

Number of Bound States of Schrödinger Operators with Matrix-Valued Potentials

Dedicated to Jean-Claude Cortet, in appreciation of his contribution to Letters in Mathematical Physics

RUPERT L. FRANK¹, ELLIOTT H. LIEB² and ROBERT SEIRINGER³

¹*Department of Mathematics, Princeton University, Washington Road, Princeton, NJ 08544, USA. e-mail: rlfrank@math.princeton.edu*

²*Departments of Mathematics and Physics, Princeton University, P. O. Box 708, Princeton, NJ 08544, USA. e-mail: lieb@princeton.edu*

³*Department of Physics, Princeton University, P. O. Box 708, Princeton, NJ 08544, USA. e-mail: rseiring@princeton.edu*

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Abstract. We give a Cwikel–Lieb–Rozenblum type bound on the number of bound states of Schrödinger operators with matrix-valued potentials using the functional integral method of Lieb. This significantly improves the constant in this inequality obtained earlier by Hundertmark.

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1. Introduction

We consider the Schrödinger operator $-\Delta - V(x)$ on \mathbb{R}^d , but with the difference from the usual case that V is a Hermitian matrix-valued potential. In other words, the Hilbert space is not $L^2(\mathbb{R}^d)$ but $L^2(\mathbb{R}^d; \mathbb{C}^N)$. The values of functions in this space, $\psi(x)$, are N -dimensional vectors. (What we say here easily generalizes to “operator-valued” potentials, i.e., \mathbb{C}^N is replaced by a Hilbert space such as $L^2(\mathbb{R}^m)$, but we stay with matrices in order to avoid technicalities.) The Cwikel–Lieb–Rozenblum (CLR) bound for $d \geq 3$ in the scalar case $N = 1$ states that $\#(-\Delta - V)$, the number of negative eigenvalues of $-\Delta - V$, can be estimated by

$$\#(-\Delta - V) \leq L_{0,d} \int_{\mathbb{R}^d} V_+(x)^{d/2} dx. \quad (1.1)$$

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(Here and below $v_{\pm} := (|v| \pm v)/2$ denotes the positive and negative part of v .) We remind the reader that the “semi-classical” approximation to $\#(-\Delta - V)$ is given in the scalar case by the phase space volume

$$(2\pi)^{-d} \iint_{\{(p,x) \in \mathbb{R}^d \times \mathbb{R}^d : p^2 - V(x) < 0\}} dp dx = L_{0,d}^{\text{cl}} \int_{\mathbb{R}^d} V_+(x)^{d/2} dx,$$

where

$$L_{0,d}^{\text{cl}} = (2\pi)^{-d} \int_{\{p \in \mathbb{R}^d : p^2 < 1\}} dp = \left(2^d \pi^{d/2} \Gamma(d/2 + 1)\right)^{-1}.$$

The bound (1.1) was obtained by completely independent methods in [3,14,15,18,19]. Later, different proofs were given in [2,13]. The best constant, which is close to optimal for $d=3$, was obtained in [14,15] using the Feynman–Kac formula and Jensen’s inequality.

Our goal here is to extend inequality (1.1) to the matrix case (with a possibly different constant $L_{0,d}$). The motivation for this extension was the work of Laptev and Weidl [11] (see also [10]) who realized that the extension allowed one to conclude that good/sharp constants obtained in low dimensions would automatically give good/sharp constants in higher dimensions. The fact that the inequality (1.1) is valid in the matrix case was proved by Hundertmark [6], confirming a conjecture in [12]. He follows Cwikel’s method and obtains a constant which is far from optimal. Hundertmark points out that “it would be nice to extend Lieb’s [...] proof of the CLR-bound to operator-valued potentials”. This is the content of this letter.

THEOREM 1.1. *Let $d \geq 3$ and assume that V is a function on \mathbb{R}^d taking values in the Hermitian $N \times N$ matrices. Then*

$$\#(-\Delta - V) \leq R_{0,d} L_{0,d}^{\text{cl}} \int_{\mathbb{R}^d} \text{Tr}_{\mathbb{C}^N} \left[V_+(x)^{d/2} \right] dx, \tag{1.2}$$

where $R_{0,d} \leq 10.332$ and $V_+ := (|V| + V)/2$.

