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 ω 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 ω. 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 $-\alpha V \leq 0$, 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 μ_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_α^Ω below μ_1 (counting multiplicities). In this paper we study Lieb-Thirring type bounds on the spectral moments[1]

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

[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_α^Ω can model various effects in quantum wires.

Compared with the usual Schrödinger operator on $L^2(\mathbb{R}^d)$, the spectral behaviour of H_α^Ω reflects the mixed dimensionality of the tube Ω. 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

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

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_α^Ω 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_α has exactly one bound state $\lambda_1(\alpha)$ below μ_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 γ 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]

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

holds. Both constants are sharp and

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

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

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

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

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

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

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

This formula allows us to extend the small coupling asymptotics

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

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 α, 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^{Ω}_{α} on the form core $C_0^{\infty}(\omega \times \mathbb{R})$, Fubini's theorem and a standard variational argument imply

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

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

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

5. Spectral Estimates on the Cross Sections

In the next step we have to find appropriate estimates on the quantities $tr\,(W^{\omega}(\alpha;x_d) - \mu_1)^{\gamma+\frac{1}{2}}_{-}$. For that end we recall that μ_k and ψ_k denote the eigenvalues and eigenfunctions of the Dirichlet Laplacian $-\Delta^{\omega}$ on $L^2(\omega)$. The lowest eigenvalue μ_1 is simple. Let P be the projection on the linear span of ψ_1 of rank one, and let Q be the projection onto its orthogonal complement in $L^2(\omega)$. Since $V \ge 0$, we have the variational estimate

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

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

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

for any $\epsilon > 0$, where

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

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

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

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

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

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

This completes the proof.

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