# LIEB-THIRRING INEQUALITIES ON TRAPPED MODES IN QUANTUM WIRES

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ABSTRACT. We prove Lieb-Thirring type bounds on the discrete spectrum of Schrödinger operators on tube-like domains and give explicit estimates on the constants involved.

## 1. INTRODUCTION

Let $\omega$ be a connected, bounded, and open set in $\mathbb{R}^{d-1}$. Consider the tube $\Omega = \omega \times \mathbb{R} \subset \mathbb{R}^d$ generated by the cross section $\omega$. Let $-\Delta^\omega$ and $-\Delta^\Omega$ be the Dirichlet Laplacians on $L^2(\omega)$ and $L^2(\Omega)$, respectively.

The spectrum of the operator $-\Delta^\omega$ is discrete. Let $\{\mu_k\}_{k=1}^\infty$ be the ordered sequence of its eigenvalues (counting multiplicities) and let $\{\psi_k\}_{k=1}^\infty$be a corresponding ortho-normed eigenbasis in $L^2(\omega)$. These give rise to generalized eigenfunctions

$$\psi_k(x')e^{i\xi x_d}, \quad x = (x', x_d),\ x' = (x_1, \dots, x_{d-1}),$$

for the operator $-\Delta^\Omega$ on $L^2(\Omega)$. Hence, by separation of variables, the spectrum of $-\Delta^\Omega$ is purely absolutely continuous and consists of the eigenvalue branches $[\mu_k, \infty)$. In particular, the point $\mu_1 > 0$ is the lower bound of the spectrum of $-\Delta^\Omega$.

If we perturb the operator $-\Delta^\Omega$ by some real-valued attractive potential $-\alpha V \le 0$, the resulting Schrödinger operator

$$H_\alpha^\Omega = -\Delta^\Omega - \alpha V, \quad \alpha > 0, \tag{1}$$

with Dirichlet boundary conditions on $L^2(\Omega)$ will have spectrum below the threshold $\mu_1$. Under certain regularity and decay assumptions on $V$ this portion of the spectrum is discrete. Let $\{\lambda_n(\alpha)\}$ stand for the respective non-decreasing sequence of the eigenvalues of $H_\alpha^\Omega$ below $\mu_1$ (counting multiplicities). In this paper we study Lieb-Thirring type bounds on the spectral moments[1]

$$S_\gamma^\Omega(\alpha) = tr(H_\alpha^\Omega - \mu_1)_-^\gamma = \sum_n (\mu_1 - \lambda_n(\alpha))^\gamma, \quad \gamma \ge 0,$$

[1]We use the notation $x_\pm = (|x| \pm x)/2$.

for tube-like domains $\Omega = \omega \times \mathbb{R}$. Such estimates are of interest, since the operators $H_\alpha^\Omega$ can model various effects in quantum wires.

Compared with the usual Schrödinger operator on $L^2(\mathbb{R}^d)$, the spectral behaviour of $H_\alpha^\Omega$ reflects the mixed dimensionality of the tube $\Omega$. One the one hand, as for any open domain, for sufficiently regular $V$ the quantity $S_\gamma^\Omega(\alpha)$ shows the $d$-dimensional large coupling Weyl asymptotics

$$S_\gamma^\Omega(\alpha) = (1+o(1))S_{\gamma,d}^{cl}(\alpha) \quad \text{as} \quad \alpha \to \infty, \tag{2}$$

where

$$S_{\gamma,d}^{cl}(\alpha) = \int\int (|\xi|^2 - \alpha V(x))_-^\gamma \frac{dxd\xi}{(2\pi)^d} = \alpha^{\gamma+\frac{d}{2}} L_{\gamma,d}^{cl} \int V_+^{\gamma+\frac{d}{2}} dx \tag{3}$$

and

$$L_{\gamma,d}^{cl} = \frac{\Gamma(\gamma+1)}{2^d \pi^{d/2} \Gamma(\gamma+\frac{d}{2}+1)}.$$

On the other hand, in the weak coupling limit $\alpha \to 0$ the ground state of $H_\alpha^\Omega$ will extend longitudinally in the tube and its respective asymptotics is similar to that of a one-dimensional Schrödinger operator. Namely, if $V \geq 0$ is continuous and compactly supported, then for sufficiently small $\alpha > 0$ the operator $H_\alpha$ has exactly one bound state $\lambda_1(\alpha)$ below $\mu_1$ and

$$S_{1/2}^\Omega(\alpha) = \frac{\alpha}{2} \int_\omega \int_{-\infty}^{+\infty} V(x', x_d) |\psi_1(x')|^2 dx' dx_d + O(\alpha^2) \tag{4}$$

as $\alpha \to 0+$ [11, 3]. Similar weak coupling asymptotics are valid also if the perturbation is of a geometric rather than potential type [1, 3, 4].

