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Eigenvalue estimates for the one-particle density matrix

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Abstract. It is shown that the eigenvalues $\lambda_k, k = 1, 2, \ldots,$ of the one-particle density matrix satisfy the bound $\lambda_k \le Ck^{-8/3}$ with a positive constant C.

1. Introduction

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

$$H = \sum_{k=1}^{N}\Big(-\Delta_k - \frac{Z}{|x_k|}\Big) + \sum_{1\le j<k\le N}\frac{1}{|x_j - x_k|}, \tag{1.1}$$

describing an atom with N electrons with coordinates $\mathbf{x} = (x_1, x_2, \ldots, x_N)$, $x_k \in \mathbb{R}^3$, $k = 1, 2, \ldots, N$, and a nucleus with charge $Z > 0$. The notation Δ_k is used for the Laplacian with respect to 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 (1.1) is an infinitesimal perturbation relative to the unperturbed operator $-\Delta = -\sum_k \Delta_k$, see, e.g., [17, 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 antisymmetric L^2-functions. Our results are not sensitive to such assumptions. Let $\psi = \psi(\mathbf{x})$, $\mathbf{x} = (\hat{\mathbf{x}}, x_N)$, $\hat{\mathbf{x}} = (x_1, x_2, \ldots, x_{N-1})$, 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

$$\gamma(x, y) = \int_{\mathbb{R}^{3N-3}} \overline{\psi(\hat{\mathbf{x}}, x)}\psi(\hat{\mathbf{x}}, y)\, d\hat{\mathbf{x}}, \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3. \tag{1.2}$$

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We do not discuss the importance of this object for multi-particle quantum mechanics and refer to [5,15,16] for details. Our focus is on spectral properties of the self-adjoint non-negative operator Γ with the kernel $\gamma(x,y)$, which we call *the one-electron 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. Our objective is to investigate the decay of the eigenvalues $\lambda_k(\Gamma) > 0$, $k = 1, 2, \dots$, of the non-negative operator Γ, labelled in descending order counting multiplicity. The significance of such information for quantum mechanical computations is discussed in the paper [11]. In particular, it is shown in [11] that Γ has infinite rank. The discussion of the case $N = 2$ in [4, Sections III and IV] suggests that $\lambda_k(\Gamma)$ should decay as $k^{-8/3}$. Our results justify this observation for arbitrary number N of particles. We obtain the bound $\lambda_k(\Gamma) = O(k^{-8/3})$, $k = 1, 2, \dots$ under the condition that ψ decays exponentially as $|\mathbf{x}| \to \infty$:

$$|\psi(\mathbf{x})| \lesssim e^{-\varkappa_0 |\mathbf{x}|_1}, \quad \mathbf{x} \in \mathbb{R}^{3N}. \tag{1.3}$$

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. Notice that instead of the standard Euclidean norm $|\mathbf{x}|$ in (1.3) we have the ℓ_1-norm which we denote by $|\mathbf{x}|_1$. This choice seems to be more convenient for computations in the proof. For the discrete eigenvalues, i.e., the ones below the bottom of the essential spectrum of H, the bound (1.3) follows from [7]. The exponential decay for eigenvalues away from the thresholds, including embedded ones, was studied in [6, 12]. For more references and detailed discussion we quote [18].

The main result of the paper is contained in the following theorem.

Theorem 1.1. *Suppose that the eigenfunction ψ satisfies the bound (1.3). Let the function $\gamma(x,y)$, $(x,y) \in \mathbb{R}^3 \times \mathbb{R}^3$, be defined by (1.2). Then the eigenvalues $\lambda_k(\Gamma)$, $k = 1, 2, \dots$, of the operator Γ satisfy the estimate*

$$0 < \lambda_k(\Gamma) \lesssim k^{-\frac{8}{3}}, \quad k = 1, 2, \dots, \tag{1.4}$$

with an implicit positive constant independent of k.

Remark 1.2. (1) The bound (1.4) is sharp. This is confirmed by the asymptotic formula for the eigenvalues $\lambda_k(\Gamma)$ which is proved in a [19]. In fact, Theorem 1.1 or, more precisely, Theorem 3.1 can be regarded as a preparation for the asymptotic formula in [19].

(2) Theorem 1.1 extends to the case of a molecule with several nuclei whose positions are fixed. The modifications are straightforward.

(3) If the function ψ is symmetric or anti-symmetric, then the kernel $N\overline{\gamma(x,y)} = N\gamma(y,x)$ coincides with the standard definition of the one-particle density, see, e.g., [15]. It is clear that the complex conjugation does not affect the bound (1.4).

In the case of a function ψ without any symmetry properties, the standard definition of the one-particle density matrix is different from (1.2). For example, under the simplifying assumption $N = 3$ the complex conjugate of the one-particle density matrix is given by

$$\int_{\mathbb{R}^3\times\mathbb{R}^3} \overline{\psi(x,s,t)}\psi(y,s,t)\,ds\,dt + \int_{\mathbb{R}^3\times\mathbb{R}^3} \overline{\psi(s,x,t)}\psi(s,y,t)\,ds\,dt \\ + \int_{\mathbb{R}^3\times\mathbb{R}^3} \overline{\psi(s,t,x)}\psi(s,t,y)\,ds\,dt.$$

The operator with this kernel satisfies the bound of the form (1.4) if each of the components does, see (2.4). The same conclusion holds for general N. Thus, taking the simplified definition (1.2) does not restrict generality of Theorem 1.1.

(4) Questions about decay of eigenvalues can be also asked for the n-particle density matrix with $1 \le n \le N-1$, see [16, Section 3.1.5] for the definition. It is the author's believe that methods similar to the ones employed in the current paper should lead to some estimates of the eigenvalues, but it is difficult to predict their form without careful analysis, which is beyond the scope of the paper.

The strategy of the proof is quite straightforward: by virtue of the factorization $\Gamma = \Psi^*\Psi$, mentioned a few lines earlier, we have $\lambda_k(\Gamma) = s_k(\Psi)^2, k = 1, 2, \dots,$ where $s_k(\Psi)$ are the singular values (s-values) of the operator Ψ. It is well known that the rate of decay of singular values for integral operators depends on the smoothness of their kernels, and the appropriate estimates via suitable Sobolev norms can be found in the monograph [2] by M. S. Birman and M. Z. Solomyak. The regularity of ψ has been well studied in the literature. To begin with, according to the classical elliptic theory, due to the analyticity of the Coulomb potential $|x|^{-1}$ for $x \ne 0$, the function ψ is real analytic away from the particle coalescence points. A more challenging problem is to understand the behaviour of ψ at the coalescence points. The first result in this direction belongs to T. Kato [14], who showed that the function ψ is Lipschitz. More detailed information on ψ at the coalescence points was obtained, e.g., in [8, 9, 13], and in the recent paper [10] by S. Fournais and T. Ø. Sørensen. The results of [2, 10] are of crucial importance for the proof of Theorem 1.1. A combination of the efficient bounds for the derivatives of the function ψ obtained in [10], and the estimates for the singular values in [2], leads to the bound $s_k(\Psi) \lesssim k^{-4/3}$, and hence to (1.4).