The constant 10.332 will be obtained for $d = 3$ and, by the Laptev–Weidl method (as used by Hundertmark [6]) it is valid uniformly for all $d \geq 3$. We emphasize that our bound on $R_{0,d}$ is slightly worse than the constant 6.87 in [14,15] for the scalar case $N = 1$. Still, it improves that of [6] by almost one order of magnitude. For $d = 3$ our bound on $R_{0,3}$ is at most a factor 2.24 bigger than the optimal constant in (1.2), since it is known that $R_{0,3} \geq 8/\sqrt{3} \approx 4.619$ [16].

It is well known that by a simple integration the bound (1.2) yields the Lieb–Thirring inequalities

$$\text{Tr}_{L_2(\mathbb{R}^d; \mathbb{C}^N)} (-\Delta - V)_-^\gamma \leq R_{\gamma,d} L_{\gamma,d}^{\text{cl}} \int_{\mathbb{R}^d} \text{Tr}_{\mathbb{C}^N} \left[V_+(x)^{\gamma+d/2} \right] dx \tag{1.3}$$

for all $\gamma > 0$, $d \geq 3$ with $R_{\gamma,d} \leq R_{0,d} \leq 10.332$ and

$$L_{\gamma,d}^{\text{cl}} = (2\pi)^{-d} \int_{\mathbb{R}^d} (1 - p^2)_+^\gamma dp. \tag{1.4}$$

Indeed, $R_{\gamma,d}$ is a monotone non-increasing function of γ [1]. Even in the scalar case $N = 1$, this yields the best known constants in this inequality for the parameter range $0 < \gamma < 1/2$. For comparison we recall that the best known bounds for larger values of γ are $R_{\gamma,d} \leq 2\pi/\sqrt{3} \approx 3.628$ if $\gamma \geq 1/2$ and $R_{\gamma,d} \leq \pi/\sqrt{3} \approx 1.814$ if $\gamma \geq 1$ [4,8]. For $\gamma \geq 3/2$ one has $R_{\gamma,d} = 1$, which is sharp [11]. We refer to the surveys [7,12] for more about inequalities (1.3).

Apart from yielding very accurate constants we believe that there is a mathematical interest in extending the path-integral method in [14,15] to the operator-valued situation. In contrast to the method of [3] used in [6], which is rather rigidly based on mapping properties of the Fourier transform, the method of [14, 15] used here works in much wider generality, e.g., on Riemannian manifolds. The only input needed is an upper bound on the heat kernel of the (scalar) unperturbed operator. For example, the Hardy–Lieb–Thirring bounds in [5] extend to the matrix-valued situation.

As already pointed out, we proceed similarly to [14,15]. Therefore we will be brief at some points and ignore some technicalities. There is an important new ingredient in our proof, however. Since matrices W_1, \dots, W_n do not commute, in general, we need to work with the “time ordering” of a function $f(\sum_j W_j)$ of their sum. In Proposition 3.1 we shall prove a modification of Jensen’s inequality valid in this setting for a certain class of convex functions f .

2. A Trace Formula

Given self-adjoint $N \times N$ -matrices W_1, \dots, W_n and a function f on \mathbb{R} , the matrix $f(\sum_j W_j)$ is defined by the spectral projections of $\sum_j W_j$. Instead, we introduce the “time-ordering” of the matrix $f(\sum_j W_j)$ as follows. We write W_j in its spectral representation

$$W_j = \sum_{k=1}^N w_k^{(j)} P_k^{(j)},$$

where $w_k^{(j)}$ are the eigenvalues and $P_k^{(j)}$ the corresponding orthogonal projections, and define

$$\mathcal{T}f(W_1, \dots, W_n) := \sum_{k_1, \dots, k_n=1}^N f\left(\sum_{j=1}^n w_{k_j}^{(j)}\right) P_{k_1}^{(1)} \dots P_{k_n}^{(n)}. \tag{2.1}$$

Intuitively, this means that when calculating $f(\sum_j W_j)$, one puts all the W_1 's left of the W_2 's, the W_2 's left of the W_3 's, and so on, without worrying about commutators. It is instructive to look at some examples.

