Mean-Field Dynamics

Singular Potentials and Rate of Convergence

Journal Article

Author(s):
Knowles, Antti; Pickl, Peter

Publication date:
2010-08

Permanent link:
https://doi.org/10.3929/ethz-b-000020676

Originally published in:
Communications in Mathematical Physics 298(1), https://doi.org/10.1007/s00220-010-1010-2

Commun. Math. Phys. 298, 101–138 (2010)
Digital Object Identifier (DOI) 10.1007/s00220-010-1010-2

Communications in
**Mathematical
Physics**

Mean-Field Dynamics: Singular Potentials and Rate of Convergence

Antti Knowles[1], **Peter Pickl**[2]

[1] Theoretische Physik, ETH Hönggerberg, CH-8093 Zürich, Switzerland.
E-mail: aknowles@itp.phys.ethz.ch
[2] Mathematisches Institut, Universität München, Theresien str. 39,
80333 München, Germany

Received: 24 July 2009 / Accepted: 7 December 2009
Published online: 19 February 2010 –

Abstract: We consider the time evolution of a system of N identical bosons whose interaction potential is rescaled by N^{-1}. We choose the initial wave function to describe a condensate in which all particles are in the same one-particle state. It is well known that in the mean-field limit $N \to \infty$ the quantum N-body dynamics is governed by the nonlinear Hartree equation. Using a nonperturbative method, we extend previous results on the mean-field limit in two directions. First, we allow a large class of singular interaction potentials as well as strong, possibly time-dependent external potentials. Second, we derive bounds on the rate of convergence of the quantum N-body dynamics to the Hartree dynamics.

1. Introduction

We consider a system of N identical bosons in d dimensions, described by a wave function $\Psi_N \in \mathcal{H}^{(N)}$. Here

$$\mathcal{H}^{(N)} := L^2_+(\mathbb{R}^{Nd}, \mathrm{d}x_1 \cdots \mathrm{d}x_N)$$

is the subspace of $L^2(\mathbb{R}^{Nd}, \mathrm{d}x_1 \cdots \mathrm{d}x_N)$ consisting of wave functions $\Psi_N(x_1, \dots, x_N)$ that are symmetric under permutation of their arguments $x_1, \dots, x_N \in \mathbb{R}^d$. The Hamiltonian is given by

$$H_N = \sum_{i=1}^{N} h_i + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j), \tag{1.1}$$

where h_i denotes a one-particle Hamiltonian h (to be specified later) acting on the coordinate x_i, and w is an interaction potential. Note the mean-field scaling $1/N$ in front of the interaction potential, which ensures that the free and interacting parts of H_N are of the same order.

The time evolution of Ψ_N is governed by the N-body Schrödinger equation

$$\mathrm{i}\partial_t \Psi_N(t) = H_N \Psi_N(t), \qquad \Psi_N(0) = \Psi_{N,0}. \tag{1.2}$$

For definiteness, let us consider factorized initial data $\Psi_{N,0} = \varphi_0^{\otimes N}$ for some $\varphi_0 \in L^2(\mathbb{R}^d)$ satisfying the normalization condition $\|\varphi_0\|_{L^2(\mathbb{R}^d)} = 1$. Clearly, because of the interaction between the particles, the factorization of the wave function is not preserved by the time evolution. However, it turns out that for large N the interaction potential experienced by any single particle may be approximated by an effective mean-field potential, so that the wave function $\Psi_N(t)$ remains approximately factorized for all times. In other words we have that, in a sense to be made precise, $\Psi_N(t) \approx \varphi(t)^{\otimes N}$ for some appropriate $\varphi(t)$. A simple argument shows that in a product state $\varphi(t)^{\otimes N}$ the interaction potential experienced by a particle is approximately $w * |\varphi(t)|^2$, where $*$ denotes convolution. This implies that $\varphi(t)$ is a solution of the nonlinear Hartree equation

$$\mathrm{i}\partial_t \varphi(t) \;=\; h\varphi(t) + \big(w * |\varphi(t)|^2\big)\varphi(t), \qquad \varphi(0) \;=\; \varphi_0. \tag{1.3}$$

