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Lieb–Thirring inequalities for the shifted Coulomb Hamiltonian

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Abstract. In this paper we prove sharp Lieb–Thirring (LT) inequalities for the family of shifted Coulomb Hamiltonians. More precisely, we prove the classical LT inequalities with the semi-classical constant for this family of operators in any dimension $d \geq 3$ and any $\gamma \geq 1$. We also prove that the semi-classical constant is never optimal for the Cwikel–Lieb–Rozenblum (CLR) inequalities for this family of operators in any dimension. In this case, we characterize the optimal constant as the minimum of a finite set and provide an asymptotic expansion as the dimension grows. Using the same method to prove the CLR inequalities for Coulomb, we obtain more information about the conjectured optimal constant in the CLR inequality for arbitrary potentials.

1. Introduction and statement of the main results

Let $V: \mathbb{R}^d \to \mathbb{R}$ be a potential, such that the Schrödinger operator $-\Delta - V$ is lower semi-bounded with a compact negative part. We denote the negative eigenvalues of $-\Delta - V$ in increasing order by

$$\lambda_0 < \lambda_1 < \lambda_2 < \cdots < 0$$

and the corresponding finite multiplicity of each λ_j by $\mu_j \in \mathbb{N}$. In the study of this negative spectrum the so-called Lieb–Thirring inequalities play an important role. Assume that $\gamma \geq 1/2$ for $d = 1$, $\gamma > 0$ for $d = 2$ or $\gamma \geq 0$ for $d \geq 3$. Then for any such admissible pair of d and γ, there exists a finite constant $R \in \mathbb{R}_+$, such that for all $V \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^d)$ with $V_+ \in \mathrm{L}^{\gamma+d/2}(\mathbb{R}^d)$, it holds

$$\mathrm{Tr}(-\Delta - V)_-^\gamma \leq R\, L^{\mathrm{cl}}_{\gamma,d} \int_{\mathbb{R}^d} V_+^{\gamma+d/2} \mathrm{d}x. \tag{1.1}$$

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(For the positive and negative parts of real numbers or self-adjoint operators we write $a_\pm := (|a| \pm a)/2$.) Here $L^{\mathrm{cl}}_{\gamma,d}$ stands for the semi-classical constant

$$L^{\mathrm{cl}}_{\gamma,d} := \frac{\Gamma(\gamma+1)}{(4\pi)^{d/2}\,\Gamma(\gamma+1+d/2)} \tag{1.2}$$

with Γ denoting the standard gamma function.

If $\gamma > 0$, the expression $\mathrm{Tr}(-\Delta - V)^\gamma_- = \sum_j \mu_j |\lambda_j|^\gamma$ is often called the *Riesz mean of order* γ of the negative eigenvalues, taking into account their multiplicities. On the other hand, if $\gamma = 0$, the left-hand side $\mathrm{Tr}(-\Delta - V)^0_- = \sum_j \mu_j$ equals the total multiplicity of all negative eigenvalues. In this case, (1.1) is commonly known as *Cwikel–Lieb–Rozenblum (CLR) inequality.*

The CLR-inequality was proven independently by Cwikel [4], Lieb [8], and Rozenblum [10]. Lieb and Thirring [9] proved the cases $\gamma > 1/2$ in $d = 1$ and $\gamma > 0$ in $d \geq 2$. The "limit" case $\gamma = 1/2$ in $d = 1$ was solved by Weidl [14]. Note that (1.1) fails for $\gamma < 1/2$ if $d = 1$ and for $\gamma = 0$ if $d = 2$.

As the validity of the bound (1.1) has been completely settled, nowadays research focuses on the optimal values $R_{\gamma,d}$ of the constants R. For the best known bounds on the optimal constant up to date, we refer the reader to the book [6], to the article [5], and to the recent works [2,3]. In particular, semi-classical analysis shows that $R_{\gamma,d} \geq 1$.

In this paper, we are interested in the family of CLR and LT inequalities for a special kind of Schrödinger operators, namely the shifted Coulomb Hamiltonian in $\mathrm{L}^2(\mathbb{R}^d)$, defined as

$$-\Delta - \frac{\kappa}{|x|} + \Lambda \quad \text{for } \kappa, \Lambda > 0.$$

This operator stands out for two reasons. For one thing, its spectrum can be computed explicitly, which allows for a direct analysis of the resulting expressions. For another, it is one of the physically most relevant Schrödinger operators, as it serves as a basic quantum model for non-interacting electrons bound to a point nucleus with charge $\kappa > 0$. Despite these facts, there are (to the best of our knowledge) only few works attempting to explicitly compute optimal constants in CLR and LT inequalities restricted to this family of operators, namely [6, 11].

The goal of this work is to fill in this gap. More precisely, our main contributions here are the following.

(i) We prove that for the family of shifted Coulomb potentials $V = \kappa|x|^{-1} - \Lambda$ the LT inequality (1.1) holds true with $R = 1$ for all dimensions $d \geq 3$ if $\gamma \in [1, d/2)$.

(ii) On the other hand, we prove that in any dimension $d \geq 3$ the CLR inequality (i.e., $\gamma = 0$) restricted to the full class of shifted Coulomb Hamiltonians does not hold with $R = 1$. Moreover, we characterize the optimal constant in this case and give an asymptotic expansion as the dimension increases.

(iii) We prove that the conjectured value of the optimal CLR constant *for arbitrary potentials* [7], which is given by the minimization of a specific function over integers, can be reduced to a minimization on an interval of length of order d around the point $d^2/6$. As a by-product of this analysis, we obtain an explicit asymptotic expansion of the conjectured optimal value as the dimension d grows.

We now present the precise statements of our main results.

1.1. Main results (i)

Our first result shows that the semi-classical constant is optimal for the Lieb–Thirring inequalities for the family of shifted Coulomb Hamiltonians with $\gamma \geq 1$. This result extends a result by Frank, Laptev, and Weidl [6, Section 5.2.2] for the case $d = 3$ to all dimensions $d \geq 3$.

Theorem 1.1 (Optimal LT inequalities for the shifted Coulomb Hamiltonian). *Let $d \geq 3$ and $\gamma \in [1, d/2)$. Then for any $\kappa, \Lambda > 0$, we have*

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_-^{\gamma} < L_{\gamma,d}^{\mathrm{cl}} \int\limits_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{\gamma+d/2} \mathrm{d}x, \tag{1.3}$$

where $L_{\gamma,d}^{\mathrm{cl}}$ is the semi-classical constant defined in (1.2).

We refer to (2.2) and (2.7) below for the explicit formulae of both sides in (1.3).

Since the family of shifted Coulomb potentials is closed with respect to the shift in energy, the general case $\gamma \in [1, d/2)$ follows by the Aizenman–Lieb argument [1] from (1.3) with $\gamma = 1$.[1] This case is of particular interest. Here one has, see (2.8),

$$L_{1,d}^{\mathrm{cl}} \int\limits_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{1+d/2} \mathrm{d}x = \frac{2^{2-d} \Lambda^{1-d/2} \kappa^d}{d!(d-2)}. \tag{1.4}$$

We point out that the bound (1.3) is strict. For $d \geq 4$, this also follows via the Aizenman–Lieb argument from the following somewhat stronger inequality in the case $\gamma = 1$, which we shall actually prove, cf. (2.18).

[1]The upper restriction $\gamma < d/2$ follows naturally from the fact that $(\kappa|x|^{-1} - \Lambda)_+ \in \mathrm{L}^p(\mathbb{R}^d)$ only for $p < d$.

Proposition 1.2 (Improved estimate). *For $d \geq 4$, it holds that*

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- \leq \Big(\frac{2^{2-d}\Lambda^{1-d/2}\kappa^d}{d!(d-2)} - \frac{\kappa^2}{4(d-1)(d-2)^2}\Big)_+ \tag{1.5}$$

for any $\kappa, \Lambda > 0$.

For $d = 3$, the bound (1.5) itself does not hold. However, straightforward computations yield the following modified elementary upper and lower bounds.

Proposition 1.3 (Sharp corrections to Lieb–Thirring for $d = 3$). *For all $\kappa, \Lambda > 0$ we have*

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- \leq \Big(\frac{\kappa^3}{12\sqrt{\Lambda}} - \frac{\kappa^2}{8} + \frac{\sqrt{\Lambda}\varkappa}{24}\Big)_+, \quad \varkappa = \sqrt{\Lambda}\Big(2\Big\lceil\frac{\kappa}{2\sqrt{\Lambda}}\Big\rceil - 1\Big), \tag{1.6}$$

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- \geq \Big(\frac{\kappa^3}{12\sqrt{\Lambda}} - \frac{\kappa^2}{8} - \frac{\sqrt{\Lambda}\kappa}{12}\Big)_+. \tag{1.7}$$

These inequalities are sharp as equality is achieved in (1.6) whenever $\kappa/\sqrt{\Lambda}$ is an odd natural number and in (1.7) whenever $\kappa/\sqrt{\Lambda}$ is an even natural number.

