Analysis and Mathematical Physics (2024) 14:13
https://doi.org/10.1007/s13324-024-00870-w

Cwikel–Lieb–Rozenblum inequalities for the Coulomb Hamiltonian

Andrés Díaz Selvi[1]

Received: 5 December 2023 / Revised: 11 December 2023 / Accepted: 5 January 2024 /
Published online: 7 February 2024

Abstract
We prove sharp Cwikel–Lieb–Rozenblum type inequalities for the Coulomb Hamiltonian in dimension higher than five. We furthermore show that the classical constant obtained from Weyl asymptotics doesn't hold in dimensions four and five.

Keywords Coulomb Hamiltonian · Cwikel–Lieb–Rozenblum inequalities · Schrödinger operator · Lieb–Thirring inequalities

Mathematics Subject Classification Primary 35J10; Secondary 47A75

1 Introduction

We consider the following Schrödinger operator in $L^2(\mathbb{R}^d)$,

$$-\Delta - \kappa|x|^{-1} + \Lambda \qquad \text{with } \kappa > 0, \Lambda > 0, d \geq 2, \tag{1}$$

known as Coulomb Hamiltonian. This is a well defined operator and the negative spectrum consists precisely of the eigenvalues

$$\left\{ \Lambda - \frac{\kappa^2}{(2k+d-1)^2} : k \in \mathbb{N}_0 \right\} \quad \text{with multiplicity } \mu_k = \frac{(d-2+k)!(d-1+2k)}{(d-1)!k!}.$$

(See for example [1]). Concerning the examination of the spectral properties of the Schrödinger operator family, Cwikel [2], Lieb [3] and Rozenblum [4] found an estimation for the number of negative eigenvalues below zero, usually denoted by $N(0, -\Delta - V)$, when the dimension is greater or equal to 3.

✉ Andrés Díaz Selvi
andres.diaz-selvi22@imperial.ac.uk

1 Department of Mathematics, Imperial College London, 180 Queen's Gate, London SW7 2AZ, UK

Theorem 1 (CLR inequality) *Let $d \geq 3$. Then there is a constant $L_{0,d} < \infty$ such that for all $V \in L^1_{loc}(\mathbb{R}^d)$ with $V_+ \in L^{d/2}(\mathbb{R}^d)$,*

$$N(0, -\Delta - V) \leq L_{0,d} \int_{\mathbb{R}^d} V(x)_+^{d/2} dx$$

Later, Lieb and Thirring [5] generalized the Cwikel–Lieb–Rozenblum inequality to obtain an estimation for the Riesz means of the negative spectrum.

Theorem 2 (Lieb–Thirring inequality) *Let $\gamma \geq 1/2$ if $d = 1$, $\gamma > 0$ if $d = 2$ and $\gamma \geq 0$ if $d \geq 3$. Then, there exist a constant $L_{\gamma,d} < \infty$ such that, for any V with $V_+ \in L^{\gamma+d/2}(\mathbb{R}^d)$ and $V_- \in L^1_{loc}(\mathbb{R}^d)$,*

$$Tr(-\Delta - V)_-^{\gamma} \leq L_{\gamma,d} \int_{\mathbb{R}^d} V(x)_+^{\gamma+d/2} dx.$$

Although the existence of the constant $L_{\gamma,d}$ is known, the sharpest value in some of this inequalities is still an open problem. In order to find the sharpest value, one approach is to study the Lieb–Thirring inequalities in specific cases that can give some information about the constant.

