ON THE SPECTRUM OF THE ONE-PARTICLE DENSITY MATRIX

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To the memory of M.Z. Solomyak

Abstract. The one-particle density matrix $\gamma(x,y)$ is one of the key objects in the quantum-mechanical approximation schemes. The self-adjoint operator Γ with kernel $\gamma(x,y)$ is trace class but no sharp results on the decay of its eigenvalues were previously known. The note presents the asymptotic formula $\lambda_k \sim (Ak)^{-8/3}$, $A \geq 0$, as $k \to \infty$, for the eigenvalues λ_k of the operator Γ, and describes the main ideas of the proof.

1. Introduction and main result

1.1. **Introduction.** Consider on $\mathsf{L}^2(\mathbb{R}^{3N})$ the Schrödinger operator

$$H = \sum_{k=1}^{N}\bigg(-\Delta_k - \frac{Z}{|x_k|}\bigg) + \sum_{1\le j<k\le N}\frac{1}{|x_j-x_k|}, \tag{1}$$

describing an atom with N particles (e.g. electrons) with coordinates $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $x_k \in \mathbb{R}^3$, $k = 1, 2, \dots, N$, and a nucleus with charge $Z > 0$. The notation Δ_k is used for the Laplacian w.r.t. the variable x_k. The operator H acts on the Hilbert space $\mathsf{L}^2(\mathbb{R}^{3N})$ and it is self-adjoint on the domain $D(H) = \mathsf{H}^2(\mathbb{R}^{3N})$, since the potential in (1) is an infinitesimal perturbation relative to the unperturbed operator $-\Delta = -\sum_k \Delta_k$, see e.g. [22, Theorem X.16]. Note that we do not need to assume that the particles are fermions, i.e. that the underlying Hilbert space consists of anti-symmetric L^2-functions. Our results are not sensitive to such assumptions. Let $\psi = \psi(\mathbf{x})$, $\mathbf{x} = (\hat{\mathbf{x}}, x_N)$, $\hat{\mathbf{x}} = (x_1, x_2, \dots, x_{N-1})$, be an eigenfunction of the operator H with an eigenvalue $E \in \mathbb{R}$, i.e. $\psi \in D(H)$ and

$$(H - E)\psi = 0.$$

We define the one-particle density matrix as the function

$$\gamma(x,y) = \int\limits_{\mathbb{R}^{3N-3}} \overline{\psi(\hat{\mathbf{x}}, x)}\psi(\hat{\mathbf{x}}, y)\, d\hat{\mathbf{x}}, \quad (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

We do not discuss the importance of this object for multi-particle quantum mechanics and refer to [10], [20], [21] for details and futher references. Our focus is on spectral

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properties of the self-adjoint non-negative operator Γ with the kernel $\gamma(x,y)$, which we call *the one-particle density operator*. Note that the operator Γ is represented as a product $\Gamma = \Psi^*\Psi$ where $\Psi : \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}^{3N-3})$ is the operator with the kernel $\psi(\hat{\mathbf{x}}, x)$. Since $\psi \in \mathsf{L}^2(\mathbb{R}^{3N})$, the operator Ψ is Hilbert-Schmidt, and hence Γ is trace class. The purpose of this note is to present the asymptotic formula (4) for the eigenvalues $\lambda_k(\Gamma) > 0$, $k = 1, 2, \dots$, of the operator Γ, labelled in descending order counting multiplicity. Apart from being a mathematically interesting and challenging question, spectral asymptotics for the operator Γ are important for quantum-mechanical computations. All computational methods of quantum chemistry rely on finite rank approximations of the operator $\boldsymbol{\Gamma}$, see e.g. [16] and [9] for discussion. The rate of decay of $\lambda_k(\Gamma)$ as $k \to \infty$ determines the precision of these approximations. It was shown in [16] that Γ has infinite rank. The results of [9] suggest that $\lambda_k(\Gamma) = O(k^{-8/3})$, which is confirmed by the formula (4).