Note that for $d = 3$ the expression (1.4) turns into $\kappa^3/12\sqrt{\Lambda}$, see (2.9). Since $\kappa^2/8 - \sqrt{\Lambda}\varkappa/24 \geq \kappa^2/8 - \Lambda(\kappa/\sqrt{\Lambda} + 1)/24 > 0$ whenever the left-hand side of (1.6) is positive, that is for $\kappa/\sqrt{\Lambda} > 2$, the bound (1.3) is strict for $d = 3$, too.

The term $-\kappa^2/8$ in (1.6) and (1.7) is related to the Scott correction [12]. The bounds in Proposition 1.3 are instructive, since the asymptotic envelopes of the eigenvalue sum, including the semi-classical term, the Scott correction, and the oscillatory third term serve also as sharp universal upper and lower bounds. For an illustration, see Figure 1.

Finally, let us point out that for $d \geq 4$ the correction term in (1.5) is *not* related to a Scott-type term, since the asymptotics of the eigenvalue sums for the Coulomb Hamiltonian show a different behavior in higher dimensions [13]. The sole purpose of this term is to show strictness of (1.3).

1.2. Main results (ii)

Our next result concerns the CLR inequality for the Coulomb Hamiltonian. In [11] it is claimed that the optimal constant of the CLR inequality for the shifted Coulomb Hamiltonian is given by the semi-classical constant in case of $d \geq 6$. However, this turns out to be incorrect.[2] In fact, as we shall see, for any $d \geq 3$ one can find (uncount-

[2]For instance, for $d = 6$ and $\kappa/\sqrt{\Lambda} = 11.1$, we have $\operatorname{Tr}(-\Delta - \kappa/|x| + \Lambda)_-^0 = 121$, but $L^{\mathrm{cl}}_{0,d} \int (\kappa/|x| - \Lambda)_+^{d/2} \mathrm{d}x \approx 81.81$.

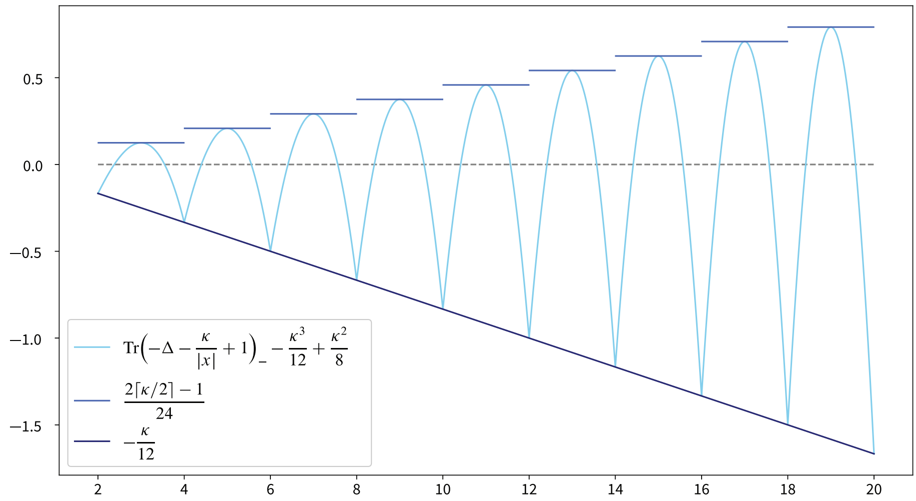

Figure 1. Behavior of the difference between left-hand side and right-hand side in (1.5) for $d = 3$, $\Lambda = 1$ and $\kappa \in (2, 20]$ oscillating between the correction terms from Proposition 1.3.

ably many) $\kappa, \Lambda > 0$, such that

$$\mathrm{Tr}\left(-\Delta - \frac{\kappa}{|x|} + \Lambda\right)_-^0 > L_{0,d}^{\mathrm{cl}} \int\limits_{\mathbb{R}^d} \left(\frac{\kappa}{|x|} - \Lambda\right)_+^{d/2} \mathrm{d}x,$$

see Figure 2.

Let us perform the corresponding analysis. For $d \geq 3$, we define the function

$$Q_d(t) := \left(t + \frac{d-1}{2}\right)^{-d} \left(t + \frac{d}{2}\right) \prod_{j=1}^{d-1} (t + j), \quad t \in \mathbb{R}, t \neq -\frac{d-1}{2}. \tag{1.8}$$

One of the main points of our analysis will be to show that $Q_d(t)$ has a unique maximum for $t \in [0, +\infty)$, at which it is larger than one. In fact, for sufficiently large d we can localize the corresponding non-negative real argument t, at which the maximum is attained, in an interval of length $d - 2$ around the point $d^2/6 - d + 5/6$, see Lemma 3.1. The optimal value of R in the CLR inequality (1.1) restricted to the shifted Coulomb Hamiltonian will correspond to the maximal value of $Q_d(t)$ over a corresponding set of natural numbers.

Indeed, set $Q_3^* := Q_3(0)$ as well as, for $d \geq 4$,

$$Q_d^* := \max\left\{Q_d(\ell) : \ell \in \mathbb{N}_0 \wedge \left\lfloor \frac{d^2}{6} - \frac{3d}{2} + \frac{7}{3} \right\rfloor \leq \ell \leq \left\lceil \frac{d^2}{6} - \frac{d}{2} - \frac{2}{3} \right\rceil\right\}.$$

It turns out that Q_d^* is the optimal choice for the factor R and that $Q_d^* > 1$ for all $d \geq 3$, see Remark 3.2. In particular, the optimal constant in the CLR inequality for the family of shifted Coulomb Hamiltonians is strictly larger than the semi-classical constant *in any dimension* $d \geq 3$.

Theorem 1.4 (Optimal CLR inequalities for the shifted Coulomb Hamiltonian). *For all* $d \geq 3$, *it holds that*

$$\inf\Big\{R : \operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_-^0 \leq R L_{0,d}^{\mathrm{cl}} \int_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{d/2} \mathrm{d}x \text{ for all } \kappa, \Lambda > 0\Big\}$$
$$= Q_d^* > 1.$$

We can also derive the following asymptotic expansion for Q_d^* as $d \to +\infty$.

Proposition 1.5 (Asymptotic expansion in high dimensions). *It holds*

$$Q_d^* = 1 + \frac{3}{2d} + \frac{45}{8d^2} + \mathcal{O}(d^{-3}) \quad \text{as } d \to +\infty.$$

Remark 1.6. In the process of proving Theorem 1.4, we shall see that the maximal excess factor $R = Q_d^*$ in the CLR inequality (1.1) restricted to the shifted Coulomb Hamiltonian is achieved in a regime of $d^2/6 + \mathcal{O}(d)$ distinct eigenvalues as $d \to +\infty$. Hence, Theorem 1.4 provides – besides the one in [7] – another class of potentials for which the optimal constant in the CLR inequality is strictly larger than both the semi-classical constant *and* the one-particle constant in high dimensions.

1.3. Main results (iii)

Our last result concerns a hypothesis on the optimal CLR constant *for arbitrary potentials* proposed by Glaser, Grosse, and Martin [7]. We briefly recall their conjecture. As above, let $R_{0,d}$ be the optimal value of the constant R in (1.1) with $d \geq 3$ and $\gamma = 0$ considered on all potentials $V \in \mathrm{L}^1_{\mathrm{loc}}(\mathbb{R}^d)$ with $V_+ \in \mathrm{L}^{d/2}(\mathbb{R}^d)$.

For $d \geq 3$, we define the function

$$A_d(t) := \Big(t + \frac{d}{2}\Big)^{1-d/2}\Big(t + \frac{d}{2} - 1\Big)^{-d/2} \prod_{k=1}^{d-1}(t+k), \tag{1.9}$$

with

$$t \in \mathbb{R}, \quad t \neq -\frac{d}{2}, \quad t \neq -\frac{d}{2} + 1,$$

and set $A_d^* := \sup\{A_d(\ell) : \ell \in \mathbb{N}_0\}$.

Conjecture 1.7 ([7]). *It holds that*

$$R_{0,d} = A_d^*.$$

The structure of the function A_d and the constant A_d^* in the aforementioned conjecture are quite similar to the one of Q_d and Q_d^* from Theorem 1.4. In fact, it is not hard to see that $Q_d \leq A_d$. Therefore, our results in Theorem 1.4 do not contradict this conjecture.

Adapting our analysis of Q_d to A_d, we can show that A_d^* and Q_d^* behave similarly to the dimension increases. The following theorem gives the precise formulation of this result.

Theorem 1.8 (On the conjectured optimal CLR excess factor). *For $d = 3, 4$, we have $A_d^* = A_d(0)$ and for $d \geq 5$, we have*

$$A_d^* = \max\Big\{A_d(\ell) : \ell \in \mathbb{N}_0 \wedge \Big\lfloor \frac{d^2}{6} - \frac{3d}{2} + \frac{5}{3} \Big\rfloor \leq \ell \leq \Big\lceil \frac{d^2}{6} - \frac{d}{2} - 1 \Big\rceil\Big\}.$$

Moreover, A_d^* and Q_d^* satisfy the asymptotic relations

$$A_d^* = Q_d^* + \mathcal{O}(d^{-3}) = 1 + \frac{3}{2d} + \frac{45}{8d^2} + \mathcal{O}(d^{-3}) \quad \text{as } d \to +\infty. \tag{1.10}$$

Remark 1.9. Theorem 1.8 shows that the conjectured value of the optimal constant in the CLR inequality approaches the semi-classical constant with convergence rate of order $1/d$ as the dimension increases, and that this value is (almost) achieved by the shifted Coulomb Hamiltonian up to an error of order $1/d^3$. To the best of our knowledge, both results are new.