Let us be a little more precise about what one means with $\Psi_N \approx \varphi^{\otimes N}$ (we omit the irrelevant time argument). One does not expect the L^2-distance $\big\|\Psi_N - \varphi^{\otimes N}\big\|_{L^2(\mathbb{R}^{Nd})}$ to become small as $N \to \infty$. A more useful, weaker, indicator of convergence should depend only on a finite, fixed[1] number, k, of particles. To this end we define the reduced k-particle density matrix

$$\gamma_N^{(k)} := \mathrm{Tr}_{k+1,\dots,N}\, |\Psi_N\rangle\langle\Psi_N|,$$

where $\mathrm{Tr}_{k+1,\dots,N}$ denotes the partial trace over the coordinates $x_{k+1}, \dots, x_N$, and $|\Psi_N\rangle\langle\Psi_N|$ denotes (in accordance with the usual Dirac notation) the orthogonal projector onto Ψ_N. In other words, $\gamma_N^{(k)}$ is the positive trace class operator on $L^2_+(\mathbb{R}^{kd}, \mathrm{d}x_1 \cdots \mathrm{d}x_k)$ with operator kernel

$$\begin{aligned}
&\gamma_N^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) \\
&\quad = \int \mathrm{d}x_{k+1} \cdots \mathrm{d}x_N\, \Psi_N(x_1, \dots, x_N)\overline{\Psi_N(y_1, \dots, y_k, x_{k+1}, \dots, x_N)}.
\end{aligned}$$

The reduced k-particle density matrix $\gamma_N^{(k)}$ embodies all the information contained in the full N-particle wave function that pertains to at most k particles. There are two commonly used indicators of the closeness $\gamma_N^{(k)} \approx (|\varphi\rangle\langle\varphi|)^{\otimes k}$: the projection

$$E_N^{(k)} := 1 - \big\langle \varphi^{\otimes k}, \gamma_N^{(k)} \varphi^{\otimes k}\big\rangle$$

and the trace norm distance

$$R_N^{(k)} := \mathrm{Tr}\,\Big|\gamma_N^{(k)} - (|\varphi\rangle\langle\varphi|)^{\otimes k}\Big|. \tag{1.4}$$

It is well known (see e.g. [9]) that all of these indicators are equivalent in the sense that the vanishing of either $R_N^{(k)}$ or $E_N^{(k)}$ for some k in the limit $N \to \infty$ implies that $\lim_N R_N^{(k')} = \lim_N E_N^{(k')} = 0$ for all k'. However, the rate of convergence may differ

[1] In fact, as shown in Corollary 3.2, k may be taken to grow like $o(N)$.

from one indicator to another. Thus, when studying rates of convergence, they are not equivalent (see Sect. 2 below for a full discussion).

The study of the convergence of $\gamma_N^{(k)}(t)$ in the mean-field limit towards $(|\varphi(t)\rangle\langle\varphi(t)|)^{\otimes k}$ for all t has a history going back almost thirty years. The first result is due to Spohn [13], who showed that $\lim_N R_N^{(k)}(t) = 0$ for all t provided that w is bounded. His method is based on the BBGKY hierarchy,

$$\mathrm{i}\partial_t \gamma_N^{(k)}(t) = \sum_{i=1}^{k} \big[h_i\,,\gamma_N^{(k)}(t)\big] + \frac{1}{N} \sum_{1\leqslant i<j\leqslant k} \big[w(x_i - x_j)\,,\gamma_N^{(k)}(t)\big] + \frac{N-k}{N} \sum_{i=1}^{k} \mathrm{Tr}_{k+1}\big[w(x_i - x_{k+1})\,,\gamma_N^{(k+1)}(t)\big], \tag{1.5}$$

an equation of motion for the family $(\gamma_N^{(k)}(t))_{k\in\mathbb{N}}$ of reduced density matrices. It is a simple computation to check that the BBGKY hierarchy is equivalent to the Schrödinger equation (1.2) for $\Psi_N(t)$. Using a perturbative expansion of the BBGKY hierarchy, Spohn showed that in the limit $N \to \infty$ the family $(\gamma_N^{(k)}(t))_{k\in\mathbb{N}}$ converges to a family $(\gamma_\infty^{(k)}(t))_{k\in\mathbb{N}}$ that satisfies the limiting BBGKY obtained by formally setting $N = \infty$ in (1.5). This limiting hierarchy is easily seen to be equivalent to the Hartree equation (1.3) via the identification $\gamma_\infty^{(k)}(t) = (|\varphi(t)\rangle\langle\varphi(t)|)^{\otimes k}$. We refer to [3] for a short discussion of some subsequent developments.

In the past few years considerable progress has been made in strengthening such results in mainly two directions. First, the convergence $\lim_N R_N^{(k)}(t) = 0$ for all t has been proven for singular interaction potentials w. It is for instance of special physical interest to understand the case of a Coulomb potential, $w(x) = \lambda|x|^{-1}$, where $\lambda \in \mathbb{R}$. The proofs for singular interaction potentials are considerably more involved than for bounded interaction potentials. The first result for the case $h = -\Delta$ and $w(x) = \lambda|x|^{-1}$ is due to Erdős and Yau [3]. Their proof uses the BBGKY hierarchy and a weak compactness argument. In [1], Schlein and Elgart extended this result to the technically more demanding case of a semirelativistic kinetic energy, $h = \sqrt{\mathbb{1} - \Delta}$ and $w(x) = \lambda|x|^{-1}$. This is a critical case in the sense that the kinetic energy has the same scaling behaviour as the Coulomb potential energy, thus requiring quite refined estimates. A different approach, based on operator methods, was developed by Fröhlich et al. in [4], where the authors treat the case $h = -\Delta$ and $w(x) = \lambda|x|^{-1}$. Their proof relies on dispersive estimates and counting of Feynman graphs. Yet another approach was adopted by Rodnianski and Schlein in [12]. Using methods inspired by a semiclassical argument of Hepp [6] focusing on the dynamics of coherent states in Fock space, they show convergence to the mean-field limit in the case $h = -\Delta$ and $w(x) = \lambda|x|^{-1}$.