The plan of the paper is as follows. In Section 2 we list the facts that serve as ingredients of the proof. Although our aim is to prove the bound $s_k(\Psi) \lesssim k^{-4/3}$, in Section 3 in Theorem 3.1 we state a bound for the operator Ψ with weights which will be useful in the study of the spectral asymptotics for Ψ. The rest of Section 3 provides some preliminary estimates for auxiliary integral operators. These estimates are put together in Section 4 to complete the proof of Theorems 3.1 and 1.1.

We conclude the introduction with some general notational conventions.

Coordinates. As mentioned earlier, we use the following standard notation for the coordinates: $\mathbf{x} = (x_1, x_2, \dots, x_N)$, where $x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, N$. The vector $\mathbf{x}$ is usually represented in the form $\mathbf{x} = (\hat{\mathbf{x}}, x_N)$ with $\hat{\mathbf{x}} = (x_1, x_2, \dots, x_{N-1}) \in \mathbb{R}^{3N-3}$. In order to write formulas in a more compact and unified way, we sometimes use the notation $x_0 = 0$.

In the space $\mathbb{R}^d$, $d \geq 1$, the notation $|x|$ stands for the Euclidean norm, whereas $|x|_1$ denotes the ℓ_1-norm.

Indicators. For any set $\Lambda \subset \mathbb{R}^d$ we denote by $\mathbb{1}_\Lambda$ its indicator function (or indicator).

Derivatives. Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. If $x = (x', x'', x''') \in \mathbb{R}^3$ and $m = (m', m'', m''') \in \mathbb{N}_0^3$, then the derivative ∂_x^m is defined in the standard way:

$$\partial_x^m = \partial_{x'}^{m'} \partial_{x''}^{m''} \partial_{x'''}^{m'''}.$$

Bounds. As explained earlier, for two non-negative numbers (or functions) X and Y depending on some parameters, we write $X \lesssim Y$ (or $Y \gtrsim X$) if $X \leq CY$ with some positive constant C independent of those parameters. To avoid confusion we may comment on the nature of (implicit) constants in the bounds.

2. Ingredients of the proof

In this section we list three ingredients of the proof of the main Theorem 1.1.

2.1. Regularity of the eigenfunction

We need some efficient bounds for the derivatives of the eigenfunction away from the coalescence points, obtained by S. Fournais and T. Ø. Sørensen in [10]. Let

$$\mathrm{d}(\hat{\mathbf{x}}, x) = \min\{|x|, |x - x_j|,\ j = 1, 2, \dots, N-1\}.$$

The following proposition is a consequence of [10, Corollary 1.3]:

Proposition 2.1. *Assume that ψ satisfies* (1.3). *Then for all multi-indices $m \in \mathbb{N}_0^3$, $|m|_1 \geq 1$, we have*

$$|\partial_x^m \psi(\hat{\mathbf{x}}, x)| \lesssim \mathrm{d}(\hat{\mathbf{x}}, x)^{1-l} e^{-\varkappa_l |\mathbf{x}|_1}, \quad l = |m|_1, \tag{2.1}$$

with some $\varkappa_l > 0$.

The precise values of the constants $\varkappa_l > 0$ are insignificant for us, and therefore we may assume that

$$\varkappa_0 = \varkappa_1 \geq \varkappa_2 \geq \cdots > 0. \tag{2.2}$$

Let us rewrite the bounds (2.1) using the notation $x_0 = 0$. With this convention, we have

$$\mathrm{d}(\hat{\mathbf{x}}, x) = \min\{|x - x_j|, j = 0, 1, 2, \ldots, N-1\}$$

and

$$\mathrm{d}(\hat{\mathbf{x}}, x)^{-1} \leq \sum_{0 \leq j \leq N-1} |x - x_j|^{-1}.$$

Therefore, (1.3) and (2.1) imply that

$$|\partial_x^m \psi(\hat{\mathbf{x}}, x)| \lesssim e^{-\varkappa_l |\mathbf{x}|_1} \Big(1 + \sum_{0 \leq j \leq N-1} |x - x_j|^{1-l}\Big), \quad l = |m|_1, \tag{2.3}$$

for all $m \in \mathbb{N}_0^3$.

Remark. (1) To elaborate on Remark 1.2(2) we should say that Proposition 2.1 also holds in the case of several nuclei, which allows one to extend Theorem 1.1 to molecules.

(2) As indicated earlier, the bounds (2.1) play the main part in the proof of (1.4). In fact, Theorem 1.1 can be recast as follows: the bound (1.4) holds for the operator Γ with kernel (1.2) if ψ is a function that satisfies the bounds (1.3) and (2.1).

2.2. Compact operators

Our main reference for compact operators is the book [3]. 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 $T = T^* \geq 0$, then $\lambda_k(T)$, $k = 1, 2, \ldots$, denote the positive eigenvalues of T numbered in descending order counting multiplicity. For arbitrary spaces $\mathcal{H}$, $\mathcal{G}$ and compact T, by $s_k(T) > 0$, $k = 1, 2, \ldots$, we denote the singular values of T defined by $s_k(T)^2 = \lambda_k(T^*T) = \lambda_k(TT^*)$. Note the useful inequality

$$s_{2k}(T_1 + T_2) \leq s_{2k-1}(T_1 + T_2) \leq s_k(T_1) + s_k(T_2), \tag{2.4}$$

which holds for any two compact T_1, T_2, see [3, formula (11.1.14)]. 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

$$\|T\|_{p,\infty} = \sup_k k^{\frac{1}{p}} s_k(T). \tag{2.5}$$

The class $\mathbf{S}_{p,\infty}$ is a complete linear space with the quasi-norm $\|T\|_{p,\infty}$, see [3, Section 11.6]. For $p \in (0, 1)$ the quasi-norm satisfies the following "triangle" inequality for operators $T_j \in \mathbf{S}_{p,\infty}$, $j = 1, 2, \dots$:

$$\Big\|\sum_j T_j\Big\|_{p,\infty}^p \le (1-p)^{-1} \sum_j \|T_j\|_{p,\infty}^p, \tag{2.6}$$

see [1, Lemmata 7.5 and 7.6], [2, Section 1] and references therein. For the case $p > 1$ see [3, Section 11.6], but we do not need it in what follows.