1.4. Outline of the paper

In Section 2 we shall first recall some basic facts about the spectrum of the shifted Coulomb Hamiltonian. Then we study the case $\gamma \geq 1$ and prove Theorem 1.1. In Section 3 we study the case $\gamma = 0$ and prove Theorem 1.4 as well as Proposition 1.5. In Section 4 we study the conjectured optimal excess factor in the CLR inequality for general potentials and prove Theorem 1.8.

Auxiliary properties and some elementary calculations will be presented in the appendix.

2. On the sharp LT inequalities for the shifted Coulomb Hamiltonian

2.1. Spectrum of the shifted Coulomb Hamiltonian

Let $d \geq 3$ and $\kappa > 0$. The negative spectrum of the Coulomb Hamiltonian $-\Delta - \kappa|x|^{-1}$ consists precisely of the eigenvalues

$$-\frac{\kappa^2}{(2j + d - 1)^2}$$

with multiplicities

$$\frac{(d-2+j)!\,(d-1+2j)}{(d-1)!\,j!} \quad \text{for } j=0,1,2,\dots.$$

For a detailed derivation of these formulae, see [6, Section 4.2.3].

Applying an energy shift $\Lambda > 0$, we see that $-\Delta - \kappa|x|^{-1} + \Lambda$ does not have negative spectrum at all as long as

$$\eta := \frac{\kappa}{\sqrt{\Lambda}} \le d-1.$$

Assume now that $\eta > d-1$, or equivalently,

$$\ell := \left\lceil \frac{\eta - d + 1}{2} \right\rceil - 1 \ge 0.$$

Then the negative spectrum of the shifted Coulomb Hamiltonian is given by the eigenvalues

$$\lambda_j = -\frac{\kappa^2}{(2j+d-1)^2} + \Lambda \quad \text{for } j=0,1,\dots,\ell,$$

with the corresponding multiplicities

$$\mu_j = \frac{(d-2+j)!\,(d-1+2j)}{(d-1)!\,j!} = \binom{d-1+j}{d-1} + \binom{d-2+j}{d-1}.$$

Using elementary properties of binomial coefficients and the *hockey-stick identity*, namely $\sum_{i=r}^{n}\binom{i}{r} = \binom{n+1}{r+1}$ for $n, r \in \mathbb{N}$ and $n \ge r$, the total multiplicity for the lowest $k+1$ eigenvalues $\lambda_0, \dots, \lambda_k$ can be computed as follows:

$$N_k := \sum_{j=0}^{k} \mu_j = \frac{(d+2k)(d+k-1)!}{d!\,k!} \quad \text{for } k=0,1,2,\dots,\ell.$$

In particular, we see that

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_-^0 = N_\ell = \frac{(d+2\ell)(d+\ell-1)!}{d!\,\ell!}. \tag{2.1}$$

For $\gamma > 0$, the Riesz means of the shifted Coulomb Hamiltonian are given by

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_-^\gamma = \sum_{j=0}^{\ell} \mu_j \Big(\frac{\kappa^2}{(2j+d-1)^2} - \Lambda\Big)^\gamma. \tag{2.2}$$

For $\gamma = 1$ this simplifies as follows:

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- = \sum_{j=0}^{\ell} \frac{\mu_j \kappa^2}{(2j+d-1)^2} - N_\ell \Lambda \tag{2.3}$$

$$= \sum_{j=0}^{\ell} \frac{\kappa^2 (d-2+j)!}{(d-1)!\, j!\, (d-1+2j)} - \frac{(d+2\ell)(d+\ell-1)!}{d!\,\ell!}\Lambda. \tag{2.4}$$

In the case $d = 3$, this turns into

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- = \frac{(\ell+1)\kappa^2}{4} - \frac{(\ell+1)(\ell+2)(2\ell+3)\Lambda}{6}. \tag{2.5}$$

2.2. Phase space integrals

The integral in the right-hand side of (1.3) can also be computed explicitly. It is finite for $0 \le \gamma < d/2$ and a standard variable transformation and the properties of the beta function yield

$$\int_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{\gamma+d/2} \mathrm{d}x = (4\pi)^{d/2} \frac{\Lambda^\gamma \eta^d}{2^{d-1}} \frac{\Gamma\big(\gamma+1+\frac{d}{2}\big)\Gamma\big(\frac{d}{2}-\gamma\big)}{\Gamma(d+1)\Gamma\big(\frac{d}{2}\big)}. \tag{2.6}$$

Combining (2.6) with the semi-classical constant (1.2), we see that the right-hand side of (1.3) reads as follows:

$$L^{\mathrm{cl}}_{\gamma,d} \int_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{\gamma+d/2} \mathrm{d}x = \frac{\Lambda^\gamma \eta^d}{2^{d-1}} \frac{\Gamma(\gamma+1)\Gamma\big(\frac{d}{2}-\gamma\big)}{\Gamma(d+1)\Gamma\big(\frac{d}{2}\big)}. \tag{2.7}$$

For $\gamma = 1$, this gives

$$L^{\mathrm{cl}}_{1,d} \int_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{1+d/2} \mathrm{d}x = \frac{\Lambda \eta^d}{2^{d-2}} \frac{1}{d!\,(d-2)}, \tag{2.8}$$

and in the case of $d = 3$, we get

$$L^{\mathrm{cl}}_{1,3} \int_{\mathbb{R}^3} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{5/2} \mathrm{d}x = \frac{\Lambda \eta^3}{12}. \tag{2.9}$$

On the other hand, for $\gamma = 0$ and $d \ge 3$ one has

$$L^{\mathrm{cl}}_{0,d} \int_{\mathbb{R}^d} \Big(\frac{\kappa}{|x|} - \Lambda\Big)_+^{d/2} \mathrm{d}x = \frac{\eta^d}{2^{d-1}\, d!}. \tag{2.10}$$

2.3. Proving the optimal LT inequality for the shifted Coulomb Hamiltonian

Proof of Proposition 1.3. We have $d = 3$. Using the notation $\eta = \kappa/\sqrt{\Lambda} > 0$ and $\ell = \lceil(\eta - 2)/2\rceil - 1 = \lceil \eta/2 \rceil - 2$, we write $\ell = \eta/2 + \delta_\eta - 2$ with $\delta_\eta := \lceil \eta/2 \rceil - \eta/2 \in [0, 1)$. For $\eta \leq 2$, the negative spectrum of $-\Delta - \kappa|x|^{-1} + \Lambda$ is empty. For $\eta > 2$, we have $\ell \in \mathbb{N}_0$ and the identity (2.5) gives

$$\begin{aligned}\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- &= \Lambda\Big(\frac{\eta^2(\ell+1)}{4} - \frac{(\ell+1)(\ell+2)(2\ell+3)}{6}\Big)\\ &= \Lambda\Big(\frac{\eta^3}{12} - \frac{\eta^2}{8} + \varphi(\eta)\Big) \qquad (2.11)\end{aligned}$$

with

$$\varphi(\eta) := \Big(\frac{\delta_\eta(1-\delta_\eta)}{2} - \frac{1}{12}\Big)\eta - \frac{\delta_\eta(1-\delta_\eta)(1-2\delta_\eta)}{6}, \quad \eta > 2.$$

Rewriting $\eta = 2\ell - 2\delta_\eta + 4 = 2m + 2\varepsilon$ with $m = \ell + 1 \in \mathbb{N}$ and $\varepsilon = 1 - \delta_\eta \in (0, 1]$, this turns into

$$\varphi(\eta) = \varphi(2m + 2\varepsilon) = -\frac{2}{3}\varepsilon^3 + \frac{1-2m}{2}\varepsilon^2 + m\varepsilon - \frac{m}{6}.$$

Elementary computations show that for fixed $m \in \mathbb{N}$ and $\varepsilon \in (0, 1]$, we have

$$-\frac{\eta}{12} = -\frac{m+\varepsilon}{6} \leq \varphi(\eta) \leq \frac{2m+1}{24} = \frac{2\lceil \frac{\eta}{2} \rceil - 1}{24}.$$

Equality is attained for each $m \in \mathbb{N}$ on the left-hand side for $\varepsilon = 1$ and in the limit $\varepsilon \to +0$, while on the right-hand side for $\varepsilon = 1/2$. If we put this back into (2.11), we arrive at

$$\begin{aligned}\Lambda\Big(\frac{\eta^3}{12} - \frac{\eta^2}{8} - \frac{\eta}{12}\Big) &\leq \operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_-\\ &\leq \Lambda\Big(\frac{\eta^3}{12} - \frac{\eta^2}{8} + \frac{2\lceil \frac{\eta}{2} \rceil - 1}{24}\Big) \quad \text{for } \eta > 2.\end{aligned}$$

It remains to observe that for $0 < \eta \leq 2$ the left term is less or equal to zero and the middle term vanishes. ■

Proof of Theorem 1.1. It remains to prove (1.5) for $d \geq 4$ and $\eta = \kappa/\sqrt{\Lambda} > d - 1$.

