection between this problem and the Lieb-Thirring conjecture in one dimension. They also proved that $\lambda_\Gamma \geq 0.5$, which seems to be the best lower bound for λ_Γ so far.

Recently, Burchard and Thomas have shown [2] that the curves in F minimize λ_Γ at least locally, i.e., there is no small variation around these curves that reduces λ_Γ. In the present article we will add further credibility to the mentioned conjecture in two ways. On the one hand, we show that $\lambda_\Gamma \geq 1$ holds for a considerable class of curves that meet a certain additional geometrical condition. Extending this method to the class of all curves of interest yields, on the other hand, an improved lower bound on λ_Γ.

2. Statement of the result

For a given smooth curve Γ with an arc length parameter s, we introduce the angle $\phi(s)$ between the tangent on Γ in s and some fixed axis, which implies $\phi'(s) =$

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$\kappa(s)$. For the sake of simplicity we will only consider strictly convex curves, i.e., $\phi' > 0$. To keep the notation compact we write

$$\phi : \Omega \to \Omega \quad \text{with} \quad \Omega := \mathbb{R}/2\pi\mathbb{Z},$$

considering numbers that differ by an integer multiple of 2π as identical. Our main result is:

Theorem 2.1. *Let Γ be a smooth, strictly convex, closed curve of length 2π in the plane and λ_Γ defined as above. Then*

$$\lambda_\Gamma > \left(1 + \frac{1}{1 + 8/\pi}\right)^{-2} > 0.6085.$$

In the proof of Theorem 2.1 we will make use of the following geometrical concept: We call $s \in \Omega$ a 'critical point' of Γ if $\phi(s+\pi) = \phi(s) + \pi$. Obviously, $s + \pi$ is then also a critical point. If s is a critical point, we call $\phi(s)$ a 'critical angle'. While open curves may have no critical points at all, the following lemma holds for the closed curves we are considering.

Lemma 2.2. *Every smooth closed curve Γ has at least six critical points.*

It is clear from the definition of a critical point and the lemma that every Γ has at least three critical points and three critical angles in $[s, s+\pi) \subset \Omega$ for any $s \in \Omega$. For a class of curves that have their critical angles distributed somewhat evenly, we can show that $\lambda_\Gamma \geq 1$ holds:

Theorem 2.3. *Let Γ be as in Theorem 2.1 and assume additionally that every interval $[\phi, \phi + \frac{\pi}{2}) \subset \Omega$ contains at least one critical angle of Γ. Then $\lambda_\Gamma \geq 1$.*

It is an immediate consequence of Theorem 2.3 and Lemma 2.2 that for any hypothetical curve Γ with $\lambda_\Gamma < 1$ there is a ϕ such that $[\phi, \phi + \frac{\pi}{2})$ and $[\phi + \pi, \phi + \frac{3\pi}{2})$ each contain at least three critical angles and $[\phi + \frac{\pi}{2}, s + \pi) \cup [\phi + \frac{3\pi}{2}, \phi + 2\pi)$ none. A few comments on the geometrical interpretation of the above are in order: Although we have defined the critical points for a certain parameterization of the curve, the location of the critical points is an intrinsic property of the curve. More precisely, two points P_1 and P_2 on a closed curve of length 2π are critical, if the arc length between P_1 and P_2 is π and the tangents in these two points are parallel.

From Theorem 2.3 it follows that only curves with a rather uneven distribution of their critical points are candidates for $\lambda_\Gamma < 1$. Roughly speaking, such curves tend to be rather symmetric, as will become clear in the proof of Theorem 2.1. In fact, the function f, that we will define and estimate in the proof, can in some sense be seen as a measure for how far away Γ is from being point-symmetric. This, on the other hand, will enable us to estimate how far λ_Γ could be below one.

We are not aware of any direct correlation between the distribution of the critical points and the ground state energy λ_Γ, except the connection that is established by Theorem 2.3, of course. There seems to be no reason why the condition of Theorem 2.3 should 'prefer' curves with a high energy, especially if one takes into account that the conjectured minimizers meet this condition. We believe that this makes the conjecture $\lambda_\Gamma \geq 1$ even more credible.

The remainder of the article is devoted to proving Lemma 2.2 and the two theorems.