The second area of recent progress in understanding the mean-field limit is deriving estimates on the rate of convergence to the mean-field limit. Methods based on expansions, as used in [13 and 4], give very weak bounds on the error $R_N^{(1)}(t)$, while weak compactness arguments, as used in [3 and 1], yield no information on the rate of convergence. From a physical point of view, where N is large but finite, it is of some interest to have tight error bounds in order to be able to address the question whether the mean-field approximation may be regarded as valid. The first reasonable estimates on the error were derived for the case $h = -\Delta$ and $w(x) = \lambda|x|^{-1}$ by Rodnianski and Schlein in their work [12] mentioned above. In fact they derive an explicit estimate on the error of the form

$$R_N^{(k)}(t) \leqslant \frac{C_1(k)}{\sqrt{N}}\, \mathrm{e}^{C_2(k)t}$$

for some constants $C_1(k), C_2(k) > 0$. Using a novel approach inspired by Lieb-Robinson bounds, Erdős and Schlein [2] further improved this estimate under the more restrictive assumption that w is bounded and its Fourier transform integrable. Their result is

$$R_N^{(k)}(t) \leqslant \frac{C_1}{N}\, \mathrm{e}^{C_2 k} \mathrm{e}^{C_3 t},$$

for some constants $C_1, C_2, C_3 > 0$.

In the present article we adopt yet another approach based on a method of Pickl [10]. We strengthen and generalize many of the results listed above, by treating more singular interaction potentials as well as deriving estimates on the rate of convergence. Moreover, our approach allows for a large class of (possibly time-dependent) external potentials, which might for instance describe a trap confining the particles to a small volume. We also show that if the solution $\varphi(\cdot)$ of the Hartree equation satisfies a scattering condition, all of the error estimates are uniform in time.

The outline of the article is as follows. Section 2 is devoted to a short discussion of the indicators of convergence $E_N^{(k)}$ and $R_N^{(k)}$, in which we derive estimates relating them to each other. In Sect. 3 we state and prove our first main result, which concerns the mean-field limit in the case of L^2-type singularities in w; see Theorem 3.1 and Corollary 3.2. In Sect. 4 we state and prove our second main result, which allows for a larger class of singularities such as the nonrelativistic critical case $h = -\Delta$ and $w(x) = \lambda |x|^{-2}$; see Theorem 4.1. For an outline of the methods underlying our proofs, see the beginnings of Sects. 3 and 4.

Notation. Except in definitions, in statements of results and where confusion is possible, we refrain from indicating the explicit dependence of a quantity $a_N(t)$ on the time t and the particle number N. When needed, we use the notations $a(t)$ and $a|_t$ interchangeably to denote the value of the quantity a at time t. The symbol C is reserved for a generic positive constant that may depend on some fixed parameters. We abbreviate $a \leqslant Cb$ with $a \lesssim b$. To simplify notation, we assume that $t \geqslant 0$.

We abbreviate $L^p(\mathbb{R}^d, \mathrm{d}x) \equiv L^p$ and $\|\cdot\|_{L^p} \equiv \|\cdot\|_p$. We also set $\|\cdot\|_{L^2(\mathbb{R}^{Nd})} = \|\cdot\|$. For $s \in \mathbb{R}$ we use $H^s \equiv H^s(\mathbb{R}^d)$ to denote the Sobolev space with norm $\|f\|_{H^s} = \big\|(1 + |k|^2)^{s/2} \hat{f}\big\|_2$, where $\hat{f}$ is the Fourier transform of f.

Integer indices on operators denote particle number: A k-particle operator A (i.e. an operator on $\mathcal{H}^{(k)}$) acting on the coordinates $x_{i_1}, \dots, x_{i_k}$, where $i_1 < \cdots < i_k$, is denoted by $A_{i_1 \dots i_k}$. Also, by a slight abuse of notation, we identify k-particle functions $f(x_1, \dots, x_k)$ with their associated multiplication operators on $\mathcal{H}^{(k)}$. The operator norm of the multiplication operator f is equal to, and will always be denoted by, $\|f\|_\infty$.