Step 1. In what follows, it is convenient to use the following (shifted) Pochhammer symbols. Let $t \in \mathbb{R}$. We define

$$p_0(t) := 1$$

and

$$p_m(t) := \prod_{k=1}^{m} (t+k) \quad \text{for } m \in \mathbb{N}.$$

By definition, we see that $p_m(-1) = 0$ for $m \in \mathbb{N}$ and that

$$p_m(t) = (t+m)p_{m-1}(t) \quad \text{for all } t \in \mathbb{R},\ m \in \mathbb{N}.$$

A key property of p_m, which can be directly verified from its definition, is the recursive relation

$$m p_{m-1}(t) = p_m(t) - p_m(t-1) \quad \text{for all } t \in \mathbb{R},\ m \in \mathbb{N}. \tag{2.12}$$

In particular, this identity allows us to explicitly evaluate the following sum:

$$m \sum_{j=0}^{\ell} p_{m-1}(j) = \sum_{j=0}^{\ell} (p_m(j) - p_m(j-1)) = p_m(\ell), \quad m \in \mathbb{N},\ \ell \in \mathbb{N}_0. \tag{2.13}$$

Step 2. Let us use this property to evaluate the sum in (2.3) and (2.4). Note that

$$\frac{(d-1)!\mu_j}{(2j+d-1)^2} = \frac{(d-2+j)!}{j!\,(d-1+2j)} = \frac{p_{d-2}(j)}{d-1+2j} = \frac{(d-2+j)\,p_{d-3}(j)}{d-1+2j}.$$

This yields

$$\frac{(d-1)!\mu_j}{(2j+d-1)^2} = \frac{p_{d-3}(j)}{2} + \frac{(d-3)\,p_{d-3}(j)}{2(d-1+2j)}.$$

Taking the sum in j from 0 to ℓ, in view of (2.13), the contribution of the first term on the right-hand side can be computed explicitly

$$(d-2)\sum_{j=0}^{\ell} \frac{(d-1)!\mu_j}{(2j+d-1)^2} = \frac{p_{d-2}(\ell)}{2} + \frac{(d-2)(d-3)}{2}\Big(\sum_{j=0}^{\ell} \frac{p_{d-3}(j)}{d-1+2j}\Big).$$

To treat the second term on the right-hand side, we first apply (2.12) to each summand individually,

$$\begin{aligned}(d-2)\sum_{j=0}^{\ell} \frac{(d-1)!\mu_j}{(2j+d-1)^2} \\ = \frac{p_{d-2}(\ell)}{2} + \frac{d-3}{2}\Big(\sum_{j=0}^{\ell} \frac{p_{d-2}(j) - p_{d-2}(j-1)}{d-1+2j}\Big).\end{aligned} \tag{2.14}$$

Now, we use Abel's formula of summation by parts, i.e.,

$$\sum_{j=0}^{\ell} A_j(B_j - B_{j-1}) = A_\ell B_\ell + \sum_{j=0}^{\ell-1}(A_j - A_{j+1})B_j, \quad A_j, B_j \in \mathbb{R}, \ B_{-1} = 0,$$

with the choice $A_j := (d-1+2j)^{-1}$ and $B_j := p_{d-2}(j)$. If $\ell = 0$, we use the convention that sums of the type $\sum_{j=0}^{-1}$ vanish. This gives

$$\sum_{j=0}^{\ell} \frac{p_{d-2}(j) - p_{d-2}(j-1)}{d-1+2j} = \frac{p_{d-2}(\ell)}{d-1+2\ell} + 2\sum_{j=0}^{\ell-1} \frac{p_{d-2}(j)}{(d-1+2j)(d+1+2j)}.$$

In view of the elementary estimate

$$4(j+1)(d-2+j) \le (d-1+2j)(d+1+2j)$$

and the definition of the Pochhammer symbol, we claim that

$$\frac{p_{d-2}(j)}{(d-1+2j)(d+1+2j)} \le \frac{p_{d-2}(j)}{4(j+1)(d-2+j)} = \frac{p_{d-3}(j)}{4(j+1)} = \frac{p_{d-4}(j+1)}{4}$$

and by (2.13),

$$\begin{aligned}\sum_{j=0}^{\ell} \frac{p_{d-2}(j) - p_{d-2}(j-1)}{d-1+2j} &\le \frac{p_{d-2}(\ell)}{d-1+2\ell} + \frac{1}{2}\sum_{j=0}^{\ell-1} p_{d-4}(j+1) \\ &= \frac{p_{d-2}(\ell)}{d-1+2\ell} + \frac{p_{d-3}(\ell) - p_{d-3}(0)}{2(d-3)}.\end{aligned}$$

Finally, we make use of the identities $p_{d-2}(\ell) = (d-2+\ell)p_{d-3}(\ell)$ and $p_{d-3}(0) = (d-3)!$ and get

$$\begin{aligned}&\frac{d-3}{2}\sum_{j=0}^{\ell} \frac{p_{d-2}(j) - p_{d-2}(j-1)}{d-1+2j} \\ &\quad\le \frac{(d-3)p_{d-2}(\ell)}{2(d-1+2\ell)} + \frac{p_{d-2}(\ell)}{4(d-2+\ell)} - \frac{(d-3)!}{4}.\end{aligned}$$

Inserting this back into (2.14), we finally arrive at

$$(d-1)!\,(d-2)\sum_{j=0}^{\ell} \frac{\mu_j}{(2j+d-1)^2} \le \alpha\, p_{d-2}(\ell) - \frac{(d-3)!}{4} \tag{2.15}$$

with

$$\alpha := \frac{1}{2} + \frac{(d-3)}{2(d-1+2\ell)} + \frac{1}{4(d-2+\ell)}. \tag{2.16}$$

Step 3. We turn now to the full expression in (2.3)–(2.4). Using the identity

$$d!N_\ell = \frac{(d+2\ell)(d+\ell-1)!}{\ell!} = (d+2\ell)(d+\ell-1)p_{d-2}(\ell)$$

together with (2.15), we find that

$$\begin{aligned}\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- &= \sum_{j=0}^{\ell} \frac{\mu_j \kappa^2}{(2j+d-1)^2} - N_\ell \Lambda \\ &\leq \frac{\Lambda\,\eta^d}{d!(d-2)} p_{d-2}(\ell)\,\omega - \frac{\kappa^2}{4(d-1)(d-2)^2}. \end{aligned} \tag{2.17}$$

Here

$$\omega := d\eta^{2-d}\alpha - \eta^{-d}(d-2)\beta,$$

where α is given in (2.16) and $\beta := (d+2\ell)(d+\ell-1)$. We can now use the fact that

$$\omega \leq \sup_{\eta\geq 0}\,(d\eta^{2-d}\alpha - \eta^{-d}(d-2)\beta) = 2\,\alpha^{d/2}\beta^{1-d/2}$$

to further estimate (2.17) from above. We obtain

$$\operatorname{Tr}\Big(-\Delta - \frac{\kappa}{|x|} + \Lambda\Big)_- \leq \frac{2^{2-d}\Lambda\,\eta^d}{d!(d-2)} G(\ell) - \frac{\kappa^2}{4(d-1)(d-2)^2} \tag{2.18}$$

with $\ell = \lceil(\eta+1-d)/2\rceil - 1 \in \mathbb{N}_0$ as before and G being defined, for $t \geq 0$, as

$$\begin{aligned} G(t) := p_{d-2}(t)\Big(1 + \frac{d-3}{d-1+2t} + \frac{1}{2(d-2+t)}\Big)^{d/2} \\ \times\Big(\Big(\frac{d}{2}+t\Big)\Big(d+t-1\Big)\Big)^{1-d/2}. \end{aligned} \tag{2.19}$$

The coefficient in front of $G(\ell)$ is precisely the value of the semi-classical phase space integral, see (2.8). The upcoming Lemma 2.1 shows that $G(\ell) \leq 1$ for all $\ell \in \mathbb{N}_0$. Consequently, (1.5) is proven. ∎

Lemma 2.1. *For $d \geq 4$, the function G defined in* (2.19) *is strictly increasing for $t \geq 0$ and satisfies* $\lim_{t\to+\infty} G(t) = 1$.

Proof. To simplify some calculations, it is more convenient to work with the translated function

$$g(t) := G\Big(t - \frac{d-1}{2}\Big),$$

which, after an index shift in the definition of the Pochhammer symbol, is given as follows:

$$g(t) = \Big[\prod_{k=0}^{d-3}\Big(t - \frac{d-3}{2} + k\Big)\Big]\Big(1 + \frac{d-3}{2t} + \frac{1}{2\big(t + \frac{d-3}{2}\big)}\Big)^{d/2}$$
$$\times\Big(\Big(t + \frac{1}{2}\Big)\Big(t + \frac{d-1}{2}\Big)\Big)^{1-d/2}.$$

Our goal is then to show that $g(t) \leq 1$ for $t \geq (d-1)/2$ and $\lim_{t\to+\infty} g(t) = 1$.