3. Proof of the results

To prepare the proofs of Lemma 2.2 and the two theorems we introduce some more notation: We consider a curve Γ as in Theorem 2.1 and assume without loss of generality that $\phi' > 0$. Because Γ is closed, ϕ meets the conditions

$$\int_\Omega \cos\phi(s)\,\mathrm{d}s = \int_\Omega \sin\phi(s)\,\mathrm{d}s = 0,$$
$$\int_\Omega \phi'(s)\,\mathrm{d}s = 2\pi.$$

We note that $\phi(s)$ has an inverse function $\phi^{-1} : \Omega \to \Omega$, and the closure conditions are equivalent to

$$\int_\Omega (\phi^{-1})'(t)\sin t\,\mathrm{d}t = \int_\Omega (\phi^{-1})'(t)\cos t\,\mathrm{d}t = 0,$$
$$\int_\Omega (\phi^{-1})'(t)\,\mathrm{d}t = 2\pi.$$

The function $(\phi^{-1})'$ can therefore be written as a Fourier series

$$(\phi^{-1})'(t) = 1 + \sum_{n=2}^{\infty} na_n\cos nt - nb_n\sin nt,$$

such that

$$\phi^{-1}(t) = C + t + \sum_{n=2}^{\infty} a_n\sin nt + b_n\cos nt.$$

By the invariance of the problem under a shift of the arc length parameter s, we can assume that $C = 0$. Then we can write ϕ^{-1} in the form

$$\phi^{-1}(t) = t + g(t) + f(t), \tag{3.1}$$

where

$$g(t) := \sum_{n=2,4,6,\ldots}^{\infty} a_n\sin nt + b_n\cos nt,$$
$$f(t) := \sum_{n=3,5,7,\ldots}^{\infty} a_n\sin nt + b_n\cos nt.$$

Note that

$$f(t+\pi) = -f(t), \quad g(t+\pi) = g(t) \quad \text{for all} \quad t\in\Omega. \tag{3.2}$$

Proof of Lemma 2.2. From (3.1) and (3.2) it is easy to see that the critical angles of Γ are just the zeroes of f. By continuity of f and (3.2), any nontrivial f clearly has at least two zeroes t_0 and $t_0+\pi$ in Ω with a change of sign. But if these were the only zeroes, we would have

$$\int_\Omega f(t)\sin(t-t_0)\,\mathrm{d}t \neq 0,$$

which is impossible by the definition of f. So f must change its sign in at least one more point. By the symmetry property (3.2) it is clear that if, say, $f(t_0+\epsilon) > 0$, then $f(t_0+\pi-\epsilon) > 0$ for small $\epsilon > 0$. That means that each of the intervals $(t_0, t_0+\pi)$ and $(t_0+\pi, t_0+2\pi)$ contains an even number of zeroes with a change of sign. In total, this leads to a minimum of six zeroes of f with a change of sign. $\square$

We now state and prove a lemma that is key to the proofs of Theorem 2.1 and Theorem 2.3.

Lemma 3.1. *Let* Γ *be as in Theorem* 2.1 *and let* $\{t_i\}_{i=1,\dots,n} \subset \Omega$ *be a set of numbers such that* $[t, t+\frac{\pi}{2}] \cap \{t_i\} \neq \emptyset$ *for all* $t \in \Omega$. *Assume that* $|f(t_i)| \leq \alpha$ *for all* i. *Then*

$$\lambda_\Gamma \geq (1 + 2\alpha/\pi)^{-2}.$$

Proof. Comparing (3.2) with (3.1) we see that

$$\phi^{-1}(t+\pi) = \phi^{-1}(t) + \pi - 2f(t) \quad \text{for all } t \in \Omega. \tag{3.3}$$

Now assume $R(s) > 0$ to be the ground state of H_Γ and define the functions

$$x(s) := R(s)\cos\phi(s), \quad y(s) := R(s)\sin\phi(s).$$

Interpreted as Euclidean coordinates, x and y define a closed curve in the plane. In these coordinates the lowest eigenvalue λ_Γ of H_Γ is

$$\lambda_\Gamma = \frac{\int_\Omega \left(R'(s)^2 + \phi'(s)^2 R(s)^2\right) \mathrm{d}s}{\int_\Omega R(s)^2 \,\mathrm{d}s} = \frac{\int_\Omega \left(x'(s)^2 + y'(s)^2\right) \mathrm{d}s}{\int_\Omega \left(x(s)^2 + y(s)^2\right) \mathrm{d}s}. \tag{3.4}$$

We now define the orthogonal projections of the curve $(x(s), y(s))$ onto straight lines through the origin:

$$h_\beta(s) := \begin{pmatrix} \sin\beta \\ -\cos\beta \end{pmatrix} \cdot \begin{pmatrix} x(s) \\ y(s) \end{pmatrix} = x(s)\sin\beta - y(s)\cos\beta. \tag{3.5}$$