For $T \in \mathbf{S}_{p,\infty}$ the following number is finite:

$$\mathsf{G}_p(T) = (\limsup_{k\to\infty} k^{\frac{1}{p}} s_k(T))^p, \tag{2.7}$$

and it clearly satisfies the inequality

$$\mathsf{G}_p(T) \le \|T\|_{p,\infty}^p. \tag{2.8}$$

More precisely, let $\mathbf{S}_{p,\infty}^\circ \subset \mathbf{S}_{p,\infty}$ be the closed subspace of all operators $R \in \mathbf{S}_{p,\infty}$ with $\mathsf{G}_p(R) = 0$. As explained in [3, Theorem 11.6.10],

$$\mathsf{G}_p(T) = \inf_{R\in\mathbf{S}_{p,\infty}^\circ} \|T + R\|_{p,\infty}^p. \tag{2.9}$$

The functional $\mathsf{G}_p(T)$, $p < 1$, also satisfies the inequality of the type (2.6):

Lemma 2.2. *Suppose that $T_j \in \mathbf{S}_{p,\infty}$, $j = 1, 2, \dots$, with some $p < 1$ and that*

$$\sum_j \|T_j\|_{p,\infty}^p < \infty. \tag{2.10}$$

Then

$$\mathsf{G}_p\Big(\sum_j T_j\Big) \le (1-p)^{-1} \sum_j \mathsf{G}_p(T_j). \tag{2.11}$$

Proof. By (2.6) the operator $T = \sum_j T_j$ belongs to $\mathbf{S}_{p,\infty}$, so that the left-hand side is finite. Furthermore, due to (2.8) and to the condition (2.10) the right-hand side of (2.11) is finite as well. Fix an $\varepsilon > 0$ and pick N such that

$$\sum_{j=N+1}^\infty \|T_j\|_{p,\infty}^p < \varepsilon.$$

Then by (2.9) and (2.6), for any $R_j \in \mathbf{S}^\circ_{p,\infty}$, $j = 1, 2, \dots, N$, we have the estimate

$$\begin{aligned} \mathsf{G}_p(T) &\le \Big\| \sum_{j=1}^{N} (T_j + R_j) + \sum_{j=N+1}^{\infty} T_j \Big\|_p^p \\ &\le (1-p)^{-1} \Big(\sum_{j=1}^{N} \|T_j + R_j\|_{p,\infty}^p + \varepsilon \Big). \end{aligned}$$

Minimizing the right-hand side over R_j, $j = 1, 2, \dots, N$, by (2.9) we get the estimate

$$\mathsf{G}_p(T) \le (1-p)^{-1} \Big(\sum_{j=1}^{N} \mathsf{G}_p(T_j) + \varepsilon \Big) \le (1-p)^{-1} \Big(\sum_{j=1}^{\infty} \mathsf{G}_p(T_j) + \varepsilon \Big).$$

Since $\varepsilon > 0$ is arbitrary, we obtain (2.11). ∎

2.3. Singular values of integral operators

The final ingredient of the proof is the result 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 [2, Proposition 2.1], see also [3, Theorem 11.8.4], which we state here in a form convenient for our purposes. Let $\mathcal{C} = (0,1)^d \subset \mathbb{R}^d$, $d \ge 1$, be the unit cube.

Proposition 2.3. *Let $T_{ba}\colon \mathsf{L}^2(\mathcal{C}) \to \mathsf{L}^2(\mathbb{R}^n)$, be the integral operator of the form*

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

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

$$s_k(T_{ba}) \lesssim k^{-\frac{1}{2} - \frac{l}{d}} \Big[\int_{\mathbb{R}^n} \|T(t,\cdot)\|_{\mathsf{H}^l}^2 |b(t)|^2\, dt \Big]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C})}, \quad k = 1, 2, \dots,$$

with some implicit constant independent of the kernel T, weights a, b and the index k. In other words, $T_{ba} \in \mathbf{S}_{q,\infty}$ with

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

and

$$\|T_{ba}\|_{q,\infty} \lesssim \Big[\int_{\mathbb{R}^n} \|T(t,\cdot)\|_{\mathsf{H}^l}^2 |b(t)|^2\, dt \Big]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C})}.$$

It is straightforward to check that if one replaces the cube $\mathcal{C}$ with its translate $\mathcal{C}_n = \mathcal{C} + n, n \in \mathbb{Z}^d$, then the bounds of Proposition 2.3 still hold with implicit constants independent of n.

3. Preliminary estimates

3.1. The weighted operator Ψ

Represent the operator Γ as the product $\Gamma = \Psi^*\Psi$, where $\Psi\colon \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}^{3N-3})$ is defined by

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

Since $\psi \in \mathsf{L}^2(\mathbb{R}^{3N})$, this operator is Hilbert–Schmidt. As explained in the Introduction, in order to prove (1.4) it suffices to show that $s_k(\Psi) \lesssim k^{-4/3}, k = 1, 2, \dots$, i.e., that $\Psi \in \mathbf{S}_{3/4,\infty}$. For future use, we obtain an estimate for the operator $b\Psi a$ with weights a and b. In order to describe these weights, denote $\mathcal{C}_n = (0,1)^3 + n, n \in \mathbb{Z}^3$. Let $\varkappa_l > 0$ be the constants in the exponential bounds (1.3) and (2.1). We assume that the weight $a \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^3)$ is such that

$$S_q^{(l)}(a) = \Big[\sum_{n\in\mathbb{Z}^3} e^{-q\varkappa_l |n|_1} \|a\|^q_{\mathsf{L}^2(\mathcal{C}_n)}\Big]^{\frac{1}{q}} < \infty, \quad q = \frac{3}{4}, \tag{3.1}$$

and that $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$, so that

$$M^{(l)}(b) = \Bigg[\int\limits_{\mathbb{R}^{3N-3}} |b(\hat{\mathbf{x}})|^2 e^{-2\varkappa_1 |\hat{\mathbf{x}}|_1} d\hat{\mathbf{x}}\Bigg]^{\frac{1}{2}} < \infty, \quad \text{for all } l = 1, 2, \dots. \tag{3.2}$$

Recall that the functional G_p is defined in (2.7). Our objective is to prove the following theorem.

Theorem 3.1. *Let $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$ and let $a \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^3)$ be such that $S^{(4)}_{3/4}(a) < \infty$. Then $b\Psi a \in \mathbf{S}_{3/4,\infty}$ and*

$$\|b\Psi a\|_{3/4,\infty} \lesssim \|b\|_{\mathsf{L}^\infty} S^{(3)}_{3/4}(a), \tag{3.3}$$

$$\mathsf{G}_{3/4}(b\Psi a) \lesssim (M^{(4)}(b) S^{(4)}_{3/4}(a))^{\frac{3}{4}}. \tag{3.4}$$

For $a = 1$ and $b = 1$ this theorem implies that $s_k(\Psi) \lesssim k^{-4/3}$, and hence $\lambda_k(\Gamma) = s_k(\Psi)^2 \lesssim k^{-8/3}$, thereby proving Theorem 1.1.

The plan of the proof is as follows. We study first the operators $\Psi_n = \Psi \mathbb{1}_{\mathcal{C}_n}$, $n \in \mathbb{Z}^3$. For each fixed n the operator Ψ_n is split in the sum of several operators depending on two parameters: $\delta > 0$ and $\varepsilon > 0$, whose singular values are estimated in different ways. None of these estimates is sharp, but in the end, when collecting all the estimates together in Section 4, we get the sharp bound (3.4) by making a clever choice of the parameters δ and ε.

For convenience we introduce the notation

$$\operatorname{Int}(T) \colon \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}^{3N-3})$$

for the integral operator with the kernel $T(\hat{\mathbf{x}}, x)$. Whenever we consider the operators $b \operatorname{Int}(\cdot) \mathbb{1}_{\mathcal{C}_n} a$ with weights a, b, the constants in all the bounds are independent on the weights or on the parameter $n \in \mathbb{Z}^3$.