Nevertheless, if we consider the classical Coulomb Hamiltonian,

$$-\Delta - \kappa|x|^{-1} \qquad \text{with } \kappa > 0, d \geq 2,$$

this operator doesn't satisfy the hypothesis of Theorem 1. Therefore, it is necessary to add the parameter $\Lambda > 0$, which acts as a shift, and enables the operator defined in 1 to be an element of $L^{d/2}(\mathbb{R}^d)$. Moreover, the integral defined in the right-hand side of Theorem 2 can be explicitely computed and equals

$$L^{cl}_{\gamma,d} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+d/2} dx = 2^{1-d}\kappa^d \Lambda^{\gamma-d/2} \frac{\Gamma(\gamma+1)\Gamma\left(\frac{d}{2}-\gamma\right)}{\Gamma(d+1)\Gamma\left(\frac{d}{2}\right)}.$$

Several months ago, Laptev, Frank and Weidl obtained the following result regarding the 3 dimensional case of the Coulomb Hamiltonian in [1].

Theorem 3 *Let $d = 3$ and $1 \leq \gamma < 3/2$. Then for all $\kappa > 0$ and $\Lambda > 0$,*

$$Tr(-\Delta - \kappa|x|^{-1} + \Lambda)_-^{\gamma} \leq L^{cl}_{\gamma,3} \int_{\mathbb{R}^3} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+3/2} dx.$$

Where

$$L^{cl}_{\gamma,d} = \frac{\Gamma(\gamma+1)}{(4\pi)^{d/2}\Gamma(\gamma+1+d/2)}$$

is the classical constant obtained through Weyl asymptotics [6].

Theorem 4 (Weyl asymptotics) *Let $\gamma \geq 0$ and let V be a continuous function on $\mathbb{R}^d$ with compact support. Then*

$$\lim_{\alpha\to\infty} \alpha^{-\gamma-d/2} Tr(0, -\Delta - \alpha V)_-^{\gamma} = L^{cl}_{\gamma,d} \int_{\mathbb{R}^d} V(x)_+^{\gamma+d/2} dx.$$

Comparing the Lieb–Thirring inequality to the Weyl asymptotics, it is clear that

$$L^{cl}_{\gamma,d} \leq L_{\gamma,d}. \tag{2}$$

A slightly different approach is to investigate the best constant concerning only the first eigenvalue, that is

$$|E_1|^{\gamma} \leq L^{(1)}_{\gamma,d} \int_{\mathbb{R}^d} V(x)_+^{\gamma+d/2} dx. \tag{3}$$

In this context, the constant $L^{(1)}_{\gamma,d}$ is sometimes referred to as the "one-particle constant". Consequently,

$$L^{(1)}_{\gamma,d} \leq L_{\gamma,d}. \tag{4}$$

In 1961, Keller [7] raised the variational problem for $L^{(1)}_{\gamma,d}$. Independently, Lieb and Thirring [5] arrived at the same optimization problem and showed that it is intimately related to the problem of finding the sharp constant in Sobolev and Gagliardo-Nirenberg inequalities. Combining 2 and 4, it follows

$$L_{\gamma,d} \geq \max\{L^{cl}_{\gamma,d}, L^{(1)}_{\gamma,d}\} \tag{5}$$

Lieb and Thirring conjectured in [5] that equality holds in 5. In other words, the optimal constant $L_{\gamma,d}$ is equal to the maximum of $L^{cl}_{\gamma,d}$ and $L^{(1)}_{\gamma,d}$. For a further discussion of this conjecture, we refer to [8].

The proof of Theorem 3 resides on the fact that the inequality holds when $\gamma = 1$, and then they extend the result using the following auxiliary lemma, known as the Aizenman–Lieb principle, presented in [9].

Lemma 1 (Aizenman–Lieb principle) *For any $d \geq 1$, the quotient $L_{\gamma,d}/L^{cl}_{\gamma,d}$ is non increasing in γ.*

In this paper we will present in which cases the classical constant $L^{cl}_{\gamma,d}$ is a valid constant for the CLR inequalities of the Coulomb Hamiltonian when working in dimension $d \geq 4$.

Moreover, we will extend those results by means of the Aizenman–Lieb principle when possible, obtaining the Lieb–Thirring inequalities. Additionally, we give an starting point γ_0 for which the Lieb–Thirring inequalities hold (with the classical constant) in those cases where the CLR inequalities don't.