We assume throughout that ψ decays exponentially as $|\mathbf{x}| \to \infty$:

$$|\psi(\mathbf{x})| \lesssim e^{-\varkappa_0|\mathbf{x}|},\ \mathbf{x} \in \mathbb{R}^{3N}. \tag{2}$$

Here $\varkappa_0 > 0$ is a constant, and the notation "$\lesssim$" means that the left-hand side is bounded from above by the right-hand side times some positive constant whose precise value is of no importance for us. This notation is used throughout the paper. For the discrete eigenvalues, i.e. the ones below the bottom of the essential spectrum of H, the bound (2) follows from [12]. The exponential decay for eigenvalues away from the thresholds, including embedded ones, was studied in [11], [17]. For more references and detailed discussion we quote [23].

1.2. **Main result.** To state the main results we need the sharp qualitative result for ψ obtained in [15]. In order to write all the formulas in a more compact and unified way, we use the notation $x_0 = 0$. As before, $\mathbf{x} = (x_1, x_2, \dots, x_N) \in \mathbb{R}^{3N}$.

Denote

$$\mathsf{S}_{ls} = \mathsf{S}_{sl} = \{\mathbf{x} \in \mathbb{R}^{3N} : x_l \neq x_s\},\ l \neq s, \quad l, s = 0, 1, 2, \dots, N.$$

Since the Coulomb potential $|x|^{-1}$ is real analytic for $x \neq 0$, by elliptic regularity, the function ψ is real-analytic away from the particle coalescence points $x_j = x_k$, i.e. on the set

$$\mathsf{U} = \bigcap_{0 \le l < s \le N} \mathsf{S}_{ls}.$$

For each $j = 0, 1, \dots, N-1$, we are interested in the behaviour of ψ on the set

$$\mathsf{U}_j = \bigcap_{0 \le l < s \le N-1} \mathsf{S}_{ls} \bigcap_{\substack{0 \le s \le N-1 \\ s \neq j}} \mathsf{S}_{sN}.$$

The set U_j includes the coalescence point $x_j = x_N$, $j = 0, 1, \dots, N-1$, but excludes all the others. Our main focus will be on the function ψ near the "diagonal" set

$$\mathsf{U}_j^{(\mathrm{d})} = \{\mathbf{x} \in \mathsf{U}_j : x_j = x_N\}.$$

Observe for completeness that the sets $\mathsf{U}_j, \mathsf{U}_j^{(\mathrm{d})}$ are of full measure in $\mathbb{R}^{3N}$ and $\mathbb{R}^{3N-3}$ respectively, and that they are connected.

The following property follows from [15, Theorem 1.4].

Proposition 1. *For each index $j = 0, 1, \dots, N-1$, there exists an open connected set $\Omega_j \subset \mathsf{U}_j$, such that $\mathsf{U}_j^{(d)} \subset \Omega_j$, and two uniquely defined functions ξ_j, η_j, both real analytic on Ω_j, such that for all $\mathbf{x} \in \Omega_j$ the following representation holds:*

$$\psi(\hat{\mathbf{x}}, x) = \xi_j(\hat{\mathbf{x}}, x) + |x_j - x|\eta_j(\hat{\mathbf{x}}, x). \tag{3}$$

Note that the above proposition does not claim that the functions ξ_j and η_j are smooth on the closure $\overline{\Omega_j}$. Moreover, Proposition 1 does not give any information on the integrability of ξ_j and η_j over Ω_j. Our first, "preparatory" theorem establishes integrability of η_j, which is necessary for the main asymptotic formula. To state this result introduce the notation

$$\tilde{\mathbf{x}}_j = (x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_{N-1}),$$

and write $\hat{\mathbf{x}} = (\tilde{\mathbf{x}}_j, x_j)$, $\mathbf{x} = (\tilde{\mathbf{x}}_j, x_j, x_N)$. Thus the function $\eta_j(\hat{\mathbf{x}}, x)$ on the diagonal $\mathsf{U}_j^{(\mathrm{d})}$ can be written as $\eta_j(\tilde{\mathbf{x}}_j, x, x)$.