Recall also that we use the notation $x_0 = 0$. The symbol $\sum_j$ (resp. $\prod_j$) assumes summation (resp. product) over all $j = 0, 1, \dots, N-1$.

3.2. Partition of Ψ_n: step 1

The first step is to estimate the contribution of the domain on which the variables x_j, $j = 0, 1, 2, \dots, N-1$, are close to each other. Fix a $\delta > 0$ and denote

$$\Omega^{(\delta)} = \bigcap_{0 \le l < s \le N-1} \{\hat{\mathbf{x}} \in \mathbb{R}^{3N-3} \colon |x_l - x_s| > 4\delta\}.$$

The indicator of this set is denoted by $\chi^{(\delta)}$, i.e.,

$$\chi^{(\delta)}(\hat{\mathbf{x}}) = \mathbb{1}_{\Omega^{(\delta)}}(\hat{\mathbf{x}}) = \prod_{0 \le l < s \le N-1} \mathbb{1}_{\{|x_l - x_s| > 4\delta\}}(\hat{\mathbf{x}}). \tag{3.5}$$

Represent ψ as follows:

$$\psi = \psi_1^{(\delta)} + \psi_2^{(\delta)}, \tag{3.6a}$$

$$\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) = \psi(\hat{\mathbf{x}}, x) \chi^{(\delta)}(\hat{\mathbf{x}}), \tag{3.6b}$$

$$\psi_2^{(\delta)}(\hat{\mathbf{x}}, x) = \psi(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x) = \psi(\hat{\mathbf{x}}, x)(1 - \chi^{(\delta)}(\hat{\mathbf{x}})). \tag{3.6c}$$

It follows from (2.3) that

$$\begin{aligned} &|\partial_x^m \psi_2^{(\delta)}(\hat{\mathbf{x}}, x)| \\ &\quad \lesssim e^{-\varkappa_{|m|_1} |\mathbf{x}|_1} \Big(1 + \sum_j |x - x_j|^{1 - |m|_1}\Big) \sum_{0 \le l < s \le N-1} \mathbb{1}_{\{|x_l - x_s| < 4\delta\}}(\hat{\mathbf{x}}), \end{aligned} \tag{3.7}$$

for all $m \in \mathbb{N}_0^3$, with an implicit constant independent of $\delta > 0$. The operator $\operatorname{Int}(\psi_2^{(\delta)})$ is considered with the weight $b = 1$ and arbitrary $a \in \mathsf{L}^2(\mathcal{C}_n)$.

In the next lemma and further on we use the straightforward inequality

$$\max_{x\in\mathcal{C}_n} e^{-\varkappa_l|\mathbf{x}|_1} \le e^{3\varkappa_1} e^{-\varkappa_1|\hat{\mathbf{x}}|_1} e^{-\varkappa_1|n|_1}. \tag{3.8}$$

Lemma 3.2. *The operator* $\mathrm{Int}(\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}$ *belongs to* $\mathbf{S}_{6/7,\infty}$ *and*

$$\| \mathrm{Int}(\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty} \lesssim e^{-\varkappa_2|n|_1}\delta^{\frac{3}{2}}\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \tag{3.9}$$

for all $n\in\mathbb{Z}^3$ *and all* $\delta>0$.

Proof. According to (3.7) and (3.8), $\psi_2^{(\delta)}(\hat{\mathbf{x}},\cdot)\in\mathsf{H}^2(\mathcal{C}_n)$ for a.e. $\hat{\mathbf{x}}\in\mathbb{R}^{3N-3}$ and

$$\begin{aligned} &e^{2\varkappa_2|\hat{\mathbf{x}}|_1}\|\psi_2^{(\delta)}(\hat{\mathbf{x}},\cdot)\|_{\mathsf{H}^2}^2\\ &\quad\lesssim e^{-2\varkappa_2|n|_1}\sum_{0\le l<s\le N-1}\mathbb{1}_{\{|x_l-x_s|<4\delta\}}(\hat{\mathbf{x}})\int_{\mathcal{C}_n}\Big(1+\sum_{0\le j\le N-1}|x-x_j|^{-2}\Big)\,dx\\ &\quad\lesssim e^{-2\varkappa_2|n|_1}\sum_{0\le l<s\le N-1}\mathbb{1}_{\{|x_l-x_s|<4\delta\}}(\hat{\mathbf{x}}). \end{aligned}$$

Using Proposition 2.3 with $l=2, d=3$ (so that $2l>d$), we get that the operator on the left-hand side of (3.9) belongs to $\mathbf{S}_{q,\infty}$ with $q=6/7$ and

$$\begin{aligned} &\| \mathrm{Int}(\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty}\\ &\quad\lesssim\Big[\int_{\mathbb{R}^{3N-3}}\|\psi_2^{(\delta)}(\hat{\mathbf{x}},\cdot)\|_{\mathsf{H}^2}^2\,d\hat{\mathbf{x}}\Big]^{\frac{1}{2}}\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}\\ &\quad\lesssim e^{-\varkappa_2|n|_1}\Big[\int_{\mathbb{R}^{3N-3}}e^{-2\varkappa_2|\hat{\mathbf{x}}|_1}\sum_{0\le l<s\le N-1}\mathbb{1}_{\{|x_l-x_s|<4\delta\}}(\hat{\mathbf{x}})\,d\hat{\mathbf{x}}\Big]^{\frac{1}{2}}.\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}\\ &\quad\lesssim e^{-\varkappa_2|n|_1}\delta^{\frac{3}{2}}\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \end{aligned}$$

which gives (3.9). ■

To study the kernel $\psi_1^{(\delta)}$, we separate the contribution from the values of x that are "far" from x_j's, $j=0,1,\dots,N-1$. Let $\theta\in\mathsf{C}_0^\infty(\mathbb{R})$ be a function such that $0\le\theta\le1$ and

$$\begin{aligned} \theta(t)&=0,\quad \text{if } |t|>2,\\ \theta(t)&=1,\quad \text{if } |t|<1. \end{aligned}$$

Denote $\zeta(t)=1-\theta(t)$. Observe that for any $\nu>0$,

$$|\partial_x^m\theta(|x|\nu^{-1})|\lesssim\mathbb{1}_{\{|x|<2\nu\}}+\nu^{-|m|_1}\mathbb{1}_{\{\nu<|x|<2\nu\}}\lesssim\nu^{-|m|_1}\mathbb{1}_{\{|x|<2\nu\}}, \tag{3.10a}$$

$$|\partial_x^m\zeta(|x|\nu^{-1})|\lesssim\mathbb{1}_{\{|x|>\nu\}}+\nu^{-|m|_1}\mathbb{1}_{\{\nu<|x|<2\nu\}}\lesssim\nu^{-|m|_1}\mathbb{1}_{\{|x|>\nu\}}, \tag{3.10b}$$

for all $m \in \mathbb{N}_0^3$. Consequently,

$$\left|\partial_x^m \theta(|x|\nu^{-1})\right| \lesssim |x|^{-|m|_1} \mathbb{1}_{\{|x|<2\nu\}}, \tag{3.11a}$$

$$|\partial_x^m \zeta(|x|\nu^{-1})| \lesssim |x|^{-|m|_1} \mathbb{1}_{\{|x|>\nu\}}, \tag{3.11b}$$

uniformly in $\nu > 0$, for all $m \in \mathbb{N}_0^3$.