2 CLR inequalities

We present now the main two results of this article. The first one shows that the classical constant is valid in the case where the dimension is greater or equal than six.

Theorem 5 *Let $d \geq 6$. Then for all $\kappa > 0$ and $\Lambda > 0$,*

$$N(0, -\Delta - \kappa|x|^{-1} + \Lambda) \leq L_{0,d}^{cl} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+d/2} dx.$$

The next one shows that in dimensions 4 and 5, the classical constant is no longer valid.

Theorem 6 *Let $d = 4$ or $d = 5$. Then, there exists some values of $\kappa > 0$ and $\Lambda > 0$ for which the CLR inequality of the correspondent Coulomb Hamiltonian don't hold with the classical constant.*

Both theorems are a consequence of the following lemma.

Lemma 2 *Let $d \geq 4$. Then, there exists $k_0 > 0$ such that for all $\kappa > 0$ and $\Lambda > 0$ satisfying $\frac{\kappa}{\sqrt{\Lambda}} \geq k_0$,*

$$N(0, -\Delta - \kappa|x|^{-1} + \Lambda) \leq L_{0,d}^{cl} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+d/2} dx.$$

Proof of Lemma 2 In order to compute $N(0, -\Delta - \kappa|x|^{-1} + \Lambda)$, the first goal is to determine when the quantity

$$\frac{\kappa^2}{(2k + d - 1)^2} - \Lambda \tag{6}$$

is positive. Making the computations, we obtain that (6) is positive for those $k \in \mathbb{N}$ such that

$$k \leq \frac{\frac{\kappa}{\sqrt{\Lambda}} - (d-1)}{2}. \tag{7}$$

In the following, we will denote $M := \lfloor \frac{\frac{\kappa}{\sqrt{\Lambda}} - (d-1)}{2} \rfloor$ the greatest integer less than or equal to $\frac{\frac{\kappa}{\sqrt{\Lambda}} - (d-1)}{2}$. Hence,

$$\begin{aligned} N(0, -\Delta - \kappa|x|^{-1} + \Lambda) &= \sum_{k=0}^{\infty} \mu_k \left(\frac{\kappa^2}{(2k + d - 1)^2} - \Lambda \right)_+^0 \\ &= \sum_{k=0}^{M} \frac{(d - 2 + k)!(d - 1 + 2k)}{(d - 1)!k!}. \end{aligned} \tag{8}$$

Similar to the case of the Laplace–Beltrami operator, since our potential only depends on $|x|$, we can reduce the study on $\mathbb{R}^d$ to problems on the real line using the spherical harmonics. If $\nu(l)$ denotes the dimension of the space of spherical harmonics of degree l, then the multiplicity μ_k associated to 6 can be written as:

$$\mu_k = \sum_{l=0}^{k} \nu(l) = \frac{(d-2+k)!(d-1+2k)}{(d-1)!k!}$$

The sum in 8 can be explicitly computed and equals

$$\sum_{k=0}^{M} \frac{(d-2+k)!(d-1+2k)}{(d-1)!k!} = \frac{(d+2M)\Gamma(d+M)}{\Gamma(d+1)\Gamma(M+1)}.$$

Simplifying the expression we get,

$$N(0, -\Delta - \kappa|x|^{-1} + \Lambda) \leq \frac{1}{2}(d-1)\left(\frac{\kappa}{\sqrt{\Lambda}} + 1\right)^2 \frac{1}{\Gamma(d+1)}.$$

On the other hand,

$$L_{0,d}^{cl} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{0+d/2} dx = 2^{1-d}\kappa^d \Lambda^{-d/2} \frac{1}{\Gamma(d+1)}.$$