Theorem 2. *If $N \geq 3$, then for each $j = 1, 2, \dots, N-1$ the function $\eta_j(\,\cdot\,, x, x)$ belongs to $\mathsf{L}^2(\mathbb{R}^{3N-6})$ a.e. $x \in \mathbb{R}^3$ and the function*

$$H(x) = \left[\sum_{j=1}^{N-1} \int_{\mathbb{R}^{3N-6}} \big|\eta_j(\tilde{\mathbf{x}}_j, x, x)\big|^2 d\tilde{\mathbf{x}}_j\right]^{\frac{1}{2}},$$

belongs to $\mathsf{L}^{\frac{3}{4}}(\mathbb{R}^3)$.

If $N = 2$, then the function $H(x) = |\eta_1(x, x)|$ belongs to $\mathsf{L}^{\frac{3}{4}}(\mathbb{R}^3)$.

Having at our disposal this theorem, we can now state the main result:

Theorem 3. *Suppose that the eigenfunction ψ satisfies the bound* (2). *Then the eigenvalues $\lambda_k(\Gamma), k = 1, 2, \dots,$ of the operator Γ satisfy the asymptotic formula*

$$\lim_{k\to\infty} k^{\frac{8}{3}}\lambda_k(\Gamma) = A^{\frac{8}{3}}, \tag{4}$$

with the constant

$$A = \frac{1}{3}\left(\frac{2}{\pi}\right)^{\frac{5}{4}} \int_{\mathbb{R}^3} H(x)^{\frac{3}{4}} dx. \tag{5}$$

One should remark that there seems to be no results in the literature claiming that at least one function $\eta_j(\hat{\mathbf{x}}, x)$ is not identically zero on the diagonal $x = x_j$. Thus, in principle, the coefficient A may be equal to zero.

Theorem 3 can be also extended to the case of a molecule with several nuclei whose positions are fixed. The modifications are straightforward.

In this note our aim is to describe the main ideas leading to the proof of Theorems 2 and 3. Complete proofs will be published elsewhere.

2. Ingredients of the proof

Here we list three ingredients of the proof of Theorems 2 and 3.

2.1. **Regularity of the eigenfunction.** The regularity of ψ has been well-studied in the literature. As mentioned earlier, according to the classical elliptic theory, due to the analyticity of the Coulomb potential $|x|^{-1}$ for $x\neq 0$, the function ψ is real analytic away from the particle coalescence points. T. Kato [19] established that the function ψ is locally Lipschitz. Note that the representation (3) is in line with this fact. More detailed information on ψ at the coalescence points was obtained, e.g. in [14], [15], [18]. We rely on the recent paper [13] by S. Fournais and T.Ø. Sørensen, where the following explicit bounds for the derivatives of ψ were obtained. Let $\mathrm{d}(\hat{\mathbf x}, x) = \min\{|x|, |x-x_j|, j = 1,\dots, N-1\}$. Then

$$|\partial_x^m\psi(\hat{\mathbf x}, x)| \lesssim \mathrm{d}(\hat{\mathbf x}, x)^{1-|m|} e^{-\varkappa_m|\mathbf x|}, |m|\ge 1, \tag{6}$$

with some $\varkappa_m > 0$. These estimates are used to derive the sharp bound (13) for the singular values of the operator Ψ.

2.2. **Compact operators.** Here we collect some basic information about the classes of compact operators relevant for the main result, see the book [8], where one can also find further references. Let $\mathcal H$ and $\mathcal G$ be separable Hilbert spaces. Let $T:\mathcal H\to\mathcal G$ be a compact operator. If $\mathcal H = \mathcal G$ and $T = T^*\ge 0$, then $\lambda_k(T)$, $k = 1, 2, \dots$, denote the positive eigenvalues of T numbered in descending order counting multiplicity. For arbitrary spaces $\mathcal H$, $\mathcal G$ and compact T, by $s_k(T) > 0$, $k = 1, 2, \dots$, we denote the singular values of T defined by $s_k(T)^2 = \lambda_k(T^*T) = \lambda_k(TT^*)$. We classify compact operators by the rate of decay of their singular values. If $s_k(T)\lesssim k^{-1/p}, k = 1, 2, \dots$, with some $p > 0$, then we say that $T\in\mathbf S_{p,\infty}$ and denote