We use the symbol $\mathcal{Q}(\cdot)$ to denote the form domain of a semibounded operator. We denote the space of bounded linear maps from X_1 to X_2 by $\mathcal{L}(X_1; X_2)$, and abbreviate $\mathcal{L}(X) = \mathcal{L}(X; X)$. We abbreviate the operator norm of $\mathcal{L}\big(L^2(\mathbb{R}^{Nd})\big)$ by $\|\cdot\|$. For two Banach spaces, X_1 and X_2, contained in some larger space, we set

$$\|f\|_{X_1 + X_2} = \inf_{f = f_1 + f_2} \big(\|f_1\|_{X_1} + \|f_2\|_{X_2}\big),$$
$$\|f\|_{X_1 \cap X_2} = \|f\|_{X_1} + \|f\|_{X_2},$$

and denote by $X_1 + X_2$ and $X_1 \cap X_2$ the corresponding Banach spaces.

2. Indicators of Convergence

This section is devoted to a discussion, which might also be of independent interest, of quantitative relationships between the indicators $E_N^{(k)}$ and $R_N^{(k)}$. Throughout this section we suppress the irrelevant index N.

Take a k-particle density matrix $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ and a one-particle condensate wave function $\varphi \in L^2$. The following lemma gives the relationship between different elements of the sequence $E^{(1)}, E^{(2)}, \ldots$, where, we recall,

$$E^{(k)} = 1 - \big\langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \big\rangle. \tag{2.1}$$

Lemma 2.1. *Let $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ satisfy*

$$\gamma^{(k)} \geqslant 0, \qquad \operatorname{Tr} \gamma^{(k)} = 1.$$

Let $\varphi \in L^2$ satisfy $\|\varphi\| = 1$. Then

$$E^{(k)} \leqslant k\, E^{(1)}. \tag{2.2}$$

Proof. Let $\big(\Phi_i^{(k)}\big)_{i \geqslant 1}$ be an orthonormal basis of $\mathcal{H}^{(k)}$ with $\Phi_1^{(k)} = \varphi^{\otimes k}$. Then

$$\begin{aligned}
\big\langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \big\rangle &= \sum_{i \geqslant 1} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \big\rangle \\
&\quad - \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \big\rangle \\
&= \langle \varphi, \gamma^{(1)} \varphi \rangle - \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \big\rangle.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&\langle \varphi, \gamma^{(1)} \varphi \rangle - \big\langle \varphi^{\otimes k}, \gamma^{(k)} \varphi^{\otimes k} \big\rangle \\
&\quad = \sum_{i \geqslant 2} \big\langle \varphi \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \varphi \otimes \Phi_i^{(k-1)} \big\rangle \\
&\quad \leqslant \sum_{i \geqslant 2} \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \big\rangle \\
&\quad = \sum_{i \geqslant 1} \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \Phi_i^{(k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \Phi_i^{(k-1)} \big\rangle \\
&\qquad - \sum_{j \geqslant 1} \big\langle \Phi_j^{(1)} \otimes \varphi^{\otimes (k-1)}, \gamma^{(k)} \Phi_j^{(1)} \otimes \varphi^{\otimes (k-1)} \big\rangle \\
&\quad = 1 - \big\langle \varphi^{\otimes (k-1)}, \gamma^{(k-1)} \varphi^{\otimes (k-1)} \big\rangle.
\end{aligned}$$

This yields

$$E^{(k)} \leqslant E^{(k-1)} + E^{(1)},$$

and the claim follows. $\square$

Remark 2.2. The bound in (2.2) is sharp. Indeed, let us suppose that $E^{(k)} \leqslant k\, f(k)\, E^{(1)}$ for some function f. Then

$$f(k) \geqslant \sup_{\gamma^{(k)}} \frac{E^{(k)}}{kE^{(1)}} \geqslant \sup_{0<\alpha<1} \frac{1-(1-\alpha)^k}{k\alpha} \geqslant \lim_{\alpha\to 0} \frac{1-(1-\alpha)^k}{k\alpha} = 1,$$

where the second inequality follows by restricting the supremum to product states $\gamma^{(k)} = (|\psi\rangle\langle\psi|)^{\otimes k}$ and writing $\alpha = E^{(1)}$.