We note that

$$h_\beta(\phi^{-1}(\beta)) = 0$$

and, by (3.3),

$$h_\beta(\phi^{-1}(\beta) + \pi - 2f(\beta)) = h_\beta(\phi^{-1}(\beta+\pi)) = 0.$$

This means that the quantity

$$I(\beta) := \frac{\int_\Omega h'_\beta(s)^2 \,\mathrm{d}s}{\int_\Omega h_\beta(s)^2 \,\mathrm{d}s}, \tag{3.6}$$

which is the Rayleigh-Ritz quotient for the Laplacian on Ω with Dirichlet conditions at $\phi^{-1}(\beta)$ and $\phi^{-1}(\beta) + \pi - 2f(\beta)$, can be estimated from below by

$$I(\beta) \geq \left(1 + \frac{2|f(\beta)|}{\pi}\right)^{-2}. \tag{3.7}$$

Now we consider two cases: First, assume that there is no β_0 for which $I(\beta_0) = (1 + 2\alpha/\pi)^{-2}$. It is clear that $I(\beta) = 1$ if β is a zero of f and we know that such a zero exists. By continuity of $I(\beta)$ in β we conclude that in this case $I(\beta) > (1 + 2\alpha/\pi)^{-2}$ for all $\beta \in \Omega$. Choosing first $\beta = \pi/2$ and then $\beta = 0$ yields

$$\frac{\int_\Omega x'^2 \,\mathrm{d}s}{\int_\Omega x^2 \,\mathrm{d}s} \geq (1 + 2\alpha/\pi)^{-2} \quad \text{and} \quad \frac{\int_\Omega y'^2 \,\mathrm{d}s}{\int_\Omega y^2 \,\mathrm{d}s} \geq (1 + 2\alpha/\pi)^{-2},$$

such that $\lambda_\Gamma \geq (1 + 2\alpha/\pi)^{-2}$ by (3.4).

In the second case there is a β_0 with $I(\beta_0) = (1 + 2\alpha/\pi)^{-2}$, and by rotational symmetry of the problem we can assume that $\beta_0 = 0$, i.e.,

$$I(0) = \frac{\int_\Omega {y'}^2 \, \mathrm{d}s}{\int_\Omega y^2 \, \mathrm{d}s} = (1 + 2\alpha/\pi)^{-2}. \tag{3.8}$$

Now put (3.5) and (3.6) into (3.7) and set $\beta = t_i$ to get

$$\int_\Omega (-x' \sin t_i + y' \cos t_i)^2 \, \mathrm{d}s \geq (1 + 2\alpha/\pi)^{-2} \int_\Omega (-x \sin t_i + y \cos t_i)^2 \, \mathrm{d}s.$$

Using (3.8) this becomes

$$\int_\Omega {x'}^2 \, \mathrm{d}s \geq (1 + 2\alpha/\pi)^{-2} \left(\int_\Omega x^2 \, \mathrm{d}s + \frac{2}{\tan t_i} \int_\Omega (x'y' - xy) \, \mathrm{d}s \right). \tag{3.9}$$

Because of the conditions on the distribution of the t_i in Ω we can choose i such that the second summand in the bracket on the right side of (3.9) is positive. Thus,

$$\int_\Omega {x'}^2 \, \mathrm{d}s \geq (1 + 2\alpha/\pi)^{-2} \int_\Omega x^2 \, \mathrm{d}s. \tag{3.10}$$

Lemma 3.1 now follows from the combination of (3.8) with (3.10). □

Proof of Theorem 2.3. Let $\{t_i\}_{i=1,\ldots,n} \subset \Omega$ be the set of critical angles of Γ. Then by the assumption of Theorem 2.3 this set also meets the conditions of Lemma 3.1. Being critical angles, the t_i's satisfy $f(t_i) = 0$. Thus α in Lemma 3.1 can be chosen to be zero, and Theorem 2.3 follows. □

Proof of Theorem 2.1. To prove Theorem 2.1 we will derive estimates on the function $f(t)$ as defined in (3.1) and then apply Lemma 3.1. It is obvious that we only have to consider curves that are not covered by Theorem 2.3. This means that our Γ has an interval larger than $\frac{\pi}{2}$ without critical angles. Recall that the critical angles of Γ are just the zeroes of f. We will thus assume, without losing generality, that t_0 (with $0 < t_0 < \frac{\pi}{2}$) and π are zeroes of f with a change of sign and that $f(t) > 0$ for $t \in (t_0, \pi)$. We define $\Omega_0 := [t_0, \pi]$. Let Ω_+ and Ω_- be the sets of all points $t \in [0, t_0)$ where $f(t)$ is positive or negative, respectively. Let us now collect some information on f:

First, we show that

$$\int_\Omega |f'(t)| \, \mathrm{d}t \leq 2\pi. \tag{3.11}$$

To do so, we note that $(\phi^{-1})' > 0$ because we assumed $\phi' > 0$ earlier. By (3.1) this means

$$f'(t) + g'(t) > -1 \quad \text{for all}\, t \in \Omega.$$

But, applying (3.2) to this inequality, we also get

$$-f'(t) + g'(t) > -1 \quad \text{for all}\, t \in \Omega.$$

Putting together the last two inequalities, we get

$$|f'(t)| < 1 - g'(t) \quad \text{for all}\, t \in \Omega.$$

Integrating over Ω and keeping in mind the periodicity of g yields (3.11).

Second, we note that for any $\Delta, t_0 \in \Omega$

$$
\begin{aligned}
0 &= \int_\Omega f(t)\sin(t+\Delta)\,\mathrm{d}t \\
&= \int_{t_0}^{t_0+\pi} f(t)\sin(t+\Delta)\,\mathrm{d}t + \int_{t_0+\pi}^{t_0+2\pi} f(t)\sin(t+\Delta)\,\mathrm{d}t \\
&= 2\int_{t_0}^{t_0+\pi} f(t)\sin(t+\Delta)\,\mathrm{d}t. \qquad (3.12)
\end{aligned}
$$

Third, let us assume that there is an interval $[t_1, t_1+\frac{\pi}{2}] \subset \Omega_0$ with $f(t) > \alpha$ on $[t_1, t_1+\frac{\pi}{2}]$ for some $\alpha \in \mathbb{R}$. Then

$$
\int_{\Omega_+} f(t)\,\mathrm{d}t \geq \alpha \quad \text{and} \quad -\int_{\Omega_-} f(t)\,\mathrm{d}t \geq \alpha. \qquad (3.13)
$$

This can be seen with the help of (3.12) via

$$
\begin{aligned}
0 &= \int_0^\pi f(t)\sin(t-t_0)\,\mathrm{d}t \\
&= \int_{\Omega_+} f(t)\sin(t-t_0)\,\mathrm{d}t + \int_{\Omega_-} f(t)\sin(t-t_0)\,\mathrm{d}t + \int_{\Omega_0} f(t)\sin(t-t_0)\,\mathrm{d}t \\
&\geq -\int_{\Omega_+} f(t)\,\mathrm{d}t + \alpha\int_{t_1}^{t_1+\pi/2} \sin(t-t_0)\,\mathrm{d}t \\
&\geq -\int_{\Omega_+} f(t)\,\mathrm{d}t + \alpha\int_0^{\pi/2} \sin(t)\,\mathrm{d}t \\
&= -\int_{\Omega_+} f(t)\,\mathrm{d}t + \alpha.
\end{aligned}
$$

The corresponding inequality for Ω_- is proven analogously, exploiting once again (3.2).

Because f vanishes at the edges of Ω_0 and because $\max\limits_{t\in\Omega_0} f(t) > \alpha$, it is clear that

$$
\int_{\Omega_0} |f'(t)|\,\mathrm{d}t > 2\alpha.
$$

From (3.13) we conclude that the inequalities

$$
\max_{t\in\Omega_+} f(t) \geq \frac{\alpha}{|\Omega_+|} \quad \text{and} \quad \max_{t\in\Omega_-} |f(t)| \geq \frac{\alpha}{|\Omega_-|}
$$

hold. Therefore

$$
\begin{aligned}
\int_\Omega |f'(t)|\,\mathrm{d}t &= 2\left(\int_{\Omega_0} |f'(t)|\,\mathrm{d}t + \int_{\Omega_+} |f'(t)|\,\mathrm{d}t + \int_{\Omega_-} |f'(t)|\,\mathrm{d}t\right) \\
&\geq 2\left(2\alpha + 2\frac{\alpha}{|\Omega_+|} + 2\frac{\alpha}{|\Omega_-|}\right) \\
&> 4\alpha\left(1+\frac{8}{\pi}\right). \qquad (3.14)
\end{aligned}
$$

In the last step we have used $|\Omega_+| + |\Omega_-| < \frac{\pi}{2}$. Comparing (3.14) with (3.11) shows that

$$
\alpha < \frac{\pi}{2(1+8/\pi)}.
$$

We conclude that for any curve Γ we can can find a sequence $\{t_i\}$ that meets the conditions of Lemma 3.1 for some $\alpha < \frac{\pi}{2(1+8/\pi)}$, proving Theorem 2.1. $\square$

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