$$\|T\|_{p,\infty} = \sup_k s_k(T) k^{\frac{1}{p}}.$$

The class $\mathbf S_{p,\infty}$ is a complete linear space with the quasi-norm $\|T\|_{p,\infty}$, see [8, §11.6]. For $p\in(0,1)$ the quasi-norm satisfies the following "triangle" inequality for operators $T_j\in\mathbf S_{p,\infty}$, $j = 1, 2, \dots$:

$$\Big\|\sum_j T_j\Big\|_{p,\infty}^p \le (1-p)^{-1}\sum_j \|T_j\|_{p,\infty}^p, \tag{7}$$

see [1, Lemmata 7.5, 7.6], [5, §1] and references therein. For the case $p > 1$ see [8, §11.6], but we do not need it in what follows.

For $T\in\mathbf S_{p,\infty}$ the following numbers are finite:

$$\begin{cases} \mathsf G_p(T) = \big(\limsup_{k\to\infty} k^{\frac{1}{p}} s_k(T)\big)^p,\\[2mm] \mathsf g_p(T) = \big(\liminf_{k\to\infty} k^{\frac{1}{p}} s_k(T)\big)^p, \end{cases} \tag{8}$$

and they clearly satisfy the inequalities

$$\mathsf{g}_p(T) \le \mathsf{G}_p(T) \le \|T\|_{p,\infty}^p.$$

Observe that

$$\mathsf{g}_p(TT^*) = \mathsf{g}_p(T^*T) = \mathsf{g}_{2p}(T), \quad \mathsf{G}_p(TT^*) = \mathsf{G}_p(T^*T) = \mathsf{G}_{2p}(T). \tag{9}$$

If $\mathsf{G}_p(T) = \mathsf{g}_p(T)$, then the singular values of T satisfy the asymptotic formula

$$s_n(T) = \big(\mathsf{G}_p(T)\big)^{\frac{1}{p}} n^{-\frac{1}{p}} + o(n^{-\frac{1}{p}}),\ n \to \infty.$$

The functionals G_p, g_p were introduced by M. Birman and M. Solomyak in the 1970's, see e.g. [2], [7]. Together with the quasi-norm $\|T\|_{p,\infty}$, the functional G_p, $p < 1$, also satisfies the inequality of the type (7) (see [24, Lemma 2.2]):

Proposition 4. *Suppose that $T_j \in \mathbf{S}_{p,\infty}$, $j = 1, 2, \dots$, with some $p < 1$ and that*

$$\sum_j \|T_j\|_{p,\infty}^p < \infty.$$

Then

$$\mathsf{G}_p\big(\sum_j T_j\big) \le (1-p)^{-1} \sum_j \mathsf{G}_p(T_j). \tag{10}$$

The functionals G_p and g_p are continuous on $\mathbf{S}_{p,\infty}$, see [8, Corollary 11.6.5]:

Proposition 5. *If $T_1, T_2 \in \mathbf{S}_{p,\infty}$, $0 < p < \infty$, then*

$$\big|\mathsf{G}_p(T_1)^{\frac{1}{p+1}} - \mathsf{G}_p(T_2)^{\frac{1}{p+1}}\big| \le \mathsf{G}_p(T_1 - T_2)^{\frac{1}{p+1}},$$
$$\big|\mathsf{g}_p(T_1)^{\frac{1}{p+1}} - \mathsf{g}_p(T_2)^{\frac{1}{p+1}}\big| \le \mathsf{G}_p(T_1 - T_2)^{\frac{1}{p+1}}.$$

We need the following two corollaries of this fact:

Corollary 6. *Suppose that $\mathsf{G}_p(T_1 - T_2) = 0$. Then*

$$\mathsf{G}_p(T_1) = \mathsf{G}_p(T_2), \quad \mathsf{g}_p(T_1) = \mathsf{g}_p(T_2).$$

The next corollary is more general: it shows that the functionals $\mathsf{G}_p(T)$ and $\mathsf{g}_p(T)$ can be found by approximating T with a family of operators $T_\nu \in \mathbf{S}_{p,\infty}$, $\nu \in \mathbb{R}$.