In what follows we consider separately the following components of $\psi_1^{(\delta)}$:

$$\psi_1^{(\delta)} = \psi_{11}^{(\delta)} + \psi_{12}^{(\delta)}, \tag{3.12a}$$

$$\psi_{11}^{(\delta)}(\hat{\mathbf{x}}, x) = \sum_j \theta(|x - x_j|\delta^{-1}) \psi_1^{(\delta)}(\hat{\mathbf{x}}, x), \tag{3.12b}$$

$$\psi_{12}^{(\delta)}(\hat{\mathbf{x}}, x) = \big[1 - \sum_j \theta\big(|x - x_j|\delta^{-1}\big)\big] \psi_1^{(\delta)}(\hat{\mathbf{x}}, x). \tag{3.12c}$$

In view of the definition of $\chi^{(\delta)}$, see (3.5), we have

$$[1 - \sum_j \theta(|x - x_j|\delta^{-1})] \chi^{(\delta)}(\hat{\mathbf{x}}) = \prod_j \zeta(|x - x_j|\delta^{-1}) \chi^{(\delta)}(\hat{\mathbf{x}}),$$

so that

$$\psi_{12}^{(\delta)}(\hat{\mathbf{x}}, x) = \psi_1^{(\delta)}(\hat{\mathbf{x}}, x) \prod_j \zeta(|x - x_j|\delta^{-1}).$$

Estimate the derivatives of this function. First observe that in view of (3.11) we have

$$\left|\partial_x^m \prod_j \zeta(|x - x_j|\delta^{-1})\right| \lesssim \Big(\sum_j |x - x_j|^{-|m|_1}\Big) \prod_j \mathbb{1}_{\{|x - x_j| > \delta\}}(\hat{\mathbf{x}}, x), \quad m \in \mathbb{N}_0^3.$$

Together with (2.3) this gives

$$|\partial_x^m \psi_{12}^{(\delta)}(\hat{\mathbf{x}}, x)| \lesssim e^{-\varkappa_{|m|_1} |\mathbf{x}|_1} \sum_j |x - x_j|^{-|m|_1} \mathbb{1}_{\{|x - x_j| > \delta\}}(\hat{\mathbf{x}}, x), \quad m \in \mathbb{N}_0^3, \tag{3.13}$$

uniformly in $\delta > 0$.

Lemma 3.3. *For any $l \geq 2$ the operator $\operatorname{Int}(\psi_{12}^{(\delta)}) a \mathbb{1}_{\mathcal{C}_n}$ belongs to $\mathbf{S}_{q,\infty}$ with*

$$\frac{1}{q} = \frac{1}{2} + \frac{l}{3}, \tag{3.14}$$

and

$$\| \operatorname{Int}(\psi_{12}^{(\delta)}) a \mathbb{1}_{\mathcal{C}_n} \|_{q,\infty} \lesssim e^{-\varkappa_l |n|_1} \delta^{-l + \frac{3}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \tag{3.15}$$

for all $\delta \in (0, \delta_0]$, with an implicit constant depending on l and δ_0 only.

Proof. According to (3.13), $\psi_{12}^{(\delta)}(\hat{\mathbf{x}},\cdot)\in \mathsf{H}^l(\mathcal{C}_n)$ for a.e. $\hat{\mathbf{x}}\in\mathbb{R}^{3N-3}$ with an arbitrary $l\ge 1$ and for $l\ge 2$ we have

$$e^{2\varkappa_l|\hat{\mathbf{x}}|_1}\|\psi_{12}^{(\delta)}(\hat{\mathbf{x}},\cdot)\|_{\mathsf{H}^l}^2 \lesssim e^{-2\varkappa_l|n|_1}\int_{\mathcal{C}_n}\Big(1+\sum_j |x-x_j|^{-2l}\mathbb{1}_{\{|x-x_j|>\delta\}}(\hat{\mathbf{x}},x)\Big)dx$$
$$\lesssim e^{-2\varkappa_l|n|_1}(1+\delta^{-2l+3})\lesssim e^{-2\varkappa_l|n|_1}\delta^{-2l+3}.$$

Now, the bound (3.15) follows from Proposition 2.3 with $d=3$ and $b(\hat{\mathbf{x}})=1$. ■

3.3. Partition of Ψ_n: step 2

It is important to note that the right-hand side of inequality (3.13) contains the factor $|x-x_j|^{-|m|_1}$ instead of $|x-x_j|^{1-|m|_1}$ that is present in (2.3). This is a consequence of the fact that the bound (2.1) holds for $|m|_1\ge 1$, but not for $m=0$. As we will see later on, in spite of this loss of one power of $|x-x_j|$, the estimate (3.15) is sufficient for derivation of the sharp bounds (3.3) and (3.4). However, when considering the term $\psi_{11}^{(\delta)}$ in (3.12) the bound by $|x-x_j|^{-|m|_1}$ is not enough, and we need to have the factor $|x-x_j|^{1-|m|_1}$, just as in (2.3). To achieve this we have to "correct" the kernel $\psi_{11}^{(\delta)}$ with the help of the auxiliary kernel

$$\eta^{(\delta)}(\hat{\mathbf{x}},x)=\sum_j\theta(|x-x_j|\delta^{-1})\psi_1^{(\delta)}(\hat{\mathbf{x}},x_j).$$

As the next lemma shows, the kernel $\eta^{(\delta)}$ has properties similar to those of $\psi_{12}^{(\delta)}$.

Lemma 3.4. *For any $l\ge 2$ the operator $\operatorname{Int}(\eta^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}$ belongs to $\mathbf{S}_{q,\infty}$ with the parameter q defined in (3.14), and*

$$\|\operatorname{Int}(\eta^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{q,\infty}\lesssim e^{-\varkappa_l|n|_1}\delta^{-l+\frac32}\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \tag{3.16}$$

for all $\delta\in(0,\delta_0]$.