An appropriate estimate should reflect this behaviour. Accordingly we prove a two-term Lieb-Thirring formula. The first term has the homogeneity of order $\alpha^{\gamma+\frac{1}{2}}$ and stands for the one-dimensional effects. The second one is a multiple of the phase space average $S_{\gamma,d}^{cl}(\alpha)$ and controls the large coupling behaviour. The sum of both gives a uniform bound on $S_\gamma^\Omega(\alpha)$ for all $\alpha \geq 0$.

Because of the one-dimensional effects, these spectral estimates hold for $\gamma \geq 1/2$ only. This agrees with the validity range of the usual Lieb-Thirring estimates in dimension one (see section 2). In particular, if $\gamma = 1/2$ then the one-dimensional term captures the asymptotics (4) and the constant in front of it is almost sharp. Based on [7, 5] we provide also reasonable explicit estimates on the constants for the semiclassical term.

## 2. Lieb-Thirring bounds on $L^2(\mathbb{R}^d)$

In this section we collect auxiliary material on Lieb-Thirring estimates on $L^2(\mathbb{R}^d)$, which shall be of use below. Usually these inequalities concern

the operator

$$H_\alpha = -\Delta - \alpha V \quad \text{on} \quad L^2(\mathbb{R}^d).$$

Assume that $V \geq 0$, $\alpha \geq 0$, and put

$$S_\gamma(\alpha) = tr\,(H_\alpha)_-^\gamma.$$

Then for $\gamma \geq 1/2$ if $d = 1$, for $\gamma > 0$ if $d = 2$, and for $\gamma \geq 0$ if $d \geq 3$, the inequality

$$S_\gamma(\alpha) \leq R(\gamma, d) S_\gamma^{cl}(\alpha) \tag{5}$$

holds true [9, 2, 8, 10]. For all other pairs of $\gamma$ and $d$ the estimate (5) fails.

The bound (5) agrees with the asymptotics (2), which on its turn implies $R(\gamma, d) \geq 1$. We mention the following known estimates for the constants $R(\gamma, d)$ in (3)

$$R(\gamma, d) = 1 \quad \text{if} \quad \gamma \geq 3/2,\ d \in \mathbb{N}, \tag{6}$$

$$R(\gamma, d) \leq 2 \quad \text{if} \quad 1 \leq \gamma < 3/2,\ d \in \mathbb{N}, \tag{7}$$

$$R(\gamma, d) \leq 2 \quad \text{if} \quad 1/2 \leq \gamma < 1,\ d = 1, \tag{8}$$

$$R(\gamma, d) \leq 4 \quad \text{if} \quad 1/2 \leq \gamma < 1,\ d \in \mathbb{N},\ d \geq 2, \tag{9}$$

see [7, 5, 6].

We point out that for $\gamma = 1/2$, $d = 1$ and non-negative integrable potentials $V$ actually a two-sided Lieb-Thirring bound [12, 6]

$$S_{1/2}^{cl}(\alpha) \leq S_{1/2}(\alpha) \leq 2 S_{1/2}^{cl}(\alpha), \quad \alpha \geq 0, \tag{10}$$

holds. Both constants are sharp and

$$S_{1/2}(\alpha) = S_{1/2}^{cl}(\alpha)(1 + o(\alpha)) \quad \text{as} \quad \alpha \to \infty, \tag{11}$$

$$S_{1/2}(\alpha) = 2 S_{1/2}^{cl}(\alpha)(1 + o(\alpha)) \quad \text{as} \quad \alpha \to 0. \tag{12}$$

Along with (5) we shall need the following generalization to Schrödinger operators with operator-valued potentials. Namely, let $G$ be a separable Hilbert space and let $W$ be a function on $\mathbb{R}^d$ which takes a.e. non-negative compact operators on $G$ as its values. We consider eigenvalue moments of the Schrödinger type operator

$$Z = 1_G \otimes (-\Delta) - W(x) \quad \text{on} \quad G \otimes L^2(\mathbb{R}^d).$$