The limit is immediate to compute. To prove the inequality, it suffices to show that the derivative of $\log g(t)$ is non-negative for $t \geq (d-1)/2$. To this end, we note that

$$\begin{aligned}(\log g)'(t) = {} & \sum_{k=0}^{d-3}\Big(\frac{1}{t - \frac{d-3}{2} + k}\Big) \\ & + \frac{d}{2}\Big(\frac{4t + 2d - 5}{2t^2 + (2d-5)t + \frac{(d-3)^2}{2}} - \frac{1}{t} - \frac{1}{t + \frac{d-3}{2}}\Big) \\ & - \frac{d-2}{2}\Big(\frac{1}{t + \frac{1}{2}} + \frac{1}{t + \frac{d-1}{2}}\Big).\end{aligned} \tag{2.20}$$

Then, we use two elementary inequalities to find a simpler lower bound for $(\log g)'(t)$. The first inequality is immediate to verify and reads, for $t \geq 0$, as follows:

$$\begin{aligned}\frac{4t + 2d - 5}{2t^2 + (2d-5)t + \frac{(d-3)^2}{2}} & \geq \frac{4t + 2d - 5}{2t^2 + (2d-5)t + \frac{(d-2)(d-3)}{2}} \\ & = \frac{1}{t + \frac{d-2}{2}} + \frac{1}{t + \frac{d-3}{2}}.\end{aligned} \tag{2.21}$$

The second inequality follows from the relation between harmonic and arithmetic means:

$$\begin{aligned}& \sum_{k=1}^{d-3}\Big(t - \frac{d-3}{2} + k\Big)^{-1} \\ & \quad \geq (d-3)^2\Big(\sum_{k=1}^{d-3}\Big(t - \frac{d-3}{2} + k\Big)\Big)^{-1} = \frac{d-3}{t + \frac{1}{2}} \quad \text{for } t \geq \frac{d-3}{2}.\end{aligned} \tag{2.22}$$

Hence, applying (2.21) and (2.22) to (2.20), we find that

$$\begin{aligned}(\log g)'(t) & \geq \frac{1}{t - \frac{d-3}{2}} + \frac{d-3}{t + \frac{1}{2}} + \frac{d}{2}\Big(\frac{1}{t + \frac{d-2}{2}} - \frac{1}{t}\Big) - \frac{d-2}{2}\Big(\frac{1}{t + \frac{1}{2}} + \frac{1}{t + \frac{d-1}{2}}\Big) \\ & = \frac{1}{t - \frac{d-3}{2}} - \frac{\frac{d}{2}}{t} + \frac{\frac{d}{2} - 2}{t + \frac{1}{2}} + \frac{\frac{d}{2}}{t + \frac{d-2}{2}} - \frac{\frac{d}{2} - 1}{t + \frac{d-1}{2}} \\ & = \frac{h(t)}{\big(t - \frac{d-3}{2}\big)t\big(t + \frac{1}{2}\big)\big(t + \frac{d-2}{2}\big)\big(t + \frac{d-1}{2}\big)}\end{aligned}$$

with

$$h(t) = \frac{(d-2)(d-4)}{4}t^2 + \frac{(5d-16)(d-1)(d-2)}{16}t + \frac{d(d-1)(d-2)(d-3)}{32}.$$

One can easily see that all coefficients of $h(t)$ are non-negative for $d \geq 4$. Therefore, we obtain $(\log g)'(t) \geq h(t) \geq 0$ for $t \geq (d-1)/2$, which completes the proof. ■

3. On the sharp CLR inequalities for the shifted Coulomb Hamiltonian

Proof of Theorem 1.4. By (2.1) and (2.10), we need to study the behaviour of the quotient

$$R_d(\eta) := \frac{\operatorname{Tr}\big(-\Delta - \frac{\kappa}{|x|} + \Lambda\big)_-^0}{L_{0,d}^{\mathrm{cl}} \int_{\mathbb{R}^d} \big(\frac{\kappa}{|x|} - \Lambda\big)_+^{d/2} \mathrm{d}x} = \frac{d+2\ell}{2^{1-d}\eta^d} \prod_{j=1}^{d-1} (\ell + j).$$

Here we use again the notation $\eta = \kappa/\sqrt{\Lambda} > 0$ and $\ell = \lceil \tau \rceil - 1$ with $\tau := (\eta + 1 - d)/2$. Observe that, in view of $\tau \geq \ell$, we have

$$R_d(\eta) = \frac{d+2\ell}{2^{1-d}\eta^d} \prod_{j=1}^{d-1} (\ell + j) \leq \frac{\tau + \frac{d}{2}}{\big(\tau + \frac{d-1}{2}\big)^d} \prod_{j=1}^{d-1} (\tau + j) = Q_d(\tau)$$

with Q_d defined in (1.8). Moreover, we note that, even though $Q_d(\tau) \neq R_d(2\tau + d - 1)$ for any $\tau > 0$, we have the equality

$$Q_d(\tau_0) = \lim_{\tau \downarrow \tau_0} R_d(2\tau + d - 1) \quad \text{for any } \tau_0 \in \mathbb{N}_0.$$

As $R_d(2\tau + d - 1)$ is strictly decreasing in any interval $(\tau_0, \tau_0 + 1]$ with $\tau_0 \in \mathbb{N}_0$, the identity above implies that the supremum of Q_d over $\mathbb{N}_0$ gives the optimal excess factor in the CLR inequality. For a visual illustration of Q_d and R_d, see Figure 2. The proof is then completed with the upcoming Lemma 3.1. ■

Lemma 3.1. *For $d = 3$, the function Q_d defined in* (1.8) *is strictly decreasing in $(-1, +\infty)$. For $d \geq 4$, Q_d has a unique maximum at $t_d^* \in (-1, +\infty)$ satisfying*

$$\frac{d^2}{6} - \frac{3d}{2} + \frac{7}{3} < t_d^* < \frac{d^2}{6} - \frac{d}{2} - \frac{2}{3}. \tag{3.1}$$

Proof of Lemma 3.1. We proceed in three steps.

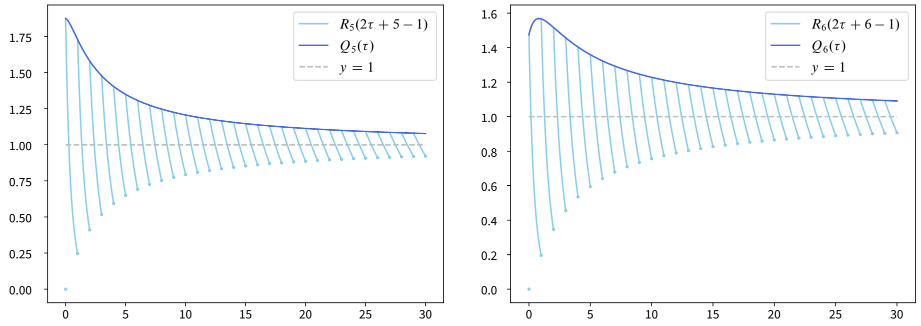

Figure 2. Comparison of $R_d(2\tau + d - 1)$, $Q_d(\tau)$ for $d = 5, 6$. The bold marked dots emphasize where R_d takes values.

Step 1. Let us define the set

$$\begin{aligned} P &:= \left\{-\frac{d}{2}, -\frac{d-1}{2}\right\} \cup \{-(d-1), -(d-2), \dots, -1\} \\ &= \left\{-\left\lceil \frac{d}{2} \right\rceil + \frac{1}{2}\right\} \cup \{-(d-1), -(d-2), \dots, -1\}, \end{aligned}$$

which consists of d elements. Then, for $t \in \mathbb{R} \setminus P$, an explicit calculation yields the representation

$$Q_d'(t) = Q_d(t)\, f_d(t) \tag{3.2}$$

with $f_d \colon \mathbb{R} \setminus P \to \mathbb{R}$ given by

$$f_d(t) := \frac{1}{t + \frac{d}{2}} - \frac{d}{t + \frac{d-1}{2}} + \sum_{k=1}^{d-1} \frac{1}{t+k}. \tag{3.3}$$

For $d = 3$, one can immediately verify that $f_3(t) < 0$ for all $t > -1$. Since $Q_3(t) > 0$ for $t > -1$, we have $Q_3'(t) < 0$ for $t > -1$ and the case $d = 3$ is proven.

Consider now $d \geq 4$. Since $Q_d(t) > 0$ for $t > -1$, by (3.2) it suffices to prove that f_d has a unique zero in $(-1, +\infty)$ located in the interval (3.1), where it changes from positive to negative values for increasing argument. To this end, we rewrite the rational function f_d as a quotient of co-prime polynomials, i.e.,

$$f_d(t) = \frac{p(t)}{q(t)}.$$

The set of poles of $f_d(t)$ matches the set P and all these poles are of order one. Hence, the polynom $q(t)$ is of degree d and can be chosen as follows:

$$q(t) := \Big(t + \Big\lceil \frac{d}{2} \Big\rceil - \frac{1}{2}\Big) \prod_{k=1}^{d-1} (t+k).$$

Due to the cancellation of the terms of order $1/t$ at infinity in (3.3), we have $f_d(t) = \mathcal{O}(t^{-2})$ as $t \to \infty$, and the degree of the polynomial p is at most $d-2$. In fact, a calculation provided in Appendix A shows that

$$p(t) = -\frac{d}{2}\Big(t^{d-2} + \Big(\frac{d^2}{3} - \Big\lfloor \frac{d}{2} \Big\rfloor - \frac{1}{3}\Big)t^{d-3} + r(t)\Big), \tag{3.4}$$

where r is a polynomial of degree at most $d-4$.