Proof. Using (3.8) and (3.10) we get

$$|\partial_x^m\eta^{(\delta)}(\hat{\mathbf{x}},x)|\lesssim \delta^{-|m|_1}e^{-\varkappa_l|n|_1-\varkappa_1|\hat{\mathbf{x}}|_1}\sum_j\mathbb{1}_{\{|x-x_j|<2\delta\}}(\hat{\mathbf{x}},x),\quad m\in\mathbb{N}_0^3, |m|_1\le l.$$

Therefore, $\eta^{(\delta)}(\hat{\mathbf{x}},\cdot)\in\mathsf{H}^l(\mathcal{C}_n)$ for a.e. $\hat{\mathbf{x}}\in\mathbb{R}^{3N-3}$ with an arbitrary $l\ge 1$ and for $l\ge 2$ we have

$$e^{2\varkappa_1|\hat{\mathbf{x}}|_1}\|\eta^{(\delta)}(\hat{\mathbf{x}},\cdot)\|_{\mathsf{H}^l}^2\lesssim e^{-2\varkappa_l|n|_1}\int_{\mathcal{C}_n}\Big(1+\delta^{-2l}\sum_j\mathbb{1}_{\{|x-x_j|<2\delta\}}(\hat{\mathbf{x}},x)\Big)dx$$
$$\lesssim e^{-2\varkappa_l|n|_1}(1+\delta^{-2l+3})\lesssim e^{-2\varkappa_l|n|_1}\delta^{-2l+3}.$$

Now, the required bound follows from Proposition 2.3 with $d=3$ and $b(\hat{\mathbf{x}})=1$. ■

Let us now investigate the "corrected" kernel $\psi_{11}^{(\delta)}$, and consider instead of it the kernel

$$\phi^{(\delta)} = \psi_{11}^{(\delta)} - \eta^{(\delta)} = \sum_j \phi_j^{(\delta)}, \tag{3.17a}$$

$$\phi_j^{(\delta)}(\hat{\mathbf{x}}, x) = \theta(|x - x_j|\delta^{-1})(\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j)). \tag{3.17b}$$

Before proceeding to the next step of the construction, we estimate the difference $\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j)$. It follows from (2.1) with $|m|_1 = 1$ that

$$\begin{aligned}|\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j)| &\le |x - x_j| \max_{t\in[0,1]} |\nabla_x \psi_1^{(\delta)}(\hat{\mathbf{x}}, t x_j + (1-t)x)| \\ &\lesssim |x - x_j| e^{-\varkappa_1 |\mathbf{x}|_1} \chi^{(\delta)}(\hat{\mathbf{x}}).\end{aligned} \tag{3.18}$$

In order to estimate the derivatives of this difference, we make the following observation. By the definition of θ, we have $|x - x_j| < 2\delta$ on the support of $\phi_j^{(\delta)}$. Furthermore, the balls $\{x \in \mathbb{R}^3 \colon |x - x_j| < 2\delta\} \subset \mathbb{R}^3$, $j = 0, 1, \dots, N-1$, are pairwise disjoint since $\hat{\mathbf{x}} \in \Omega^{(\delta)}$. As a consequence,

$$\mathrm{d}(\hat{\mathbf{x}}, x) = |x - x_j|, \quad \text{if } |x - x_j| < 2\delta, \hat{\mathbf{x}} \in \Omega^{(\delta)}.$$

Consequently, the bound (2.1) together with (3.18) lead to

$$\begin{aligned}&|\partial_x^m (\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j))| \\ &\quad\lesssim |x - x_j|^{1-|m|_1} e^{-\varkappa_{|m|_1} |\mathbf{x}|_1} \chi^{(\delta)}(\hat{\mathbf{x}}), \quad \text{if } |x - x_j| < 2\delta,\end{aligned} \tag{3.19}$$

for *all* $m \in \mathbb{N}_0^3$. Here we have also used our convention that $\varkappa_0 = \varkappa_1$, see (2.2).

Now, return to the functions $\phi_j^{(\delta)}$, see (3.17). The $\phi_j^{(\delta)}(\hat{\mathbf{x}}, x)$ is again partitioned in the sum of two new kernels. At this (last) stage of the partition we introduce a new parameter $\varepsilon \le \delta/2$. With this choice of ε we have $\theta(t\varepsilon^{-1}) = \theta(t\varepsilon^{-1})\theta(t\delta^{-1})$, so that

$$\phi_j^{(\delta)} = \xi_j^{(\delta,\varepsilon)} + \beta_j^{(\delta,\varepsilon)}, \quad j = 0, 1, 2, \dots, N-1,$$

with

$$\begin{aligned}\xi_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, x) &= \theta(|x - x_j|\varepsilon^{-1})(\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j)), \\ \beta_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, x) &= \theta(|x - x_j|\delta^{-1})\zeta(|x - x_j|\varepsilon^{-1})(\psi_1^{(\delta)}(\hat{\mathbf{x}}, x) - \psi_1^{(\delta)}(\hat{\mathbf{x}}, x_j)).\end{aligned}$$

Therefore

$$\phi^{(\delta)} = \xi^{(\delta,\varepsilon)} + \beta^{(\delta,\varepsilon)}, \quad \text{where } \xi^{(\delta,\varepsilon)} = \sum_j \xi_j^{(\delta,\varepsilon)}, \ \beta^{(\delta,\varepsilon)} = \sum_j \beta_j^{(\delta,\varepsilon)}. \tag{3.20}$$

In the next lemma we introduce a weight $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$. Recall that under this condition the integral $M^{(l)}(b)$ defined in (3.2) is finite for all $l \ge 1$.

Lemma 3.5. *Let $a \in \mathsf{L}^2(\mathcal{C}_n)$ and $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$. Then $b\,\mathrm{Int}(\xi^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n} \in \mathbf{S}_{6/7,\infty}$ and*

$$\|b\,\mathrm{Int}(\xi^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty} \lesssim e^{-\varkappa_2|n|_1}\varepsilon^{\frac{1}{2}}M^{(2)}(b)\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \tag{3.21}$$

for all $\varepsilon \in (0,1]$ and $\delta \in [2\varepsilon, 2]$.

Proof. According to (2.6), it suffices to prove (3.21) for each $j = 0, 1, \dots, N-1$, individually. It follows from (3.11) that

$$|\partial_x^m \theta(|x - x_j|\varepsilon^{-1})| \lesssim |x - x_j|^{-|m|_1}\mathbb{1}_{\{|x-x_j|<2\varepsilon\}}(\hat{\mathbf{x}}, x),$$

uniformly in $\varepsilon > 0, \delta > 2\varepsilon$, for all $m \in \mathbb{N}_0^3$. Together with (3.19) this implies that

$$|\partial_x^m \xi_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, x)| \lesssim |x - x_j|^{1-|m|_1}e^{-\varkappa_l|\mathbf{x}|_1}\mathbb{1}_{\{|x-x_j|<2\varepsilon\}}(\hat{\mathbf{x}}, x),$$

for all $m \in \mathbb{N}_0^3$, $|m|_1 \le l$. Thus, $\xi_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot) \in \mathsf{H}^2(\mathcal{C}_n)$ for a.e. $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$ and

$$\begin{aligned} e^{2\varkappa_2|\hat{\mathbf{x}}|_1}\|\xi_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot)\|_{\mathsf{H}^2}^2 &\lesssim e^{-2\varkappa_2|n|_1}\int_{\mathcal{C}_n}(1 + |x - x_j|^{-2})\mathbb{1}_{\{|x-x_j|<2\varepsilon\}}\,dx \\ &\lesssim e^{-2\varkappa_2|n|_1}(\varepsilon^3 + \varepsilon) \lesssim e^{-2\varkappa_2|n|_1}\varepsilon. \end{aligned}$$