EXAMPLE 2.1. If $f(\mu) = \mu^k$, $k \in \mathbb{N}$, then the definition immediately implies

$$\mathcal{T}f(W_1, \dots, W_n) = \sum_{j_1 + \dots + j_n = k} \frac{k!}{j_1! \dots j_n!} W_1^{j_1} \dots W_n^{j_n}.$$

EXAMPLE 2.2. If $f(\mu) = e^{\alpha\mu}$, $\alpha \in \mathbb{R}$, then again by the definition (2.1)

$$\mathcal{T}f(W_1, \dots, W_n) = e^{\alpha W_1} \dots e^{\alpha W_n}.$$

Similarly, one shows that if $f(\mu) = \mu e^{\alpha\mu}$, $\alpha \in \mathbb{R}$, then

$$\begin{aligned} \mathcal{T}f(W_1, \dots, W_n) &= \\ &= W_1 e^{\alpha W_1} e^{\alpha W_2} \dots e^{\alpha W_n} + e^{\alpha W_1} W_2 e^{\alpha W_2} \dots e^{\alpha W_n} + \dots + e^{\alpha W_1} e^{\alpha W_2} \dots W_n e^{\alpha W_n}. \end{aligned}$$

We have introduced the notion of time-ordering in order to generalize the trace formula in [14,15], which is the starting point of the analysis leading to (1.1).

PROPOSITION 2.3. *Let f be a non-negative, lower semi-continuous function with $f(0) = 0$, and let*

$$F(\lambda) := \int_0^\infty f(\mu) e^{-\mu/\lambda} \mu^{-1} d\mu, \quad \lambda > 0. \tag{2.2}$$

Then for any sufficiently regular and decaying functions V on \mathbb{R}^d , $d \geq 3$, taking values in the non-negative $N \times N$ -matrices, one has

$$\begin{aligned} \text{Tr}_{L_2(\mathbb{R}^d; \mathbb{C}^N)} F(V^{1/2}(-\Delta)^{-1}V^{1/2}) &= \\ &= \int_0^\infty \frac{dt}{t} \lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} \dots \int_{\mathbb{R}^d} dx_1 \dots dx_n \times \\ &\quad \times \prod_{j=1}^n k\left(x_j, x_{j-1}, \frac{t}{n}\right) \text{Tr}_{\mathbb{C}^N} \left[\mathcal{T}f\left(\frac{t}{n}V(x_1), \dots, \frac{t}{n}V(x_n)\right) \right] \end{aligned} \tag{2.3}$$

with the convention that $x_0 = x_n$. Here, $k(x, y, t) = (4\pi t)^{-d/2} \exp(-|x - y|^2/(4t))$.

In the limit $n \rightarrow \infty$ the multiple integral on the right side of (2.3) converges to a Wiener integral (the Feynman–Kac integral); in fact, the right side of (2.3) is the Trotter product approximation to this integral [9,17,21].

Proof. By an approximation argument [21, Theorem 8.2] it suffices to prove this formula for

$$F(\lambda) = \lambda / (1 + \alpha\lambda), \quad f(\mu) = \mu e^{-\alpha\mu},$$

where $\alpha > 0$ is a constant. Using the resolvent identity and Trotter’s product formula, one easily verifies that in this case

$$\begin{aligned} F(V^{1/2}(-\Delta)^{-1}V^{1/2}) &= V^{1/2}(-\Delta + \alpha V)^{-1}V^{1/2} = \\ &= \int_0^\infty V^{1/2} \exp(-t(-\Delta + \alpha V))V^{1/2} dt = \\ &= \int_0^\infty \lim_{n \rightarrow \infty} T_n(t) dt. \end{aligned}$$