The next lemma describes the relationship between $E^{(k)}$ and $R^{(k)}$, where, we recall,

$$R^{(k)} = \operatorname{Tr}\big|\gamma^{(k)} - (|\varphi\rangle\langle\varphi|)^{\otimes k}\big|.$$

Lemma 2.3. *Let $\gamma^{(k)} \in \mathcal{L}(\mathcal{H}^{(k)})$ be a density matrix and $\varphi \in L^2$ satisfy $\|\varphi\| = 1$. Then*

$$E^{(k)} \leqslant R^{(k)}, \tag{2.3a}$$
$$R^{(k)} \leqslant \sqrt{8\, E^{(k)}}. \tag{2.3b}$$

Proof. It is convenient to introduce the shorthand

$$p^{(k)} := (|\varphi\rangle\langle\varphi|)^{\otimes k}.$$

Thus,

$$E^{(k)} = 1 - \big\langle \varphi^{\otimes k}, \gamma^{(k)}\, \varphi^{\otimes k}\big\rangle = \operatorname{Tr}\big(p^{(k)} - p^{(k)}\gamma^{(k)}\big) \leqslant \|p^{(k)}\| \operatorname{Tr}\big|p^{(k)} - \gamma^{(k)}\big| = R^{(k)},$$

which is (2.3a). In order to prove (2.3b) it is easiest to use the identity

$$\operatorname{Tr}\big|p^{(k)} - \gamma^{(k)}\big| = 2\,\big\|p^{(k)} - \gamma^{(k)}\big\|, \tag{2.4}$$

valid for any one-dimensional projector $p^{(k)}$ and nonnegative density matrix $\gamma^{(k)}$. This was first observed by Seiringer; see [12]. For the convenience of the reader we recall the proof of (2.4). Let $(\lambda_n)_{n\in\mathbb{N}}$ be the sequence of eigenvalues of the trace class operator $A := \gamma^{(k)} - p^{(k)}$. Since $p^{(k)}$ is a rank one projection, A has at most one negative eigenvalue, say λ_0. Also, $\operatorname{Tr} A = 0$ implies that $\sum_n \lambda_n = 0$. Thus, $\sum_n |\lambda_n| = 2|\lambda_0|$, which is (2.4).

Now (2.4) yields

$$R^{(k)} = \operatorname{Tr}\big|p^{(k)} - \gamma^{(k)}\big| = 2\,\|p^{(k)} - \gamma^{(k)}\| \leqslant 2\sqrt{\operatorname{Tr}\big(p^{(k)} - \gamma^{(k)}\big)^2}.$$

Then (2.3b) follows from

$$\operatorname{Tr}\big(p^{(k)} - \gamma^{(k)}\big)^2 = 1 - 2\operatorname{Tr}\big(p^{(k)}\gamma^{(k)}\big) + \operatorname{Tr}(\gamma^{(k)})^2 \leqslant E^{(k)} - \operatorname{Tr}\big(p^{(k)}\gamma^{(k)}\big) + 1 = 2E^{(k)}.$$

Alternatively, one may prove (2.3b) without (2.4) by using the polar decomposition and the Cauchy-Schwarz inequality for Hilbert-Schmidt operators. □

Remark 2.4. Up to constant factors the bounds (2.3) are sharp, as the following examples show. Here we drop the irrelevant index k. Consider first

$$\varphi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} 1-a & 0 \\ 0 & a \end{pmatrix},$$

where $0 \leqslant a \leqslant 1$. As above we set $p := |\varphi\rangle\langle\varphi|$. One finds

$$E = 1 - \langle \varphi, \gamma\, \varphi \rangle = a, \qquad R = \operatorname{Tr}|p - \gamma| = 2a,$$

so that (2.3a) is sharp up to a constant factor.

It is not hard to see that if γ and p commute then (2.3b) can be replaced with the stronger bound $R \lesssim E$. In order to show that in general (2.3b) is sharp up to a constant factor, consider

$$\varphi = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \gamma = \begin{pmatrix} 1-a & \sqrt{a-a^2} \\ \sqrt{a-a^2} & a \end{pmatrix},$$

where $0 \leqslant a \leqslant 1$. One readily sees that γ is a density matrix (in fact, a one-dimensional projector). A short calculation yields

$$E = 1 - \langle \varphi, \gamma\, \varphi \rangle = a$$

as well as

$$\operatorname{Tr}\big|\gamma(1-p)\big| = \sqrt{a}.$$

Using

$$\operatorname{Tr}\big|\gamma(1-p)\big| = \operatorname{Tr}\big|\gamma - p + p - \gamma p\big| \leqslant 2 \operatorname{Tr}|p - \gamma|$$

we therefore find

$$R = \operatorname{Tr}|p-\gamma| \geqslant \frac{\sqrt{a}}{2} = \frac{\sqrt{E}}{2},$$

as desired.

3. Convergence for L^2-type Singularities

This section is devoted to the case $w \in L^2 + L^\infty$.