It follows from Proposition 2.3 with $l = 2, d = 3$ that $b\,\mathrm{Int}(\xi_j^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n} \in \mathbf{S}_{6/7,\infty}$ and

$$\begin{aligned} &\|b\,\mathrm{Int}(\xi_j^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty} \\ &\quad\lesssim e^{-\varkappa_2|n|_1}\bigg[\int_{\mathbb{R}^{3N-3}}|b(\hat{\mathbf{x}})|^2\|\xi_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot)\|_{\mathsf{H}^2}^2 e^{-2\varkappa_2|\hat{\mathbf{x}}|_1}\,d\hat{\mathbf{x}}\bigg]^{\frac{1}{2}}\|a\|_{\mathsf{L}^2(\mathcal{C}_n)} \\ &\quad\lesssim e^{-\varkappa_2|n|_1}\varepsilon^{\frac{1}{2}}M^{(2)}(b)\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}. \end{aligned}$$

This completes the proof of (3.21). ∎

Lemma 3.6. *Let $a \in \mathsf{L}^2(\mathcal{C}_n)$ and $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$. Then for any $l \ge 3$ the operator $b\,\mathrm{Int}(\beta^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n}$ belongs to $\mathbf{S}_{q,\infty}$ with the parameter q defined in (3.14), and*

$$\|b\,\mathrm{Int}(\beta^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n}\|_{q,\infty} \lesssim e^{-\varkappa_l|n|_1}\varepsilon^{-l+\frac{5}{2}}M^{(l)}(b)\|a\|_{\mathsf{L}^2(\mathcal{C}_n)}, \tag{3.22}$$

for all $\varepsilon \in (0,1]$ and $\delta \in [2\varepsilon, 2]$.

Proof. As in the previous lemma, due to (2.6), it suffices to prove (3.22) for each $j = 0, 1, \dots, N-1$, individually. It follows from (3.11) that

$$|\partial_x^m(\theta(|x - x_j|\delta^{-1})\zeta(|x - x_j|\varepsilon^{-1}))| \lesssim |x - x_j|^{-|m|_1}\mathbb{1}_{\{\varepsilon<|x-x_j|<2\delta\}}(\hat{\mathbf{x}}, x),$$

uniformly in $\varepsilon > 0, \delta > 2\varepsilon$, for all $m \in \mathbb{N}_0^3$. Together with (3.19) this implies that

$$|\partial_x^m \beta_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, x)| \lesssim |x - x_j|^{1-|m|_1} e^{-\varkappa_1 |\mathbf{x}|_1} \mathbb{1}_{\{|x-x_j|>\varepsilon\}}(\hat{\mathbf{x}}, x),$$

for all $m \in \mathbb{N}_0^3$, $|m|_1 \le l$. Thus, $\beta_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot) \in \mathsf{H}^l(\mathcal{C}_n)$ for a.e. $\hat{\mathbf{x}} \in \mathbb{R}^{3N-3}$ with an arbitrary $l \ge 1$, and for $l \ge 3$ we have

$$\begin{aligned} e^{2\varkappa_l |\hat{\mathbf{x}}|_1} \|\beta_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot)\|_{\mathsf{H}^l}^2 &\lesssim e^{-2\varkappa_l |n|_1} \int_{\mathcal{C}_n} (1 + |x - x_j|^{2-2l}) \mathbb{1}_{\{|x-x_j|>\varepsilon\}} dx \\ &\lesssim e^{-2\varkappa_l |n|_1} (1 + \varepsilon^{5-2l}) \lesssim e^{-2\varkappa_l |n|_1} \varepsilon^{5-2l}. \end{aligned}$$

Using Proposition 2.3 with $d = 3$ and arbitrary $l \ge 3$, we get that $b \operatorname{Int}(\beta_j^{(\delta,\varepsilon)}) a \mathbb{1}_{\mathcal{C}_n} \in \mathbf{S}_{q,\infty}$ and

$$\begin{aligned} &\|b \operatorname{Int}(\beta_j^{(\delta,\varepsilon)}) a \mathbb{1}_{\mathcal{C}_n}\|_{q,\infty} \\ &\quad \lesssim e^{-\varkappa_l |n|_1} \Bigg[\int_{\mathbb{R}^{3N-3}} |b(\hat{\mathbf{x}})|^2 \|\beta_j^{(\delta,\varepsilon)}(\hat{\mathbf{x}}, \cdot)\|_{\mathsf{H}^l}^2 e^{-2\varkappa_1 |\hat{\mathbf{x}}|_1} \, d\hat{\mathbf{x}} \Bigg]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C}_n)} \\ &\quad \lesssim e^{-\varkappa_l |n|_1} \varepsilon^{-l+\frac{5}{2}} M^{(l)}(b) \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}. \end{aligned}$$

This completes the proof of (3.22). ■

4. Proof of Theorems 3.1 and 1.1

Her we put together the estimates obtained in the previous section to complete the proof of Theorem 3.1. Recall again that the quantities $S_q^{(l)}(a)$ and $M^{(l)}(b)$ are defined in (3.1) and (3.2) respectively.

Lemma 4.1. *Suppose that $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$ and $a \in \mathsf{L}^2(\mathcal{C}_n)$. Then $b\Psi_n a \in \mathbf{S}_{3/4,\infty}$ and*

$$\|b\Psi_n a\|_{3/4,\infty} \lesssim e^{-\varkappa_3 |n|_1} \|b\|_{\mathsf{L}^\infty} \|a\|_{\mathsf{L}^2(\mathcal{C})}, \tag{4.1}$$

$$\mathsf{G}_{3/4}(b\Psi_n a) \lesssim (e^{-\varkappa_4 |n|_1} M^{(4)}(b) \|a\|_{\mathsf{L}^2(\mathcal{C}_n)})^{\frac{3}{4}}, \tag{4.2}$$

for all $n \in \mathbb{Z}^3$.

Proof. Now, we can put together all the estimates for the singular numbers, obtained above. Without loss of generality assume that $\|b\|_{\mathsf{L}^\infty} \le 1$ and $\|a\|_{\mathsf{L}^2(\mathcal{C})} \le 1$.