Here,

$$T_n(t) := V^{1/2} (\exp(t\Delta/n) \exp(-t\alpha V/n))^n V^{1/2}.$$

The latter is an integral operator and we evaluate its trace by integrating its kernel on the diagonal. Let k denote the heat kernel

$$k(x, y, t) := (4\pi t)^{-d/2} \exp(-|x - y|^2/(4t)).$$

Then

$$\begin{aligned} \text{Tr}_{L_2(\mathbb{R}^d; \mathbb{C}^N)} T_n(t) &= \\ &= \int \cdots \int dx_1 \cdots dx_n \prod_{j=1}^n k\left(x_j, x_{j-1}, \frac{t}{n}\right) \text{Tr}_{\mathbb{C}^N} \left[e^{-\frac{\alpha t}{n} V(x_1)} \cdots e^{-\frac{\alpha t}{n} V(x_n)} V(x_n) \right]. \end{aligned}$$

Cyclical relabeling of the variables leads to

$$\begin{aligned} \text{Tr}_{L_2(\mathbb{R}^d; \mathbb{C}^N)} T_n(t) &= \\ &= \frac{1}{t} \int \cdots \int dx_1 \cdots dx_n \prod_{j=1}^n k\left(x_j, x_{j-1}, \frac{t}{n}\right) \text{Tr}_{\mathbb{C}^N} [T f(tV(x_1)/n, \dots, tV(x_n)/n)] \end{aligned}$$

(compare with Example 2.2). The claimed formula (2.3) follows if one interchanges the trace with the t -integration and the n -limit. □

3. Jensen’s Inequality and Time Ordering

To apply (2.3) we need to estimate the trace of a time-ordered sum. Recall that Jensen’s inequality says that $\text{Tr} f(\sum W_j) \leq n^{-1} \sum \text{Tr} f(nW_j)$ for f convex. The analog for the time-ordered case, and a certain class of f ’s, is

PROPOSITION 3.1. *Assume that*

$$f(\mu) = \sum_{j=0}^{\infty} \alpha_j \mu^j + \int_{\mathbb{R}} e^{-\alpha \mu} d\nu(\alpha) \tag{3.1}$$

for some $\alpha_0, \alpha_1 \in \mathbb{R}, \alpha_j \geq 0$ for $j \geq 2$ and a non-negative measure ν . Then for any non-negative $N \times N$ -matrices W_1, \dots, W_n

$$\text{Re Tr}_{\mathbb{C}^N} [\mathcal{T} f(W_1, \dots, W_n)] \leq \frac{1}{n} \sum_{j=1}^n \text{Tr}_{\mathbb{C}^N} f(nW_j). \tag{3.2}$$

Note that the f in (3.1) is convex on $[0, \infty)$. We do not know whether the statement is true for an arbitrary convex function on $[0, \infty)$. If it were, the constant in Theorem 1.1 could be improved, as explained at the end of this letter.

Proof. By linearity of the trace it suffices to consider the cases $f(\mu) = \mu^k, k \in \mathbb{N}$, and $f(\mu) = e^{\alpha \mu}$. In the former case, one has by Hölder’s inequality for traces (see, e.g., [20, Theorem 2.8])

$$\begin{aligned} \text{Re Tr}_{\mathbb{C}^N} [\mathcal{T} f(W_1, \dots, W_n)] &= \sum_{j_1 + \dots + j_n = k} \frac{k!}{j_1! \dots j_n!} \text{Re Tr}_{\mathbb{C}^N} [W_1^{j_1} \dots W_n^{j_n}] \leq \\ &\leq \sum_{j_1 + \dots + j_n = k} \frac{k!}{j_1! \dots j_n!} (\text{Tr}_{\mathbb{C}^N} W_1^k)^{j_1/k} \dots (\text{Tr}_{\mathbb{C}^N} W_n^k)^{j_n/k} = \\ &= f \left(\sum_{j=1}^n (\text{Tr}_{\mathbb{C}^N} W_j^k)^{1/k} \right), \end{aligned}$$