3.1. Outline and main result. Our method relies on controlling the quantity

$$\alpha_N(t) \;:=\; E_N^{(1)}(t). \tag{3.1}$$

To this end, we derive an estimate of the form

$$\dot{\alpha}_N(t) \;\leqslant\; A_N(t) + B_N(t)\,\alpha_N(t), \tag{3.2}$$

which, by Grönwall's Lemma, implies

$$\alpha_N(t) \;\leqslant\; \alpha_N(0)\,\mathrm{e}^{\int_0^t B_N} + \int_0^t A_N(s)\,\mathrm{e}^{\int_s^t B_N}\,\mathrm{d}s. \tag{3.3}$$

In order to show (3.2), we differentiate $\alpha_N(t)$ and note that all terms arising from the one-particle Hamiltonian vanish. We control the remaining terms by introducing the time-dependent orthogonal projections

$$p(t) := |\varphi(t)\rangle\langle\varphi(t)|, \qquad q(t) := \mathbb{1} - p(t).$$

We then partition $\mathbb{1} = p(t) + q(t)$ appropriately and use the following heuristics for controlling the terms that arise in this manner. Factors $p(t)$ are used to control singularities of w by exploiting the smoothness of the Hartree wave function $\varphi(t)$. Factors $q(t)$ are expected to yield something small, i.e. proportional to $\alpha_N(t)$, in accordance with the identity $\alpha_N(t) = \langle \Psi_N(t)\,, q_1(t)\Psi_N(t)\rangle$.

For the following it is convenient to rewrite the Hamiltonian (1.1) as

$$H_N \;=\; \sum_{i=1}^N h_i + \frac{1}{N}\sum_{1\leqslant i<j\leqslant N} W_{ij} \;=:\; H_N^0 + H_N^W, \tag{3.4}$$

where $W_{ij} \;:=\; w(x_i - x_j)$. We may now list our assumptions.

(A1) The one-particle Hamiltonian h is self-adjoint and bounded from below. Without loss of generality we assume that $h \geqslant 0$. We define the Hilbert space $X_N = \mathcal{Q}(H_N^0)$ as the form domain of H_N^0 with norm

$$\|\Psi\|_{X_N} := \big\|(1 + H_N^0)^{1/2}\Psi\big\|.$$

(A2) The Hamiltonian (3.4) is self-adjoint and bounded from below. We also assume that $\mathcal{Q}(H_N) \subset X_N$.

(A3) The interaction potential w is a real and even function satisfying $w \in L^{p_1} + L^{p_2}$, where $2 \leqslant p_1 \leqslant p_2 \leqslant \infty$.

(A4) The solution $\varphi(\cdot)$ of (1.3) satisfies

$$\varphi(\cdot) \in C(\mathbb{R}; X_1 \cap L^{q_1}) \cap C^1(\mathbb{R}; X_1^*),$$

where $2 \leqslant q_2 \leqslant q_1 \leqslant \infty$ are defined through

$$\frac{1}{2} = \frac{1}{p_i} + \frac{1}{q_i}, \qquad i = 1, 2. \tag{3.5}$$

Here X_1^* denotes the dual space of X_1, i.e. the closure of L^2 under the norm $\|\varphi\|_{X_1^*} := \|(\mathbb{1} + h)^{-1/2}\varphi\|$.

We now state our main result.

Theorem 3.1. *Let $\Psi_{N,0} \in \mathcal{Q}(H_N)$ satisfy $\|\Psi_{N,0}\| = 1$, and $\varphi_0 \in X_1 \cap L^{q_1}$ satisfy $\|\varphi_0\| = 1$. Assume that Assumptions* (A1) – (A4) *hold. Then*

$$\alpha_N(t) \leqslant \left(\alpha_N(0) + \frac{1}{N}\right) \mathrm{e}^{\phi(t)},$$

where

$$\phi(t) := 32\|w\|_{L^{p_1}+L^{p_2}} \int_0^t \mathrm{d}s \big(\|\varphi(s)\|_{q_1} + \|\varphi(s)\|_{q_2}\big).$$

We may combine this result with the observations of Sect. 2.

Corollary 3.2. *Let the sequence $\Psi_{N,0} \in \mathcal{Q}(H_N)$, $N \in \mathbb{N}$, satisfy the assumptions of Theorem 3.1 as well as*

$$E_N^{(1)}(0) \lesssim \frac{1}{N}.$$

Then we have

$$E_N^{(k)}(t) \lesssim \frac{k}{N}\,\mathrm{e}^{\phi(t)}, \qquad R_N^{(k)}(t) \lesssim \sqrt{\frac{k}{N}}\,\mathrm{e}^{\phi(t)/2}.$$

Remark 3.3. Corollary 3.2 implies that we can control the condensation of $k = o(N)$ particles.

Remark 3.4. Assumption (A3) allows for singularities in w up to, but not including, the type $|x|^{-3/2}$ in three dimensions. In the next section we treat a larger class of interaction potentials.

Remark 3.5. Assumption (A4) is typically verified by solving the Hartree equation in a Sobolev space of high index (see e.g. Sect. 3.2.2). Instead of requiring a global-in-time solution $\varphi(\cdot)$, it is enough to have a local-in-time solution on $[0, T)$ for some $T > 0$.