Corollary 7. *Suppose that $T \in \mathbf{S}_{p,\infty}$ and that for every $\nu > 0$ there exists an operator $T_\nu \in \mathbf{S}_{p,\infty}$ such that $\mathsf{G}_p(T - T_\nu) \to 0$, $\nu \to 0$. Then the functionals $\mathsf{G}_p(T_\nu), \mathsf{g}_p(T_\nu)$ have limits as $\nu \to 0$ and*

$$\lim_{\nu \to 0} \mathsf{G}_p(T_\nu) = \mathsf{G}_p(T), \quad \lim_{\nu \to 0} \mathsf{g}_p(T_\nu) = \mathsf{g}_p(T).$$

2.3. **Singular values of integral operators.** The final ingredients of the proof are two results due to M.S. Birman and M.Z. Solomyak, investigating the membership of integral operators in the class $\mathbf{S}_{p,\infty}$ with some $p > 0$.

For estimates of the singular values we rely on [5, Proposition 2.1], see also [8, Theorem 11.8.4], which we state here in a form convenient for our purposes. Let $\Lambda \subset \mathbb{R}^d, d \geq 1$, be a bounded domain with a piece-wise C^1-boundary.

Proposition 8. *Let $T_{ba} : \mathsf{L}^2(\Lambda) \to \mathsf{L}^2(\mathbb{R}^n)$, be the integral operator of the form*

$$(T_{ba}u)(t) = b(t) \int T(t,x)a(x)u(x)\, dx,$$

where $a \in \mathsf{L}^2(\Lambda)$, $b \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$, and the kernel $T(t,x)$, $t \in \mathbb{R}^n$, $x \in \Lambda$, is such that $T(t,\ \cdot\ ) \in \mathsf{H}^l(\Lambda)$ with some $l = 1, 2, \dots,\ 2l > d$, a.e. $t \in \mathbb{R}^n$ and the function $\|T(t,\ \cdot\ )\|_{\mathsf{H}^l}$ is in $\mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$. Then

$$s_k(T_{ba}) \lesssim k^{-\frac{1}{2}-\frac{l}{d}} \bigg[\int \|T(t,\ \cdot\ )\|^2_{\mathsf{H}^l}\, |b(t)|^2\, dt\bigg]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\Lambda)},$$

$k = 1, 2, \dots$. In other words, $T_{ba} \in \mathbf{S}_{q,\infty}$ with

$$\frac{1}{q} = \frac{1}{2} + \frac{l}{d},$$

and

$$\|T_{ba}\|_{q,\infty} \lesssim \bigg[\int \|T(t,\ \cdot\ )\|^2_{\mathsf{H}^l}\, |b(t)|^2\, dt\bigg]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\Lambda)}.$$

The implicit constants in the above estimates are independent of the functions T, a, b or index k, but may depend on the domain Λ.

The next result establishes the spectral asymptotics for an integral operator with a homogeneous kernel. We do not need the most general result, but content ourselves with a special case. The following proposition follows from [5, Theorem 10.9], see also [3], [4], [6].

Proposition 9. *Let $X, Y \subset \mathbb{R}^d, d \geq 1$, be bounded Borel sets. Let $T : \mathsf{L}^2(Y) \to \mathsf{L}^2(X)$ be the operator with the kernel*

$$T(x,y) = \rho_1(x)|x-y|^\alpha \phi(x,y)\rho_2(y), \tag{11}$$

where $\alpha > -d$, $\rho_1 \in \mathsf{L}^\infty(X), \rho_2 \in \mathsf{L}^\infty(Y)$, and $\phi \in \mathsf{C}^\infty(\overline{X} \times \overline{Y})$. Then for $p^{-1} = 1 + \alpha d^{-1}$ we have

$$\mathsf{g}_p(T) = \mathsf{G}_p(T) = \mu_{\alpha,d} \int\limits_{X \cap Y} |\rho_1(x)\phi(x,x)\rho_2(x)|^p dx,$$

with

$$\mu_{\alpha,d} = \frac{1}{\Gamma\big(d/2+1\big)}\left[\frac{\Gamma\big((d+\alpha)/2\big)}{\pi^{\alpha/2}|\Gamma(-\alpha/2)|}\right]^p, \qquad \alpha \neq 0,2,4,\dots,$$
$$\mu_{\alpha,d} = 0, \quad \alpha = 0,2,4,\dots.$$

3. Proof of Theorems 2 and 3

The complete proof of Theorems 2, 3 will be published elsewehere. In this note we briefly describe its main steps.