Comparing both expressions, it is easy to see that CLR inequality hold if and only if

$$(d-1)\left(1 + \frac{1}{\left(\frac{\kappa}{\sqrt{\Lambda}}\right)}\right)^2 \leq \left(\frac{\kappa}{2\sqrt{\Lambda}}\right)^{d-2}. \tag{9}$$

We now recall two well known facts. Firstly, for any non zero $x \in \mathbb{R}$, $1 + x < e^x$. Secondly, by the definition of exponentiation,

$$\left(\frac{\kappa}{2\sqrt{\Lambda}}\right)^{d-2} = e^{(d-2)ln\left(\frac{\kappa}{2\sqrt{\Lambda}}\right)}.$$

Combining both of them with the strictly increasing condition of the exponential function we get,

$$d - 1 = 1 + (d-2) < e^{d-2} \leq e^{(d-2)ln\left(\frac{\kappa}{2\sqrt{\Lambda}}\right)} \text{ if } \frac{\kappa}{\sqrt{\Lambda}} \geq 2e.$$

To finish our argument, we conclude considering the following limits:

$$\lim_{\alpha\to\infty}\left(1 + \frac{1}{\alpha}\right)^2 = 1 \text{ and } \lim_{\alpha\to\infty} ln\left(\frac{\alpha}{2}\right) = \infty.$$

Therefore, if the coefficient $\frac{\kappa}{\sqrt{\Lambda}}$ is big enough, the last inequality holds. We denote by k_0 the number such that if $\frac{\kappa}{\sqrt{\Lambda}} \geq k_0$ then the inequality holds for all $d \geq 4$. Although we can not give an explicit computation of that value for the moment, numerical analysis show us that the inequality is valid when considering a really low value k_0. Namely,

$$4.27451 < k_0 < 4.27452.$$

However, we can proof analytically that the inequality 9 holds when $\frac{\kappa}{\sqrt{\Lambda}} \geq 4.5$. Although it is not the optimal value for k_0, will be sufficient to justify the argument in the following proofs. If $\frac{\kappa}{\sqrt{\Lambda}} \geq 4.5$, then

$$\left(1+\frac{1}{\left(\frac{\kappa}{\sqrt{\Lambda}}\right)}\right)^2 \leq \left(1+\frac{1}{(4.5)}\right)^2 \text{ and } \left(\frac{4.5}{2}\right)^{d-2} \leq \left(\frac{\kappa}{2\sqrt{\Lambda}}\right)^{d-2} \text{ for any } d \geq 4.$$

Hence, inequality 9 will hold if the function $h(d) = (d-1)(1+\frac{1}{(4.5)})^2 - (\frac{4.5}{2})^{d-2} \leq 0$ when $d \geq 4$. We note that $h(4) < 0$ and computing the derivative we see that $h(d)$ is strictly decreasing in $[4.5, \infty)$, completing the proof. □

Proof of Theorem 5 We move now to study the case where $\frac{\kappa}{\sqrt{\Lambda}} < k_0$. We first observe that there exist some cases for which the CLR inequalities hold trivially. In particular, in those cases where we do not have eigenvalues.

$$\frac{\frac{\kappa}{\sqrt{\Lambda}} - (d-1)}{2} < 0 \iff \begin{cases} d = 4 \text{ or } d = 5 : \frac{\kappa}{\sqrt{\Lambda}} < d-1. \\ d \geq 6 : \frac{\frac{\kappa}{\sqrt{\Lambda}} - (d-1)}{2} < \frac{k_0 - (d-1)}{2} < 0. \end{cases}$$

Therefore, if $d \geq 6$ the CLR inequalities hold trivially when $\frac{\kappa}{\sqrt{\Lambda}} < k_0$. This completes the proof of Theorem 5. □

Proof of Theorem 6 For the two remaining cases, $d = 4$ and $d = 5$, we have already proved that if

$$\frac{\kappa}{\sqrt{\Lambda}} \in (0, d-1) \cup [k_0, \infty),$$

then the CLR inequalities for the classical constant are valid. If we move to the remaining case, due to the value of k_0, the condition 7 holds if and only if $k = 0$. Therefore, we consider the CLR inequalities associated with one eigenvalue, $-\frac{\kappa^2}{(d-1)^2}$.