Step 2. Every zero of f_d must be a zero of p and, in particular, the function f_d has at most $d-2$ zeros. Analysing the sign changes of f_d in the intervals between two consecutive poles, we can infer the location of the zeros of f_d. Indeed, from (3.3) we conclude that

$$\lim_{t\uparrow\tau_k} f_d(t) = -\infty \quad \text{and} \quad \lim_{t\downarrow\tau_k} f_d(t) = +\infty \quad \text{for } \tau_k \in P \setminus \Big\{-\frac{d-1}{2}\Big\}, \tag{3.5}$$

as well as

$$\lim_{t\uparrow-(d-1)/2} f_d(t) = +\infty \quad \text{and} \quad \lim_{t\downarrow-(d-1)/2} f_d(t) = -\infty.$$

Let us define the disjoint open intervals $I_j = (-j-1, -j)$ for $j = 1, \dots, d-1$ with $j \notin \{\lfloor d/2 \rfloor - 1, \lfloor d/2 \rfloor\}$ and

$$I_j := \begin{cases} \Big(-\frac{d}{2}, -\Big\lfloor \frac{d}{2} \Big\rfloor + 1\Big) & \text{for } j = \Big\lfloor \frac{d}{2} \Big\rfloor - 1, \\ \Big(-\Big\lfloor \frac{d}{2} \Big\rfloor - 1, -\frac{d}{2}\Big) & \text{for } j = \Big\lfloor \frac{d}{2} \Big\rfloor. \end{cases}$$

Note that $-(d-1)/2 \in I_j$ for $j = \lfloor d/2 \rfloor - 1$, while each open interval I_j for $j \in \{1, \dots, d-2\} \setminus \{\lfloor d/2 \rfloor - 1\}$ has two poles of the type (3.5) as its endpoints and does not contain any poles inside. By the intermediate value theorem, we see that $f_d(t)$ has at least one zero in each of the latter intervals. This means that $f_d(t)$ has at least $d-3$ distinct zeros inside the interval $(-d+1, -1)$.

Moreover, the leading coefficient of p is negative and therefore

$$\lim_{t\to+\infty} p(t) = -\infty.$$

Since $q(t) > 0$ for $t > -1$, we see that $f_d(t)$ is negative for sufficiently large t.

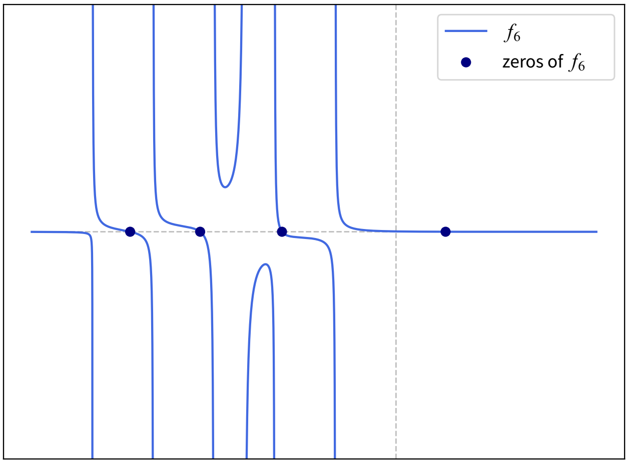

Figure 3. The function f_d for $d = 6$ and its four zeros: 3 negative ones and 1 positive one, as stated in the proof of Lemma 3.1.

On the other hand, in view of $d \geq 4$ we have $\lim_{t\downarrow -1} f_d(t) = +\infty$. Again, by the intermediate value theorem we deduce that f_d has at least one zero in the interval $(-1, +\infty)$. Since f_d has at most $d-2$ zeros in total, we conclude that f_d must have exactly one zero in each of the intervals I_j for $j \in \{1, \dots, d-2\} \setminus \{\lfloor d/2 \rfloor - 1\}$ and additionally one zero in the interval $(-1, +\infty)$ (see Figure 3 for an example of f_d), where it changes from positive to negative sign as the argument increases. Hence, this rightmost zero corresponds to the unique local maximum of Q_d in the interval $(-1, +\infty)$.

Step 3. We now proceed to prove the bound in (3.1). To this end, note that the previous arguments do not only give us a qualitative picture of the function f_d, but they also allow for a quantitative estimate on the negative zeros of the polynomial p.

From the previous discussion, we know that p has together with f_d exactly $d-2$ distinct zeros, one in each interval I_j for $j \neq \lceil (d-1)/2 \rceil - 1$ and one zero $t_d^* > -1$. Since p has the degree $d-2$, all these zeros are of order one. Therefore, taking the leading coefficient in (3.4) into account, we can write p in the factorized form

$$p(t) = -\frac{d}{2}(t - t_d^*) \prod_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor - 1}}^{d-2} (t + k + \varepsilon_k), \tag{3.6}$$

where all $\varepsilon_k \in (0, 1)$.[3]

[3]Note that we include the factor for $k = \lfloor d/2 \rfloor$ directly in the product, as all points from $I_{\lfloor \frac{d}{2} \rfloor} = (d/2, \lfloor d/2 \rfloor + 1)$ permit the necessary representation as well.

To estimate t_d^*, we compare (3.6) with (3.4) and apply Vieta's formula applied to the term of order t^{d-3}. This gives

$$-t_d^* + \sum_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor - 1}}^{d-2} (k + \varepsilon_k) = \frac{d^2}{3} - \left\lfloor \frac{d}{2} \right\rfloor - \frac{1}{3}.$$

In view of $0 < \varepsilon_k < 1$, the upper and lower bounds (3.1) follow. ∎

Remark 3.2. Since by our analysis $Q_d(t)$ is strictly increasing for all $t > t_d^*$ and $\lim_{t\to+\infty} Q_d(t) = 1$, we conclude that $Q_d(\ell) > 1$ for all $\ell \in \mathbb{N}$ with $\ell > t_d^*$. Therefore, $Q_d^* > 1$ for all $d \geq 3$.

Let us now turn to the proof of Proposition 1.5.

Proof of Proposition 1.5. By Lemma 3.1, for $d \geq 4$, the point t_d^* at which Q_d maximizes over the positive real numbers satisfies

$$\frac{d^2}{6} - \frac{3d}{2} + \frac{7}{3} \leq t_d^* \leq \frac{d^2}{6} - \frac{d}{2} - \frac{2}{3}.$$

Let us estimate $\log Q_d(t_d^*)$. For this, we use the Taylor expansion of $Q_d(t)$ around t_d^*. Since f_d is the logarithmic derivative of Q_d and $f_d(t_d^*) = 0$, the Lagrange remainder term gives for $t = d^2/6$

$$\begin{aligned} \left|\log Q_d\Big(\frac{d^2}{6}\Big) - \log Q_d(t_d^*)\right| &\leq \frac{1}{2} \sup_{s\in[t_d^*, d^2/6]} |f_d'(s)| \cdot \left|\frac{d^2}{6} - t_d^*\right|^2 \\ &\leq \frac{9d^2}{8} \sup_{s\in[t_d^*, d^2/6]} |f_d'(s)|. \end{aligned} \tag{3.7}$$

By (3.3), the derivative $f_d'(s)$ is equal to

$$\begin{aligned} f_d'(s) &= -\frac{1}{\big(s + \frac{d}{2}\big)^2} + \frac{d}{\big(s + \frac{d-1}{2}\big)^2} - \sum_{k=1}^{d-1} \frac{1}{(s+k)^2} \\ &= \frac{4s - 1 + 2d}{4\big(s + \frac{d}{2}\big)^2\big(s + \frac{d-1}{2}\big)^2} + \frac{d-1}{\big(s + \frac{d-1}{2}\big)^2} - \sum_{k=1}^{d-1} \frac{1}{(s+k)^2}, \qquad s \in \mathbb{R} \setminus P. \end{aligned}$$

Note that, for $s > 0$, the sum $\sum_{k=1}^{d-1} (s+k)^{-2}$ can be estimated from above and below as follows:

$$\begin{aligned} \frac{d-1}{(s+1)(s+d)} = \int_1^d \frac{1}{(s+k)^2} \mathrm{d}k \leq \sum_{k=1}^{d-1} \frac{1}{(s+k)^2} &\leq \int_0^{d-1} \frac{1}{(s+k)^2} \mathrm{d}k \\ &= \frac{d-1}{t(s+d-1)}. \end{aligned} \tag{3.8}$$