Assume that $tr_G W^{\gamma + \frac{d}{2}}(\cdot) \in L^{\gamma + \frac{d}{2}}(\mathbb{R}^d)$. Then for $\gamma \geq 1/2$ if $d = 1$, and for $\gamma > 0$ if $d \geq 2$, the following estimate holds true:

$$tr_{G \times L^2(\mathbb{R}^d)}\, Z_-^\gamma \leq r(\gamma, d) L_{\gamma, d}^{cl} \int_{\mathbb{R}^d} tr_G\, W^{\gamma + \frac{d}{2}}(x) dx. \tag{13}$$

The constants $r(\gamma, d)$ satisfy the inequalities (6)-(9) if one replaces $R(\gamma, d)$ by $r(\gamma, d)$. For the proof of this generalization we refer to [7] for $\gamma \geq 3/2$ and to [5] for $1/2 \leq \gamma < 3/2$.

While the validity of (5) is settled, it seems not to be clear whether (13) holds for $\gamma = 0$ and $d \geq 3$.[2] Moreover, it is obvious that $R(\gamma, d) \leq r(\gamma, d)$. In all cases where their sharp values are known, these constants coincide. However, to our knowledge it is not clear whether $R(\gamma, d) = r(\gamma, d)$ holds in general.

## 3. Statement of the Result

The main result of this paper is the following:

**Theorem.** *Let us assume that $\Omega = \omega \times \mathbb{R}$, $V \geq 0$, and $V \in L^{\gamma+\frac{d}{2}}(\Omega) \cap L^{\gamma+\frac{1}{2}}(\mathbb{R}, dx_d; L^2(\omega, |\psi_1(x')|^2 dx'))$. Then for $\gamma \geq 1/2$, $\alpha \geq 0$, and all $\epsilon > 0$ the following estimate holds true*

(14)

$$S^{\Omega}_{\gamma}(\alpha) \leq c_1 \alpha^{\gamma+\frac{1}{2}} \int_{\mathbb{R}} \left( \int_{\omega} V(x', x_d) |\psi_1(x')|^2 dx' \right)^{\gamma+\frac{1}{2}} dx_d + c_2 S^{cl}_{\gamma,d}(\alpha).$$

*The constants $c_1$ and $c_2$ satisfy the bounds*

$$\begin{aligned} c_1 &\leq (1+\epsilon)^{\gamma+\frac{1}{2}} r(\gamma, 1) L^{cl}_{\gamma,1}, \\ c_2 &\leq (1+\epsilon^{-1})^{\gamma+\frac{d}{2}} \left( \frac{\mu_2}{\mu_2 - \mu_1} \right)^{\frac{d-1}{2}} r(\gamma, 1) R(\gamma + \frac{1}{2}, d-1), \end{aligned}$$

*where $R(\cdot, \cdot)$ are the sharp constant in (5) and $r(\cdot, \cdot)$ are the sharp constants in (13).*

*Remark.* If $\gamma = 1/2$ then (14) gives rise to

$$\begin{aligned} S^{\Omega}_{1/2}(\alpha) &\leq (1+\epsilon) \frac{\alpha}{2} \int_{\Omega} V(x', x_d) |\psi_1(x')|^2 dx \\ &\quad + 4(1+\epsilon^{-1})^{\frac{d+1}{2}} \alpha^{\frac{d+1}{2}} \left( \frac{\mu_2}{\mu_2 - \mu_1} \right)^{\frac{d-1}{2}} \int_{\Omega} V^{\frac{d+1}{2}}(x) dx. \end{aligned}$$

This formula allows us to extend the small coupling asymptotics

$$S^{\Omega}_{1/2}(\alpha) = \frac{\alpha}{2} \int_{\Omega} V(x', x_d) |\psi_1(x')|^2 dx + o(\alpha) \quad \text{as} \quad \alpha \to 0$$

to all non-negative potentials $V \in L^{\frac{d+1}{2}}(\Omega) \cap L^1(\Omega, |\psi_1(x')|^2 dx' dx_d)$. The constant in the first term on the r.h.s. of the above estimate is sharp up to the factor $(1+\epsilon)$. Minimizing in $\epsilon = \epsilon(\alpha, V)$ one can extract a three-term formula with an additional intermediate homogeneity in $\alpha$, such that the term serving for small perturbations appears with the optimal constant.