At the heart of the proof is the factorization formula $\Gamma = \Psi^*\Psi$, where $\Psi : \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}^{3N-3})$ is the integral operator

$$(\Psi u)(\hat{\mathbf{x}}) = \int_{\mathbb{R}^3} \psi(\hat{\mathbf{x}}, x) u(x) dx, \quad u \in \mathsf{L}^2(\mathbb{R}^3).$$

Using the functionals (8) the formula (4) can be rewritten as $\mathsf{G}_{3/8}(\Gamma) = \mathsf{g}_{3/8}(\Gamma) = A$. Thanks to the formula $\Gamma = \Psi^*\Psi$, by (9) we have

$$\mathsf{G}_{3/8}(\Gamma) = \mathsf{G}_{3/4}(\Psi), \quad \mathsf{g}_{3/8}(\Gamma) = \mathsf{g}_{3/4}(\Psi).$$

Therefore Theorem 3 is equivalent to the following result.

Theorem 10. *Suppose that the eigenfunction ψ satisfies the bound* (2)*. Then the singular values $s_k(\Psi), k = 1,2,\dots,$ of the operator Ψ satisfy the asymptotic formula*

$$\mathsf{G}_{3/4}(\Psi) = \mathsf{g}_{3/4}(\Psi) = A. \tag{12}$$

The proof of Theorem 10 splits into two parts.

3.1. **Proof of Theorem 10: an upper bound for $\mathsf{G}_{3/4}(\Psi)$.** The first stage of the asymptotic analysis is to obtain convenient upper bounds. We need the bounds for the operator $b\Psi a$ with weights $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$ and $a \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^3)$. The function a is assumed to satisfy the condition

$$\sup_{n\in\mathbb{Z}^3} \|a\|_{\mathsf{L}^2(\mathcal{C}_n)} < \infty,$$

where $\mathcal{C}_n = [0,1)^3 + n, n \in \mathbb{Z}^3$. Thus, for any $\varkappa > 0$ the functionals

$$S_\varkappa(a) = \bigg[\sum_{n\in\mathbb{Z}^3} e^{-\frac{3}{4}\varkappa|n|}\|a\|^{\frac{3}{4}}_{\mathsf{L}^2(\mathcal{C}_n)}\bigg]^{\frac{4}{3}}, \quad M_\varkappa(b) = \bigg[\int_{\mathbb{R}^{3N-3}} |b(\hat{\mathbf{x}})|^2 e^{-2\varkappa|\hat{\mathbf{x}}|} d\hat{\mathbf{x}}\bigg]^{\frac{1}{2}}$$

are both finite. In the literature functionals of the form $S_\varkappa$ are sometimes called *lattice norms* (or *quasi-norms*, if appropriate). Lattice norms emerge in a natural way when one studies integral operators in classes $\mathbf{S}_{p,\infty}$ with $p < 1$, see e.g. [5, Section 6.4].

Theorem 11. *Assume* (2)*. Then for some $\varkappa \in (0, \varkappa_0]$ we have*

$$\mathsf{G}_{3/4}\big(b\Psi a\big) \lesssim \big[M_\varkappa(b) S_\varkappa(a)\big]^{3/4}. \tag{13}$$

The complete proof of this theorem is given in [24]. Here we present only a short sketch illustrating the emergence of lattice norms.