Remark 3.6. If $\sup_t \phi(t) < \infty$, or in other words if $\|\varphi(t)\|_{q_1}$ and $\|\varphi(t)\|_{q_2}$ are integrable in t over $\mathbb{R}$, then all estimates are uniform in time. This describes a scattering regime where the time evolution is asymptotically free for large times. Such an integrability condition requires large exponents q_i, which translates to small exponents p_i, i.e. an interaction potential with strong decay.

Remark 3.7. The result easily extends to time-dependent one-particle Hamiltonians $h \equiv h(t)$. Replace (A1) and (A2) with

(A1') The Hamiltonian $h(t)$ is self-adjoint and bounded from below. We assume that there is an operator $h_0 \geqslant 0$ that such that $0 \leqslant h(t) \leqslant h_0$ for all t. Define the Hilbert space $X_N = \mathcal{Q}\big(\sum_i (h_0)_i\big)$ as in (A1).

(A2') The Hamiltonian $H_N(t)$ is self-adjoint and bounded from below. We assume that $\mathcal{Q}(H_N(t)) \subset X_N$ for all t. We also assume that the N-body propagator $U_N(t,s)$, defined by

$$\mathrm{i}\partial_t U_N(t,s) = H_N(t) U_N(t,s), \qquad U_N(s,s) = \mathbb{1},$$

exists and satisfies $U_N(t,0)\Psi_{N,0} \in \mathcal{Q}(H_N(t))$ for all t.

It is then straightforward that Theorem 3.1 holds with the same proof.

Remark 3.8. In some cases (see e.g. Sect. 3.2.1 below) it is convenient to modify the assumptions as follows. Replace (A3) and (A4) with

(A3') The interaction potential w is a real and even function satisfying

$$\left\| w^2 * |\varphi|^2 \right\|_\infty \leqslant K \, \|\varphi\|_{X_1}^2 \tag{3.6}$$

for some constant $K > 0$. Without loss of generality we assume that $K \geqslant 1$.

(A4') The solution $\varphi(\cdot)$ of (1.3) satisfies

$$\varphi(\cdot) \in C(\mathbb{R}; X_1) \cap C^1(\mathbb{R}; X_1^*).$$

Then Theorem 3.1 and Corollary 3.2 hold with

$$\phi(t) = 32K \int_0^t \mathrm{d}s \, \|\varphi(s)\|_{X_1}^2 .$$

The proof remains virtually unchanged. One replaces (3.24) with (3.6), as well as (3.20) with

$$\left\| w * |\varphi|^2 \right\|_\infty \leqslant 2K \, \|\varphi\|_{X_1}^2 ,$$

which is an easy consequence of (3.6).

3.2. Examples. We list two examples of systems satisfying the assumptions of Theorem 3.1.

3.2.1. Particles in a trap. Consider nonrelativistic particles in $\mathbb{R}^3$ confined by a strong trapping potential. The particles interact by means of the Coulomb potential: $w(x) = \lambda |x|^{-1}$, where $\lambda \in \mathbb{R}$. The one-particle Hamiltonian is of the form $h = -\Delta + v$, where v is a measurable function on $\mathbb{R}^3$. Decompose v into its positive and negative parts: $v = v_+ - v_-$, where $v_+, v_- \geqslant 0$. We assume that $v_+ \in L^1_{\mathrm{loc}}$ and that v_- is $-\Delta$-form bounded with relative bound less than one, i.e. there are constants $0 \leqslant a < 1$ and $0 \leqslant b < \infty$ such that

$$\langle \varphi \,, v_- \varphi \rangle \leqslant a \langle \varphi \,, -\Delta \varphi \rangle + b \langle \varphi \,, \varphi \rangle . \tag{3.7}$$

Thus $h + b\mathbb{1}$ is positive, and it is not hard to see that h is essentially self-adjoint on $C_c^\infty(\mathbb{R}^3)$. This follows by density and a standard argument using Riesz's representation theorem to show that the equation $(h + (b+1)\mathbb{1})\varphi = f$ has a unique solution $\varphi \in \{\varphi \in L^2 \,:\, h\varphi \in L^2\}$ for each $f \in L^2$.

It is now easy to see that Assumptions (A1) and (A2) hold with the one-particle Hamiltonian $h + c\mathbb{1}$ for some $c > 0$. Let us assume without loss of generality that $c = 0$. Next, we verify Assumptions (A3') and (A4') (see Remark 3.8). We find

$$\begin{aligned} \left\| w^2 * |\varphi|^2 \right\|_\infty &= \sup_x \left| \int \mathrm{d}y \frac{\lambda^2}{|x-y|^2} |\varphi(y)|^2 \right| \lesssim \langle \varphi \,, -\Delta \varphi \rangle \\ &\lesssim \langle \varphi \,, h\varphi \rangle + \langle \varphi \,, \varphi \rangle = \|\varphi\|_{X_1}^2 , \end{aligned}$$

where the second step follows from Hardy's inequality and translation invariance of Δ, and the third step is a simple consequence of (3.7). This proves (A3').