By (3.6), (3.12), (3.17), and (3.20) we have

$$\psi = \xi^{(\delta,\varepsilon)} + \beta^{(\delta,\varepsilon)} + \eta^{(\delta)} + \psi_{12}^{(\delta)} + \psi_2^{(\delta)}.$$

According to (3.9), (3.21), and the inequality (2.6),

$$\begin{aligned}&\|b\,\mathrm{Int}(\xi^{(\delta,\varepsilon)}+\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty}^{6/7}\\&\quad\le 7(\|b\,\mathrm{Int}(\xi^{(\delta,\varepsilon)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty}^{6/7}+\|\,\mathrm{Int}(\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{6/7,\infty}^{6/7})\\&\quad\lesssim e^{-6\varkappa_2|n|_1/7}(\varepsilon^{\frac12}M^{(2)}(b)+\delta^{\frac32})^{6/7},\end{aligned}$$

so that, by definition (2.5),

$$\begin{aligned}&s_k(b\,\mathrm{Int}(\xi^{(\delta,\varepsilon)}+\psi_2^{(\delta)})a\mathbb{1}_{\mathcal{C}_n})\\&\quad\lesssim e^{-\varkappa_2|n|_1}(\varepsilon^{\frac12}M^{(2)}(b)+\delta^{\frac32})\,k^{-\frac76},\quad k=1,2,\dots.\end{aligned}\tag{4.3}$$

Similarly, using (3.15), (3.16) and (3.22) with one and the same $l\ge 3$, we obtain that

$$\|b\,\mathrm{Int}(\beta^{(\delta,\varepsilon)}+\eta^{(\delta)}+\psi_{12}^{(\delta)})a\mathbb{1}_{\mathcal{C}_n}\|_{q,\infty}\lesssim e^{-\varkappa_l|n|_1}(\varepsilon^{-l+\frac52}M^{(l)}(b)+\delta^{-l+\frac32}),$$

with $1/q=1/2+l/3$ and hence,

$$\begin{aligned}&s_k\big(b\,\mathrm{Int}\big(\beta^{(\delta,\varepsilon)}+\eta^{(\delta)}+\psi_{12}^{(\delta)}\big)a\mathbb{1}_{\mathcal{C}_n}\big)\\&\quad\lesssim e^{-\varkappa_l|n|_1}(\varepsilon^{-l+\frac52}M^{(l)}(b)+\delta^{-l+\frac32})k^{-\frac12-\frac{l}{3}},\quad k=1,2,\dots.\end{aligned}\tag{4.4}$$

Due to (2.4) and (2.2), combining (4.3) and (4.4), we get the estimate

$$\begin{aligned}&s_{2k}(b\Psi_n a)\le s_{2k-1}(b\Psi_n a)\\&\quad\lesssim e^{-\varkappa_l|n|_1}[(\varepsilon^{\frac12}M^{(l)}(b)+\delta^{\frac32})k^{-\frac76}+(\varepsilon^{-l+\frac52}M^{(l)}(b)+\delta^{-l+\frac32})k^{-\frac12-\frac{l}{3}}],\end{aligned}\tag{4.5}$$

where we have used that $M^{(2)}(b)\le M^{(l)}(b)$. Rewrite the expression in the square brackets, gathering the terms containing ε and δ in two different groups:

$$\begin{aligned}&\big(\varepsilon^{\frac12}M^{(l)}(b)k^{-\frac76}+\varepsilon^{-l+\frac52}M^{(l)}(b)k^{-\frac12-\frac{l}{3}}\big)+(\delta^{\frac32}k^{-\frac76}+\delta^{-l+\frac32}k^{-\frac12-\frac{l}{3}})\\&\quad=\varepsilon^{\frac12}M^{(l)}(b)k^{-\frac76}(1+\varepsilon^{-l+2}k^{\frac{2-l}{3}})+\delta^{\frac32}k^{-\frac76}(1+\delta^{-l}k^{\frac{2-l}{3}}).\end{aligned}$$

Since $\varepsilon\in(0,1]$ and $\delta\in[2\varepsilon,2]$ are arbitrary, we can pick $\varepsilon=\varepsilon_k=k^{-1/3}$ and $\delta=\delta_k=2k^{2/(3l)-1/3}$, so that the condition $\delta\in[2\varepsilon,2]$ is satisfied for all $k=1,2,\dots,$ and

$$\begin{aligned}\varepsilon^{-l+2}k^{\frac{2-l}{3}}&=1,\qquad \varepsilon^{\frac12}k^{-\frac76}=k^{-\frac43},\\ \delta^{-l}k^{\frac{2-l}{3}}&=2^{-l},\quad \delta^{\frac32}k^{-\frac76}=2^{\frac32}k^{\frac1l-\frac53}.\end{aligned}$$

Thus, the bound (4.5) rewrites as

$$s_{2k}(b\Psi_n a)\le s_{2k-1}(b\Psi_n a)\lesssim e^{-\varkappa_l|n|_1}(M^{(l)}(b)k^{-\frac43}+k^{\frac1l-\frac53}).\tag{4.6}$$

Using the bound $M^{(l)}(b) \lesssim \|b\|_{\mathsf{L}^\infty} \le 1$, and taking $l = 3$ we conclude that

$$s_k(b\Psi_n a) \lesssim e^{-\varkappa_3 |n|_1} k^{-\frac{4}{3}}.$$

This leads to (4.1).

In order to obtain (4.2), we use (4.6) to write

$$\limsup_{k\to\infty} k^{\frac{4}{3}} s_k(b\Psi_n a) \lesssim e^{-\varkappa_l |n|_1} \limsup_{k\to\infty} (M^{(l)}(b) + k^{\frac{1}{l}-\frac{1}{3}}).$$

Taking $l = 4$ we ensure that the second term in the brackets tends to zero. Therefore,

$$\limsup_{k\to\infty} k^{\frac{4}{3}} s_k(b\Psi_n a) \lesssim e^{-\varkappa_4 |n|_1} M^{(4)}(b).$$

Applying definition (2.7), we arrive at (4.2). ■

Proof of Theorems 3.1 *and* 1.1. Since $\Psi = \sum_{n\in\mathbb{Z}^3} \Psi_n$, we have, by (2.6) and (4.1),

$$\begin{aligned}\|b\Psi a\|_{3/4,\infty}^{3/4} &\le 4 \sum_{n\in\mathbb{Z}^3} \|b\Psi_n a\|_{3/4,\infty}^{3/4} \\ &\lesssim \|b\|_{\mathsf{L}^\infty}^{\frac{3}{4}} \sum_{n\in\mathbb{Z}^3} e^{-\frac{3}{4}\varkappa_3 |n|_1} \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}^{\frac{3}{4}} = \|b\|_{\mathsf{L}^\infty}^{\frac{3}{4}} (S_{3/4}^{(3)}(a))^{\frac{3}{4}} < \infty.\end{aligned}$$

This proves (3.3).

To prove (3.4) we use Lemma 2.2. According to (2.11) and (4.2),

$$\begin{aligned}\mathsf{G}_{3/4}(b\Psi a) &\le 4 \sum_{n\in\mathbb{Z}^3} \mathsf{G}_{3/4}(b\Psi_n a) \\ &\lesssim (M^{(4)}(b))^{\frac{3}{4}} \sum_{n\in\mathbb{Z}^3} e^{-\frac{3}{4}\varkappa_4 |n|_1} \|a\|_{\mathsf{L}^2(\mathcal{C}_n)}^{\frac{3}{4}} = (M^{(4)}(b))^{\frac{3}{4}} (S_{3/4}^{(4)}(a))^{\frac{3}{4}} < \infty.\end{aligned}$$

This completes the proof of Theorem 3.1.

Using (3.3) with $a(x) = 1$ and $b(\hat{\mathbf{x}}) = 1$ we get $\|\Psi\|_{3/4,\infty} < \infty$, which implies that $s_k(\Psi) \lesssim k^{-4/3}$, and hence $\lambda_k(\Gamma) = s_k(\Psi)^2 \lesssim k^{-8/3}$. This proves Theorem 1.1. ■

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