Sketch of the proof of Theorem 11. Represent $b\Psi a$ as

$$\sum_{n\in\mathbb{Z}^3} b\Psi_n a, \quad \Psi_n = \Psi \mathbb{1}_n,$$

where we have denoted by $\mathbb{1}_n$ the indicator of the cube $\mathcal{C}_n = [0,1)^3 + n, n \in \mathbb{Z}^3$. Relying on the bounds (2), (6) and using Proposition 8 we prove that for some $\varkappa \in (0, \varkappa_0]$, the estimate holds:

$$\mathsf{G}_{3/4}(b\Psi_n a) \lesssim \big(e^{-\varkappa|n|} M_\varkappa(b) \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}\big)^{3/4}, \quad n \in \mathbb{Z}^3.$$

By (10),

$$\mathsf{G}_{3/4}(b\Psi a) \le 4 \sum_{n\in\mathbb{Z}^3} \mathsf{G}_{3/4}(b\Psi_n a) \lesssim M_\varkappa(b)^{3/4} \sum_{m\in\mathbb{Z}^3} e^{-\frac{3}{4}\varkappa|n|} \, \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}^{3/4},$$

which leads to (13). □

3.2. **Proof of Theorem 10: asymptotic relation** (12) **and formula** (5)**.** We conduct the proof for the case $N = 2$ only. Under this assumption the proof retains all its crucial features, but permits to avoid some tedious technical details.

The representation from Proposition 1 is of central importance:

$$\psi(x_1, x) = \xi_1(x_1, x) + |x_1 - x|\eta_1(x_1, x), \quad (x_1, x) \in \Omega. \tag{14}$$

Assume for simplicity that $\Omega_1 = (\mathbb{R}^3 \setminus \{0\}) \times (\mathbb{R}^3 \setminus \{0\})$. Note that the kernel $\psi(x_1, x)$ contains the homogeneous factor $|x_1 - x|$ which points to the possible use of Proposition 9. However, as mentioned earlier, Proposition 1 provides no information on the smoothness of the functions ξ_1 and η_1 on the set $\overline{\Omega_1}$, or on their integrability on Ω_1. In order to apply Proposition 9 we approximate ξ_1 and η_1 by C_0^∞-functions supported in Ω_1. Let $\zeta \in \mathsf{C}_0^\infty(\mathbb{R})$ be s.t. $\zeta(t) = 0, |t| \ge 1$, $\zeta(t) = 1, |t| \le 1/2$, and let $\omega(t) = 1 - \zeta(t)$. For convenience we also assume that

$$\zeta(t) = \zeta(-t), \ \forall t \in \mathbb{R}, \quad \text{and} \quad \zeta \text{ is non-increasing on } [0, \infty). \tag{15}$$

For arbitrary $\varepsilon > 0$, $R > \varepsilon$, consider now the kernel

$$\psi_{\varepsilon,R}(x_1, x) = \omega(|x_1|/\varepsilon)\zeta(|x_1|/R)\omega(|x|/\varepsilon)\zeta(|x|/R)\psi(x_1, x). \tag{16}$$

It is supported on the domain $\Omega_{\varepsilon,R} = \{x_1 : \varepsilon/2 < |x_1| < R\} \times \{x : \varepsilon/2 < |x| < R\}$, on which both ξ_1 and η_1 are uniformly bounded together with their derivatives of arbitrary order. Similarly to the notation Ψ, denote by $\Psi_{\varepsilon,R}$ the integral operator with the kernel $\psi_{\varepsilon,R}(x_1, x)$. An important fact is that the operator $\Psi_{\varepsilon,R}$ is an approximation of Ψ in the following sense:

Lemma 12.

$$\mathsf{G}_{3/4}(\Psi - \Psi_{\varepsilon,R}) \to 0, \quad \text{as} \quad \varepsilon \to 0, R \to \infty. \tag{17}$$

Proof. The kernel of $\Psi - \Psi_{\varepsilon,R}$ has the form

$$\psi(x_1,x) - \psi_{\varepsilon,R}(x_1,x) = \Big[\zeta(|x_1|/\varepsilon) + \omega(|x_1|/\varepsilon)\zeta(|x|/\varepsilon) + \omega(|x_1|/\varepsilon)\omega(|x|/\varepsilon)\omega(|x|/R)$$

$$+ \omega(|x_1|/\varepsilon)\omega(|x_1|/R)\omega(|x|/\varepsilon)\zeta(|x|/R)\Big]\psi(x_1,x). \tag{18}$$