In particular, for values s from $\mathcal{I} = [d^2/6 - 3d/2, d^2/6]$, the lower bound in (3.8) leads to

$$\begin{aligned} f_d'(s) &\leq \frac{4s-1+2d}{4\big(s+\frac{d}{2}\big)^2\big(s+\frac{d-1}{2}\big)^2} + \frac{d-1}{\big(s+\frac{d-1}{2}\big)^2} - \frac{d-1}{(s+1)(s+d)} \\ &= \frac{4s-1+2d}{4\big(s+\frac{d}{2}\big)^2\big(s+\frac{d-1}{2}\big)^2} + \frac{(d-1)\big(2s+d-\big(\frac{d-1}{2}\big)^2\big)}{\big(s+\frac{d-1}{2}\big)^2(s+1)(s+d)} \leq C_+ d^{-5}, \quad s \in \mathcal{I}, \end{aligned} \tag{3.9}$$

with some uniform constant $C_+ > 0$ for all sufficiently large d. In a similar way, the upper bound in (3.8) gives for the same admissible values of s

$$\begin{aligned} f_d'(s) &\geq \frac{4s-1+2d}{4\big(s+\frac{d}{2}\big)^2\big(s+\frac{d-1}{2}\big)^2} + \frac{d-1}{\big(s+\frac{d-1}{2}\big)^2} - \frac{d-1}{s(s+d-1)} \\ &= \frac{4s-1+2d}{4\big(s+\frac{d}{2}\big)^2\big(s+\frac{d-1}{2}\big)^2} - \frac{(d-1)^3}{4\big(s+\frac{d-1}{2}\big)^2 s(s+d-1)} \geq -C_- d^{-5}, \quad s \in \mathcal{I}, \end{aligned} \tag{3.10}$$

with some uniform constant $C_- > 0$ for all sufficiently large d. Thus, by (3.7), (3.9), and (3.10), it holds

$$\left|\log Q_d\Big(\frac{d^2}{6}\Big) - \log Q_d(t_d^*)\right| = \mathcal{O}(d^{-3}) \quad \text{as } d \to +\infty.$$

By the way f_d changes sign at t_d^*, we see that $Q_d(t)$ is strictly increasing for $0 \leq t < t_d^*$ and strictly decreasing for $t > t_d^*$. Hence, the maximum of Q_d over all non-negative integers is taken at $\ell = \lfloor t_d^* \rfloor$ or at $\ell = \lceil t_d^* \rceil$. Using again the Taylor expansion of $Q_d(t)$ at t_d^*, (3.9), and (3.10), we see that

$$\begin{aligned} &|\log Q_d(\ell) - \log Q_d(t_d^*)| \\ &\quad \leq \frac{1}{2} \sup_{s \in [\lfloor t_d^* \rfloor, \lceil t_d^* \rceil]} |f_d'(s)| \cdot |\ell - t_d^*|^2 \leq C d^{-5} \quad \text{as } d \to +\infty. \end{aligned}$$

Therefore,

$$Q_d(\ell) = Q_d\Big(\frac{d^2}{6}\Big)(1 + \mathcal{O}(d^{-3})) \quad \text{as } d \to +\infty.$$

It remains to compute that

$$Q_d\Big(\frac{d^2}{6}\Big) = 1 + \frac{3}{2d} + \frac{45}{8d^2} + \mathcal{O}(d^{-3}) \quad \text{as } d \to +\infty.$$

This is best done computing the asymptotics for $\log Q_d(d^2/6)$ and inserting the result into the Taylor expansion for the exponential function at zero. ∎

4. On the CLR conjecture

Proof of Theorem 1.8. Let A_d be the function given in (1.9). For $t \in \mathbb{R} \setminus \{-1,-2,\dots,-d+1\}$ the derivative of A_d satisfies the identity $A'_d(t) = A_d(t)g_d(t)$ with

$$g_d(t) := \frac{1-\frac{d}{2}}{t+\frac{d}{2}} - \frac{\frac{d}{2}}{t+\frac{d}{2}-1} + \sum_{k=1}^{d-1} \frac{1}{t+k}.$$

As A_d is positive for $t \geq 0$, it suffices to study the behavior of g_d for $t \geq 0$. For $d \leq 4$, it is immediate to see that $g_d \leq 0$ and therefore A_d is decreasing, which completes the proof in this case.

For $d \geq 5$, we divide the proof into two cases. First, we consider the case when d is even. Later, we deal with the case when d is odd. In the even case, the proof follows the exact same steps of the proof of Theorem 1.4. For convenience of the reader, we sketch these steps below.

Step 1. *The case $d > 5$ even.* For d even, we note that the poles of the first two terms also appear as poles within the sum term. Rewriting g_d as a quotient of co-prime polynomials, we obtain

$$g_d(t) = \frac{p(t)}{q(t)},$$

where $q(t) := \prod_{k=1}^{d-1}(t+k)$ and $p(t)$ is a polynomial of order $d-3$ satisfying

$$p(t) = -\frac{d}{2}\Big(t^{d-3} + \Big(\frac{d^2}{3} - d + \frac{2}{3}\Big)t^{d-4} + \mathcal{O}(t^{d-5})\Big). \tag{4.1}$$

Thus, p (and consequently g_d) has at most $d-3$ zeros. Analysing the behavior of g_d near its poles and using the intermediate value theorem, as we did in the proof of Theorem 1.4, we conclude that g_d has at least one zero in each of the intervals $(-k-1,-k)$ for $k \in \{1,\dots,d-2\} \setminus \{d/2, d/2-2\}$, and at least one zero in the interval $(-1,+\infty)$. Therefore, g_d (and consequently p) has exactly one zero of order one in each of the described intervals. Hence, $p(t)$ can be written as a product as follows:

$$p(t) = -\frac{d}{2}(t-\tilde{t}_d)\prod_{\substack{k=1\\ k\notin\{d/2,d/2-2\}}}^{d-2}(t+k+\varepsilon_k), \tag{4.2}$$

where $\tilde{t}_d$ is the unique zero in the interval $(-1,+\infty)$. Expanding the right-hand side of (4.2) then yields

$$p(t) = -\frac{d}{2}t^{d-3} + \frac{d}{2}\Big(\tilde{t}_d - \sum_{\substack{k=1\\ k\notin\{d/2,d/2-2\}}}^{d-2}(k+\varepsilon_k)\Big)t^{d-4} + \mathcal{O}(t^{d-5}). \tag{4.3}$$

By comparing the coefficient in front of t^{d-4} in (4.3) with the corresponding one in (4.1) and using the estimates $0 \le \varepsilon_k \le 1$, we conclude that

$$\frac{d^2}{6} - \frac{3d}{2} + \frac{7}{3} \le \tilde{t}_d \le \frac{d^2}{6} - \frac{d}{2} - \frac{5}{3},$$

which is within the interval in Theorem 1.8.

Step 2. *The case $d \ge 5$ odd.* For d odd, we cannot apply the same argument because $g_d(t)$ has five consecutive poles with different sign, namely

$$\Big\{-\frac{d+1}{2}, -\frac{d}{2}, -\frac{d-1}{2}, -\frac{d}{2}+1, -\frac{d-3}{2}\Big\},$$

and therefore the counting poles argument does not add up. Hence, we shall first use a simple estimate to get rid of the middle pole $t = \{-(d-1)/2\}$, and then proceed as in the previous step. To this end, it is more convenient for calculations to work with the shifted function

$$\tilde{g}_d(s) := g_d\Big(s - \frac{d-1}{2}\Big) = \frac{1-\frac{d}{2}}{s+\frac{1}{2}} - \frac{\frac{d}{2}}{s-\frac{1}{2}} + \sum_{j=-(d-3)/2}^{j=(d-1)/2} \frac{1}{s+j}.$$

Note that it suffices to study the behaviour of the shifted function for $s \ge (d-3)/2$. Moreover, the set of poles of $\tilde{g}_d(s)$ is

$$P := \Big\{-\frac{d-1}{2}, -\frac{d-1}{2}+1, \dots, -1, -\frac{1}{2}, 0, \frac{1}{2}, 1, \dots, \frac{d-3}{2}\Big\},$$

and the pole at $t = -(d-1)/2$ is now located at $s = 0$. The simple estimate we use to get rid of this pole is the following:

$$\frac{1-a_d}{s-\frac{1}{2}} + \frac{a_d}{s+\frac{1}{2}} \le \frac{1}{s} \le \frac{1/2}{s-\frac{1}{2}} + \frac{1/2}{s+\frac{1}{2}}, \quad \text{for } s \ge \frac{d-3}{2}, \tag{4.4}$$

where

$$a_d := \frac{1}{2} + \frac{1}{2(d-3)}.$$

Precisely, we note that by (4.4) we have

$$h_{a_d}(s) < \tilde{g}_d(s) < h_{1/2}(s) \quad \text{for } s > \frac{d-3}{2}, \tag{4.5}$$

where $h_a(s)$ is the function defined for $s \in (\mathbb{R} \setminus P) \cup \{0\}$ by

$$h_a(s) := \frac{1-\frac{d}{2}}{s+\frac{1}{2}} - \frac{\frac{d}{2}}{s-\frac{1}{2}} + \frac{1-a}{s-\frac{1}{2}} + \frac{a}{s+\frac{1}{2}} + \sum_{\substack{k=-(d-3)/2 \\ k \neq 0}}^{(d-1)/2} \frac{1}{s+k}.$$