$$1 \leq 2^{1-d} \kappa^d \Lambda^{-d/2} \frac{1}{\Gamma(d+1)} = 2^{1-d} \frac{1}{\Gamma(d+1)} \left(\frac{\kappa}{\sqrt{\Lambda}}\right)^d$$

In those cases, the CLR inequalities hold if the quotient $\frac{\kappa}{\sqrt{\Lambda}}$ satisfies the following condition:

$$2^{(1-1/d)}\Gamma(d+1)^{1/d} \leq \frac{\kappa}{\sqrt{\Lambda}}$$

Nevertheless, the interval $[d-1, 2^{(1-1/d)}\Gamma(d+1)^{1/d})$ is non empty in both these cases. In particular, if we take $\Lambda = 1$ and $\kappa = d-1$, we get an example of the Coulomb Hamiltonian for which the CLR inequalities with the classical constant don't hold in dimension 4 and dimension 5. Concluding the proof of Theorem 6. □

3 Lieb–Thirring inequalities

As we advanced in the introduction, we extend Theorem 5 by means of the Aizenman–Lieb principle (Lemma 1), obtaining

Corollary 1 *Let $d \geq 6$ and $0 \leq \gamma < d/2$. Then for all $\kappa > 0$ and $\Lambda > 0$,*

$$Tr(-\Delta - \kappa|x|^{-1} + \Lambda)_-^{\gamma} \leq L_{\gamma,d}^{cl} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+d/2} dx.$$

In the cases where $d = 4$ or $d = 5$, we obtain the following corolary.

Corollary 2 *Let $d = 4$ or $d = 5$. Then, there exist $0 < \gamma_{0,d} < \frac{d}{2}$ as in (14) such that for all $\gamma_{0,d} \leq \gamma < d/2$, $\kappa > 0$ and $\Lambda > 0$,*

$$Tr(-\Delta - \kappa|x|^{-1} + \Lambda)_-^{\gamma} \leq L_{\gamma,d}^{cl} \int_{\mathbb{R}^d} (\kappa|x|^{-1} - \Lambda)_+^{\gamma+d/2} dx.$$

Proof of Corolary 2 From Lemma 2, the study of trivial cases in the proof of Theorem 5 and the study of the CLR inequalities associated with one eigenvalue in the proof of Theorem 6, we know that if

$$\frac{\kappa}{\sqrt{\Lambda}} \in (0, d-1) \cup [2^{(1-1/d)}\Gamma(d+1)^{1/d}, \infty),$$

then we can use the Aizenman–Lieb principle to extend the validity of the classical constant. To solve the remaining case, $\frac{\kappa}{\sqrt{\Lambda}} \in [d-1, 2^{(1-1/d)}\Gamma(d+1)^{1/d})$, we consider the following variational problem associated to one eigenvalue,

$$|E_1|^{\gamma} \leq L_{\gamma,d}^{cl} \int_{\mathbb{R}^d} V(x)_+^{\gamma+d/2} dx.$$

In our case, it reads as

$$\left(\frac{\kappa}{d-1}\right)^{2\gamma} \leq 2^{1-d}\kappa^d \Lambda^{\gamma-d/2} \frac{\Gamma(\gamma+1)\Gamma\left(\frac{d}{2}-\gamma\right)}{\Gamma(d+1)\Gamma\left(\frac{d}{2}\right)}.$$

When $d = 4$, can be rewritten as

$$\left(\frac{\kappa}{\sqrt{\Lambda}}\right)^{2(\gamma-2)} \leq \frac{3^{2\gamma-1}}{2^6}\Gamma(\gamma+1)\Gamma(2-\gamma). \tag{10}$$