and the assertion follows from the convexity of f . In the latter case, one has similarly by Hölder’s inequality and the geometric-arithmetric mean inequality

$$\begin{aligned} \text{Re Tr}_{\mathbb{C}^N} [\mathcal{T} f(W_1, \dots, W_n)] &= \text{Re Tr}_{\mathbb{C}^N} [e^{\alpha W_1} \dots e^{\alpha W_n}] \leq \\ &\leq (\text{Tr}_{\mathbb{C}^N} e^{\alpha n W_1})^{1/n} \dots (\text{Tr}_{\mathbb{C}^N} e^{\alpha n W_n})^{1/n} \leq \\ &\leq \frac{1}{n} \sum_{j=1}^n \text{Tr}_{\mathbb{C}^N} e^{n \alpha W_j}, \end{aligned}$$

as claimed. □

COROLLARY 3.2. *Assume that f is a non-negative function of the form considered in Proposition 3.1 and let F be as in (2.2). Then for any sufficiently regular and decaying function V on \mathbb{R}^d taking values in the non-negative $N \times N$ -matrices, one has*

$$\begin{aligned} & \text{Tr}_{L^2(\mathbb{R}^d; \mathbb{C}^N)} F(V^{1/2}(-\Delta)^{-1}V^{1/2}) \leq \\ & \leq \frac{1}{(4\pi)^{d/2}} \left(\int_0^\infty \frac{f(s) \, ds}{s^{d/2} \, s} \right) \int_{\mathbb{R}^d} \text{Tr}_{\mathbb{C}^N} [V(x)^{d/2}] \, dx. \end{aligned} \tag{3.3}$$

Proof. Combining Propositions 3.1 and 2.3 we obtain

$$\begin{aligned} & \text{Tr}_{L^2(\mathbb{R}^d; \mathbb{C}^N)} F(V^{1/2}(-\Delta)^{-1}V^{1/2}) \leq \\ & \leq \int_0^\infty \frac{dt}{t} \lim_{n \rightarrow \infty} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \prod_{j=1}^n k\left(x_j, x_{j-1}, \frac{t}{n}\right) \frac{1}{n} \sum_{j=1}^n \text{Tr}_{\mathbb{C}^N} f(tV(x_j)) \, dx_1 \dots dx_n. \end{aligned}$$

(Here we have used that the left side of (2.3) is real, hence only the real part of $\text{Tr} \mathcal{T} f$ contributes to the integral.) The semi-group property implies

$$\begin{aligned} & \frac{1}{n} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \prod_{j=1}^n k\left(x_j, x_{j-1}, \frac{t}{n}\right) \sum_{j=1}^n \text{Tr}_{\mathbb{C}^N} f(tV(x_j)) \, dx_1 \dots dx_n = \\ & = \frac{1}{n} \sum_{j=1}^n \int_{\mathbb{R}^d} k(x_j, x_j, t) \text{Tr}_{\mathbb{C}^N} f(tV(x_j)) \, dx_j = \frac{1}{(4\pi t)^{d/2}} \int_{\mathbb{R}^d} \text{Tr}_{\mathbb{C}^N} f(tV(x)) \, dx. \end{aligned}$$

Denoting the eigenvalues of $V(x)$ by $v_1(x) \leq \dots \leq v_N(x)$ one finds that

$$\int_0^\infty \frac{dt}{t} \frac{\text{Tr}_{\mathbb{C}^N} f(tV(x))}{t^{d/2}} = \sum_{j=1}^N \int_0^\infty \frac{dt}{t} \frac{f(tv_j(x))}{t^{d/2}} = \sum_{j=1}^N v_j(x)^{d/2} \int_0^\infty \frac{ds}{s} \frac{f(s)}{s^{d/2}},$$

thereby proving the assertion. □

4. Proof of Theorem 1.1

First we assume that $d=3$. By the variational principle we can assume that $V(x)$ is a non-negative matrix for all x , and by an approximation argument we can assume that V is smooth and rapidly decaying. For any increasing function F on $(0, \infty)$ the Birman–Schwinger principle implies that

$$\#(-\Delta - V) \leq F(1)^{-1} \text{Tr}_{L^2(\mathbb{R}^3; \mathbb{C}^N)} F(V^{1/2}(-\Delta)^{-1}V^{1/2}). \tag{4.1}$$