In the remaining part of this paper we sketch the proof of the theorem.

[2] Recently D. Hundertmark has announced that (13) holds true for $\gamma = 0$ and $d \geq 3$.

## 4. Reduction in Dimension

As the first step we apply (13) to reduce bounds for $S^{\Omega}_{\gamma}(\alpha)$ to appropriate integrals of spectral estimates on the operator

$$W^{\omega}(\alpha; x_d) = -\Delta^{\omega} - \alpha V(\cdot, x_d) \quad \text{on} \quad L^2(\omega)$$

(satisfying Dirichlet boundary conditions) for fixed coordinate parameter $x_d \in \mathbb{R}$. Indeed, evaluating the quadratic form of $H^{\Omega}_{\alpha}$ on the form core $C^{\infty}_0(\omega \times \mathbb{R})$, Fubini's theorem and a standard variational argument imply

$$\begin{aligned} S^{\Omega}_{\gamma}(\alpha) &= tr_{L^2(\Omega)} \left(-\Delta - \mu_1 - \alpha V\right)^{\gamma}_{-} \\ &\leq tr_{L^2(\omega)\otimes L^2(\mathbb{R})} \left( -\frac{d}{dx_d} \otimes 1_{L^2(\omega)} - (W^{\omega}(\alpha; x_d) - \mu_1)_{-} \right)^{\gamma}_{-}. \end{aligned}$$

The bound (13) with $W(x_d) = (W^{\omega}(\alpha; x_d) - \mu_1)_{-}$, $d = 1$ and $G = L^2(\omega)$ gives now

$$S^{\Omega}_{\gamma}(\alpha) \leq r(\gamma, 1) L^{cl}_{\gamma,1} \int_{\mathbb{R}} tr \left(W^{\omega}(\alpha; x_d) - \mu_1\right)^{\gamma+\frac{1}{2}}_{-} dx_d. \tag{15}$$

## 5. Spectral Estimates on the Cross Sections

In the next step we have to find appropriate estimates on the quantities $tr \left(W^{\omega}(\alpha; x_d) - \mu_1\right)^{\gamma+\frac{1}{2}}_{-}$. For that end we recall that $\mu_k$ and $\psi_k$ denote the eigenvalues and eigenfunctions of the Dirichlet Laplacian $-\Delta^{\omega}$ on $L^2(\omega)$. The lowest eigenvalue $\mu_1$ is simple. Let $P$ be the projection on the linear span of $\psi_1$ of rank one, and let $Q$ be the projection onto its orthogonal complement in $L^2(\omega)$. Since $V \geq 0$, we have the variational estimate

$$W^{\omega}(\alpha; x_d) \geq PW((1+\epsilon)\alpha; x_d)P + QW((1+\epsilon^{-1})\alpha; x_d)Q.$$

Since $P(-\Delta^{\omega} - \mu_1)P = 0$, one claims that

$$W^{\omega}(\alpha; x_d) - \mu \geq \hat{W}^{\omega}((1+\epsilon)\alpha; x_d) + \tilde{W}^{\omega}((1+\epsilon^{-1})\alpha; x_d)$$

for any $\epsilon > 0$, where

$$\hat{W}^{\omega}(\alpha; x_d) = -\alpha PV(\cdot, x_d)P, \tag{16}$$

$$\tilde{W}^{\omega}(\alpha; x_d) = Q(W(\alpha; x_d) - \mu_1)Q. \tag{17}$$

Obviously, the operators (16) and (17) reduce on the orthogonal subspaces $L^2(\omega) = PL^2(\omega) \oplus QL^2(\omega)$ and

$$\begin{aligned} tr \left(W^{\omega}(\alpha; x_d) - \mu\right)^{\gamma+\frac{1}{2}}_{-} &\leq tr \left(\hat{W}^{\omega}((1+\epsilon)\alpha; x_d)\right)^{\gamma+\frac{1}{2}}_{-} \\ &\quad + tr \left(\tilde{W}^{\omega}((1+\epsilon^{-1})\alpha; x_d)\right)^{\gamma+\frac{1}{2}}_{-}. \end{aligned}$$

Now we shall estimate the last two terms separately. Since $P$ is a perturbation of rank one and $V \geq 0$, by (16) it is clear that