Let us consider for example the functional $\mathsf{G}_{3/4}(T_\varepsilon)$ for the operator T_ε with kernel $\zeta(|x_1|/\varepsilon)\psi(x_1,x)$, which is the first term on the right-hand side of (18). By (13) with $a = 1$ and $b(x_1) = \zeta(|x_1|/\varepsilon)$, we get

$$\mathsf{G}_{3/4}(T_\varepsilon) \lesssim M_\varkappa(b)^{3/4} \le \left[\int_{\mathbb{R}^3} \zeta(|x_1|/\varepsilon)^2 dx_1\right]^{\frac{3}{8}} \lesssim \varepsilon^{\frac{9}{8}} \to 0, \quad \varepsilon \to 0.$$

The remaining kernels on the right-hand side of (18) are handled in a similar way with the help of Theorem 11. In view of (10) this implies (17). □

Lemma 12, together with Corollary 7 implies that

$$\mathsf{G}_{3/4}(\Psi) = \lim_{\varepsilon\to 0, R\to\infty} \mathsf{G}_{3/4}(\Psi_{\varepsilon,R}), \quad \mathsf{g}_{3/4}(\Psi) = \lim_{\varepsilon\to 0, R\to\infty} \mathsf{g}_{3/4}(\Psi_{\varepsilon,R}). \tag{19}$$

In line with (14) the kernel (16) consists of two components. The kernel

$$\omega(|x_1|/\varepsilon)\zeta(|x_1|/R)\omega(|x|/\varepsilon)\zeta(|x|/R)\xi_1(x_1,x)$$

is infinitely smooth, and hence, by Proposition 8 the associated functional $\mathsf{G}_{3/4}$ equals zero. Therefore, by Corollary 6, this operator gives a zero contribution to $\mathsf{G}_{3/4}(\Psi_{\varepsilon,R})$. The kernel

$$\omega(|x_1|/\varepsilon)\zeta(|x_1|/R)|x - x_1|\eta_1(|x_1|, x)\omega(|x|/\varepsilon)\zeta(|x|/R) \tag{20}$$

has the form (11) with

$$\rho_1(x) = \rho_2(x) = 1, \quad \phi(x_1,x) = \eta_1(x_1,x)\omega(|x_1|/\varepsilon)\zeta(|x_1|/R)\omega(|x|/\varepsilon)\zeta(|x|/R)$$

and $\alpha = 1$, $d = 3$, $p = 3/4$. Considering (20) as the kernel of an operator on $\mathsf{L}^2(\Omega_{\varepsilon,R})$, by Proposition 9 we obtain that

$$\mathsf{G}_{3/4}(\Psi_{\varepsilon,R}) = \mathsf{g}_{3/4}(\Psi_{\varepsilon,R}) = \mu_{1,3}\int_{\mathbb{R}^3} |\omega(x/\varepsilon)|^{3/2}\zeta(x/R)^{3/2}|\eta_1(x,x)|^{3/4}dx.$$

Because of the relations (19) all three terms have finite limits as $\varepsilon \to 0, R \to \infty$, and

$$\mathsf{G}_{3/4}(\Psi) = \mathsf{g}_{3/4}(\Psi) = A := \lim_{\varepsilon\to 0, R\to\infty} \mu_{1,3}\int_{\mathbb{R}^3} |\omega(x/\varepsilon)|^{3/2}\zeta(x/R)^{3/2}|\eta_1(x,x)|^{3/4}dx. \tag{21}$$

To complete the proof of Theorem 10 (and hence of Theorem 3), we need to show that Theorem 2 holds and that A is given by (5).

To prove Theorem 2 note that the integral on the right-hand side of (21) is bounded uniformly in ε and R. Furthermore, $\omega(x/\varepsilon) \to 1, \varepsilon \to 0$, and $\zeta(x/R) \to 1, R \to \infty$, for all $x \ne 0$, and by (15), this convergence is monotone. By the Monotone Convergence

Theorem, this implies that $\eta_1 \in \mathsf{L}^{3/4}(\mathbb{R})$, which proves Theorem 2 for $N = 2$. Moreover, this entails that

$$A = \mu_{1,3} \int_{\mathbb{R}^3} |\eta_1(x,x)|^{3/4} dx.$$

Calculating $\mu_{1,3}$ we obtain the formula (5) for the coefficient A, thus completing the proof of Theorems 10 and 3.

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