And when $d = 5$, we obtain

$$\left(\frac{\kappa}{\sqrt{\Lambda}}\right)^{2\gamma-5} \leq \frac{2^{4\gamma-5}}{5 \cdot 3^2 \cdot \sqrt{\pi}}\Gamma(\gamma+1)\Gamma\left(\frac{5}{2}-\gamma\right). \tag{11}$$

In order to solve 10 and 11 with respect to the parameter γ, we note that for any $0 < \gamma < \frac{d}{2}$ the left hand side of both expressions is always less or equal to it's value at the point $d-1$. If we substitute the value and simplify, we can rewrite 10 and 11 as

$$\frac{2^6}{3^3} \leq \Gamma(\gamma+1)\Gamma(2-\gamma). \tag{12}$$

$$\frac{5 \cdot 3^2 \cdot \sqrt{\pi}}{2^5} \leq \Gamma(\gamma+1)\Gamma\left(\frac{5}{2}-\gamma\right). \tag{13}$$

Using the properties of the Gamma function, in particular using the fact that the right hand side of both equations tends to infinity when γ tends to $\frac{d}{2}$, we know both equations have solution. We will denote it by $\gamma_{0,d}$. Solving numerically,

$$1,5 < \gamma_{0,4} < 1,51 \text{ and } 1,86 < \gamma_{0,5} < 1,87. \tag{14}$$

Therefore, we can extend the result by the Aizenman–Lieb principle. □

Acknowledgements The author wants to thank Prof. Ari Laptev for his invaluable help to get this manuscript ready.

Author Contributions Both authors contributed equally to this work.

Funding The author was supported by JAEINT_22_00810 Grant at the ICMAT - Institute of Mathematical Sciences.

Data Availibility Statement No datasets were generated or analysed during the current study.

Declaration

Conflicts of interest The authors have no relevant financial or non-financial interests to disclose. The authors have no conflicts of interest to declare that are relevant to the content of this article. All authors certify that they have no affiliations with or involvement in any organization or entity with any financial interest or non-financial interest in the subject matter or materials discussed in this manuscript. The authors have no financial or proprietary interests in any material discussed in this article.

References

1. Frank, R.L., Laptev, A., Weidl, T.: Schrödinger Operators: Eigenvalues and Lieb–Thirring Inequalities. Cambridge Studies in Advanced Mathematics. Cambridge University Press, London (2022)
2. Cwikel, M.: Weak type estimates for singular values and the number of bound states of Schrödinger operators. Ann. Math. **106**(1), 93–100 (1977)
3. Lieb, E.H.: The Number of Bound States of One-Body Schrödinger Operators and the Weyl Problem, pp. 245–256. Springer, Berlin (2005)
4. Rozenblum, G.: Distribution of the discrete spectrum of singular differential operators. Izv. Vyssh. Uchebn. Zaved. Mat. **20**(1), 63–71 (1976)
5. Lieb, E.H., Thirring, W.E.: Inequalities for the Moments of the Eigenvalues of the Schrödinger Hamiltonian and Their Relation to Sobolev Inequalities, pp. 135–169. Springer, Berlin (1991)
6. Weyl, H.: Über die asymptotische verteilung der eigenwerte. *Nachrichten der Königlichen Gesellschaft der Wissenschaften zu Göttingen*, pp. 110–117 (1911)
7. Keller, J.B.: Lower bounds and isoperimetric inequalities for eigenvalues of the Schrödinger equation. J. Math. Phys. **2**(2), 262–266 (2004)
8. Schimmer, L.: The state of the Lieb–Thirring conjecture. In: The Physics and Mathematics of Elliott Lieb, vol. 2, pp. 253–275. EMS Press (2022)
9. Aizenman, M., Lieb, E.H.: On semi-classical bounds for eigenvalues of Schrödinger operators. Phys. Lett. A **66**(6), 427–429 (1978)