(18)

$$tr\,(\hat{W}^\omega((1+\epsilon)\alpha; x_d))_-^{\gamma+\frac{1}{2}} = \alpha^{\gamma+\frac{1}{2}}(1+\epsilon)^{\gamma+\frac{1}{2}} \left( \int_\omega V(x', x_d)|\psi_1(x')|^2 dx' \right)^{\gamma+\frac{1}{2}}.$$

With regard to the second term we note, that because of $\mu_k \geq \mu_2 > \mu_1 > 0$ for $k = 2, 3, \ldots$, the operator inequality

$$\begin{aligned} Q(-\Delta^\omega - \mu_1)Q &= \sum_{k=2}^{\infty} (\mu_k - \mu_1)\psi_k(\cdot, \psi_k)_{L^2(\omega)} \\ &\geq \sum_{k=2}^{\infty} \frac{\mu_2 - \mu_1}{\mu_2} \mu_k \psi_k(\cdot, \psi_k)_{L^2(\omega)} \\ &= \frac{\mu_2 - \mu_1}{\mu_2} Q(-\Delta^\omega)Q \end{aligned}$$

holds true. Hence,

$$\begin{aligned} tr\,(\tilde{W}^\omega((1+\epsilon^{-1})\alpha; x_d))_-^{\gamma+\frac{1}{2}} &\leq tr\,(Q(-\tau\Delta^\omega - \tau\rho V(\cdot, x_d))Q)_-^{\gamma+\frac{1}{2}} \\ &= \tau^{\gamma+\frac{1}{2}} tr\,(QW(\rho; x_d)Q)_-^{\gamma+\frac{1}{2}} \\ &\leq \tau^{\gamma+\frac{1}{2}} tr\,(W(\rho; x_d))_-^{\gamma+\frac{1}{2}}, \end{aligned}$$

where $\tau = \mu_2^{-1}(\mu_2 - \mu_1)$ and $\rho = \tau^{-1}\alpha(1+\epsilon^{-1})$. Clearly, the negative eigenvalues of the operator $W(\rho; x_d)$ on $L^2(\omega)$ with Dirichlet boundary conditions at $\partial\omega$ can be estimated from below by the respective negative eigenvalues of

$$H_\rho(x_d) = -\Delta - \rho V(\cdot, x_d) \quad \text{on} \quad L^2(\mathbb{R}^{d-1}).$$

Now the usual Lieb-Thirring inequality (5) for $\gamma' = \gamma + \frac{1}{2}$ and $d' = d - 1$ implies that

$$\begin{aligned} tr\,(\tilde{W}^\omega((1+\epsilon^{-1})\alpha; x_d))_-^{\gamma'} &\leq \tau^{\gamma'} S_{\gamma'}(\rho) \\ &\leq \tau^{\gamma'} R(\gamma', d') L^{cl}_{\gamma', d'} S^{cl}_{\gamma', d'}(\rho) \\ &= R(\gamma', d') L^{cl}_{\gamma', d'} \tau^{\gamma'} \rho^{\gamma+\frac{d}{2}} \int_\omega V^{\gamma+\frac{d}{2}}(x', x_d) dx'. \end{aligned}$$

In the last expression we made use of the relation $\gamma' + \frac{d'}{2} = \gamma + \frac{d}{2}$.

Now we insert the spectral estimates on (16) and (17) into (15). In view of $L^{cl}_{\gamma',d'}L^{cl}_{\gamma,1} = L^{cl}_{\gamma,d}$ this gives

$$\begin{aligned} S^{\Omega}_{\gamma}(\alpha) \;\leq\; & \alpha^{\gamma+\frac{1}{2}}(1+\epsilon)^{\gamma+\frac{1}{2}} r(\gamma,1) L^{cl}_{\gamma,1} \int_{\mathbb{R}} \left( \int_{\Omega} V(x)|\psi_1(x')|^2 dx \right)^{\gamma+\frac{1}{2}} dx_d \\ & + (1+\epsilon^{-1})^{\gamma+\frac{d}{2}} \left( \frac{\mu_2}{\mu_2-\mu_1} \right)^{\frac{d-1}{2}} r(\gamma,1) R(\gamma',d') S^{cl}_{\gamma,d}(\alpha). \end{aligned}$$

This completes the proof.

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