We can now apply the "counting poles" argument to the function $h_a(s)$ for $0 \le a \le 1$ to show that $h_a(s)$ has a unique zero inside the interval $(-\frac{(d-3)}{2}, +\infty)$ and to localize this zero. More precisely, by following the arguments in the previous step, one can show that

$$h_a(s) \ge 0 \quad \text{for } s \le \Big(\frac{d-1}{2}+a\Big)^{-1}\Big(\frac{d^3-6d^2+11d-3}{12}-\frac{d-2}{2}a\Big) \tag{4.6}$$

and

$$h_a(s) \le 0 \quad \text{for } s \ge \Big(\frac{d-1}{2}+a\Big)^{-1}\Big(\frac{d^3-6d^2+11d-3}{12}-\frac{d-2}{2}a\Big)+d-3. \tag{4.7}$$

Hence, by setting $a = 1/2$ in (4.7) and using (4.5), we find that

$$\tilde{g}_d(s) < 0 \quad \text{for } s \ge \frac{d^2}{6}-\frac{5}{3}+\frac{1}{2d}.$$

Shifting back, $g_d(t) = \tilde{g}_d(t+(d-1)/2)$, and using the trivial estimate $1/2d \le 1/6$ we obtain

$$g_d(t) < 0 \quad \text{for } t \ge \frac{d^2}{6}-\frac{d}{2}-1. \tag{4.8}$$

Similarly, by setting

$$a = a_d = \frac{1}{2}+\frac{1}{2(d-3)}$$

in (4.6) and using (4.5) we find

$$\tilde{g}_d(s) > 0 \quad \text{for } \frac{d-3}{2} < s \le \frac{d^2}{6}-d+\frac{7}{6}+\frac{3d-10}{6(d^2-3d+1)}.$$

Shifting back and using the trivial estimate

$$\frac{3d-10}{6(d^2-3d+1)} \ge 0$$

(valid for $d \ge 4$) we get

$$g_d(t) > 0 \quad \text{for } -1 < t \le \frac{d^2}{6}-\frac{3d}{2}+\frac{5}{3}. \tag{4.9}$$

In particular, any zeros of $g_d(t)$ for $t > -1$ are within the interval in Theorem 1.8. Together with (4.8) and (4.9), this implies that the maximum of $A_d(t)$ is achieved inside the desired interval.

Step 3. *Proving the asymptotic expression* (1.10). Let now $t \geq 0$. We note that

$$\frac{A_d(t)}{Q_d(t)} = \frac{\left(t + \frac{d-1}{2}\right)^d}{\left(t + \frac{d}{2}\right)^{d/2}\left(t + \frac{d}{2} - 1\right)^{d/2}} = \left(1 + \frac{1}{(2t + d - 1)^2 - 1}\right)^{d/2}.$$

Thus, one has $A_d(t) > Q_d(t)$. We know the maximizing points of both Q_d and A_d are contained within the interval $\mathcal{J} := [d^2/6 - 3d/2, d^2/6]$. For such t, we see that

$$\log A_d(t) - \log Q_d(t) = \frac{d}{2} \log\left(1 + \frac{1}{(2t + d - 1)^2 - 1}\right) \leq C d^{-3}, \quad t \in \mathcal{J},$$

with some uniform $C > 0$ for sufficiently large d. This implies the first equality in (1.10). The second equality in (1.10) follows from the expansion from Proposition 1.5. ∎

A. Proof of (3.4)

Proof of equation (3.4). First let us rewrite f_d from (3.3) as follows

$$\begin{aligned} f_d(t) &= \frac{1}{t + \frac{d}{2}} - \frac{1}{t + \frac{d-1}{2}} + \sum_{k=1}^{d-1}\left(\frac{1}{t + k} - \frac{1}{t + \frac{d-1}{2}}\right) \\ &= -\frac{1}{2\left(t + \frac{d-1}{2}\right)\left(t + \frac{d}{2}\right)} + \sum_{k=1}^{d-1} \frac{\frac{d-1}{2} - k}{\left(t + \frac{d-1}{2}\right)(t + k)}. \end{aligned}$$

Multiplying this expression by $q(t)$ yields

$$\begin{aligned} p(t) &= f_d(t)\left(t + \left\lceil\frac{d}{2}\right\rceil - \frac{1}{2}\right)\prod_{k=1}^{d-1}(t + k) \\ &= -\frac{1}{2}\prod_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1}(t + k) + \sum_{k=1}^{d-1}\left(\frac{d-1}{2} - k\right)\frac{t + \frac{d}{2}}{t + \left\lfloor\frac{d}{2}\right\rfloor}\prod_{\substack{j=1 \\ j \neq k}}^{d-1}(t + j). \end{aligned}$$

Note that the two different shapes the summand for $k = \lfloor d/2 \rfloor$ takes for odd and even d can be combined into one expression:

$$\left(\frac{d-1}{2} - \left\lfloor\frac{d}{2}\right\rfloor\right)\prod_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1}(t + k).$$

Hence, we have $p(t) = I(t) + J(t)$ with

$$I(t) := \Big(\frac{d-1}{2} - \Big\lfloor \frac{d}{2} \Big\rfloor - \frac{1}{2}\Big) \prod_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1} (t+k),$$

$$J(t) := \sum_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1} \Big(\frac{d-1}{2} - k\Big)\Big(t + \frac{d}{2}\Big) \prod_{\substack{j=1 \\ j \notin \{k, \lfloor d/2 \rfloor\}}}^{d-1} (t+j).$$

The term $I(t)$ expands as follows:

$$I(t) = \Big(\frac{d}{2} - \Big\lfloor \frac{d}{2} \Big\rfloor - 1\Big) t^{d-2} + T_1(d) t^{d-3} + r_1(t),$$

where the polynomial r_1 is at most of degree $d-4$. Let

$$S(d) := \sum_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1} k = \frac{(d-1)d}{2} - \Big\lfloor \frac{d}{2} \Big\rfloor.$$

By Vieta's theorem, the factor in front of t^{d-3} in $I(t)$ is then given by

$$T_1(d) = \Big(\frac{d}{2} - \Big\lfloor \frac{d}{2} \Big\rfloor - 1\Big) S(d) = \Big\lfloor \frac{d}{2} \Big\rfloor^2 + \Big(-\frac{d^2}{2} + 1\Big)\Big\lfloor \frac{d}{2} \Big\rfloor + \frac{d^3}{4} - \frac{3d^2}{4} + \frac{d}{2}.$$

Regarding $J(t)$, we find that

$$\begin{aligned} J(t) &= \sum_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1} \Big(\frac{d-1}{2} - k\Big)\Big(t^{d-2} + \Big(\frac{d}{2} + \sum_{\substack{j=1 \\ j \notin \{k, \lfloor d/2 \rfloor\}}}^{d-1} j \Big) t^{d-3} + r_{2,k}(t)\Big) \\ &= \Big(1 - d + \Big\lfloor \frac{d}{2} \Big\rfloor\Big) t^{d-2} + T_2(d)\, t^{d-3} + r_3(t), \end{aligned}$$

where $r_{2,k}$ and r_3 are polynomials of degree of at most $d-4$. We compute the factor in front of t^{d-3} in $J(t)$ as follows:

$$\begin{aligned} T_2(d) &= \sum_{\substack{k=1 \\ k \neq \lfloor d/2 \rfloor}}^{d-1} \Big(\frac{d-1}{2} - k\Big)\Big(\frac{d}{2} + S(d) - k\Big) \\ &= \frac{d^2 - 3d + 2}{2}\Big(\frac{d}{2} + S(d)\Big) \\ &\quad - \Big(d - \frac{1}{2} + S(d)\Big) S(d) + \frac{(d-1)d(2d-1)}{6} - \Big\lfloor \frac{d}{2} \Big\rfloor^2 \\ &= -2\Big\lfloor \frac{d}{2} \Big\rfloor^2 + \Big(\frac{d^2}{2} + \frac{3d}{2} - \frac{3}{2}\Big)\Big\lfloor \frac{d}{2} \Big\rfloor - \frac{5d^3}{12} + \frac{d^2}{2} - \frac{d}{12}. \end{aligned}$$

Combining these results, we find that

$$I(t) + J(t) = -\frac{d}{2}t^{d-2} + (T_1(d) + T_2(d))t^{d-3} + (r_1(t) + r_3(t)),$$

where

$$\begin{aligned} T_1(d) + T_2(d) &= -\Big\lfloor \frac{d}{2} \Big\rfloor^2 + \Big(\frac{3d}{2} - \frac{1}{2}\Big)\Big\lfloor \frac{d}{2} \Big\rfloor - \frac{d^3}{6} - \frac{d^2}{4} + \frac{5d}{12} \\ &= -\frac{d}{2}\Big(\frac{d^2}{3} - \Big\lfloor \frac{d}{2} \Big\rfloor - \frac{1}{3}\Big). \end{aligned}$$

This implies (3.4). ∎

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