We choose $F = F_a$ of the form (2.2) where $a > 0$ is a parameter and $f = f_a$ is defined by

$$f_a(\mu) = \frac{\mu^2}{\mu + a} = \mu - a + \frac{a^2}{\mu + a} = \mu - a + a^2 \int_0^\infty e^{-t(\mu+a)} dt.$$

Since this function is of the form considered in Proposition 3.1 we can apply Corollary 3.2 and get in view of (4.1)

$$\#(-\Delta - V) \leq C_a \int_{\mathbb{R}^3} \text{Tr}_{\mathbb{C}^N} \left[V(x)^{3/2} \right] dx,$$

where

$$\begin{aligned} C_a &:= (4\pi)^{-3/2} F_a(1)^{-1} \left(\int_0^\infty \frac{f_a(s) ds}{s^{3/2} s} \right) \\ &= \frac{1}{8} (\pi a)^{-1/2} \left(1 + a e^a \int_a^\infty e^{-s} \frac{ds}{s} \right)^{-1}. \end{aligned}$$

The result follows by choosing $a = 1.13$, which approximately minimizes C_a .

Now we assume that $d \geq 4$. We will use the Laptev–Weidl strategy to reduce this case to the case $d = 3$. This argument is already contained in [6] but we include it for the sake of completeness. We note that by a straightforward approximation argument as in [11] the inequality for $d = 3$ holds also for $N = \infty$, i.e., if $V(x)$ assumes values in the compact self-adjoint operators on a separable Hilbert space. Introduce variables $x = (x_1, x_2) \in \mathbb{R}^d$ where $x_1 \in \mathbb{R}^3$ and $x_2 \in \mathbb{R}^{d-3}$. We decompose the Laplacian correspondingly as $-\Delta = -\Delta_1 - \Delta_2$ and define, for fixed $x_1 \in \mathbb{R}^3$, $W(x_1) := (-\Delta_1 - V(x_1, \cdot))_-$. If V is, say, smooth with compact support, then $W(x_1)$ is a compact operator in $L^2(\mathbb{R}^{d-3}, \mathbb{C}^N)$ for every x_1 . The variational principle and the inequality for $d = 3$ imply that

$$\#(-\Delta - V) \leq \#(-\Delta_1 - W) \leq R_{0,3} L_{0,3}^{\text{cl}} \int_{\mathbb{R}^3} \text{Tr}_{L^2(\mathbb{R}^{d-3}, \mathbb{C}^N)} \left[W(x_1)^{3/2} \right] dx_1.$$

By the result of Laptev and Weidl [11], one has

$$\text{Tr}_{L^2(\mathbb{R}^{d-3}, \mathbb{C}^N)} \left[W(x_1)^{3/2} \right] \leq L_{3/2, d-3}^{\text{cl}} \int_{\mathbb{R}^{d-3}} \text{Tr}_{\mathbb{C}^N} \left[V(x_1, x_2)^{d/2} \right] dx_2$$

with the constant $L_{3/2, d-3}^{\text{cl}}$ from (1.4). Noting that $L_{0,3}^{\text{cl}} L_{3/2, d-3}^{\text{cl}} = L_{0,d}^{\text{cl}}$ we obtain the assertion of Theorem 1.1.

Remark 4.1. If the estimate in Proposition 3.1 held for all convex functions on $[0, \infty)$ [not merely for those of the form (3.1)], then we could choose $f_a(\mu) = (\mu - a)_+$ in the preceding proof, as in [14, 15], and would get the same constant as in the scalar case. If estimate (3.2) held for the absolute value instead of merely for the real part, our proof would extend to Schrödinger operators with magnetic fields. This follows as in the scalar case by means of the diamagnetic inequality.

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