Next, take $\varphi_0 \in X_1$. By standard methods (see e.g. the presentation of [7]) one finds that (A4') holds. Moreover, the mass $\|\varphi(t)\|^2$ and the energy

$$E^{\varphi}(t) = \left[\langle\varphi, h\varphi\rangle + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\; w(x-y)|\varphi(x)|^2|\varphi(y)|^2\right]\Bigg|_t$$

are conserved under time evolution. Using the identity $|x|^{-1} \leqslant \mathbb{1}_{\{|x|\leqslant\varepsilon\}}\varepsilon|x|^{-2} + \mathbb{1}_{\{|x|>\varepsilon\}}\varepsilon^{-1}$ and Hardy's inequality one sees that

$$\|\varphi(t)\|_{X_1}^2 \lesssim E^{\varphi}(t) + \|\varphi(t)\|^2,$$

and therefore $\|\varphi(t)\|_{X_1} \leqslant C$ for all t. We conclude: Theorem 3.1 holds with $\phi(t) = Ct$. More generally, the preceding discussion holds for interaction potentials $w \in L^3_w + L^\infty$, where L^p_w denotes the weak L^p space (see e.g. [11]). This follows from a short computation using symmetric-decreasing rearrangements; we omit further details. This example generalizes the results of [3,12 and 4].

3.2.2. A boson star. Consider semirelativistic particles in $\mathbb{R}^3$ whose one-particle Hamiltonian is given by $h = \sqrt{\mathbb{1} - \Delta}$. The particles interact by means of a Coulomb potential: $w(x) = \lambda|x|^{-1}$. We impose the condition $\lambda > -4/\pi$. This condition is necessary for both the stability of the N-body problem (i.e. Assumption (A2)) and the global well-posedness of the Hartree equation. See [7,8] for details. It is well known that Assumptions (A1) and (A2) hold in this case.

In order to show (A4) we need some regularity of $\varphi(\cdot)$. To this end, let $s > 1$ and take $\varphi_0 \in H^s$. Theorem 3 of [7] implies that (1.3) has a unique global solution in H^s. Therefore Sobolev's inequality implies that (A4) holds with

$$\frac{1}{q_1} = \frac{1}{2} - \frac{s}{3}.$$

Thus $q_1 > 6$, and (A3) holds with appropriately chosen values of p_1, p_2. We conclude: Theorem 3.1 holds for some continuous function $\phi(t)$. (In fact, as shown in [7], one has the bound $\phi(t) \lesssim \mathrm{e}^{Ct}$.) This example generalizes the result of [1].

3.3. Proof of Theorem 3.1.

3.3.1. A family of projectors. Define the time-dependent projectors

$$p(t) := |\varphi(t)\rangle\langle\varphi(t)|, \qquad q(t) := \mathbb{1} - p(t).$$

Write

$$\mathbb{1} = (p_1 + q_1)\cdots(p_N + q_N), \tag{3.8}$$

and define P_k, for $k = 0, \dots, N$, as the term obtained by multiplying out (3.8) and selecting all summands containing k factors q. In other words,

$$P_k = \sum_{\substack{a\in\{0,1\}^N :\\ \sum_i a_i = k}} \prod_{i=1}^N p_i^{1-a_i} q_i^{a_i}. \tag{3.9}$$

If $k \neq \{0, \dots, N\}$ we set $P_k = 0$. It is easy to see that the following properties hold:

(i) P_k is an orthogonal projector,
(ii) $P_k P_l = \delta_{kl} P_k$,
(iii) $\sum_k P_k = \mathbb{1}$.

Next, for any function $f : \{0, \dots, N\} \to \mathbb{C}$ we define the operator

$$\widehat{f} := \sum_k f(k) P_k. \tag{3.10}$$

It follows immediately that

$$\widehat{f}\widehat{g} = \widehat{fg},$$

and that $\widehat{f}$ commutes with p_i and P_k. We shall often make use of the functions

$$m(k) := \frac{k}{N}, \qquad n(k) := \sqrt{\frac{k}{N}}.$$

We have the relation

$$\frac{1}{N}\sum_i q_i = \frac{1}{N}\sum_k \sum_i q_i P_k = \frac{1}{N}\sum_k k P_k = \widehat{m}. \tag{3.11}$$

Thus, by symmetry of Ψ, we get

$$\alpha = \langle \Psi , q_1 \Psi \rangle = \langle \Psi , \widehat{m}\, \Psi \rangle. \tag{3.12}$$

The correspondence $q_1 \sim \widehat{m}$ of (3.11) yields the following useful bounds.

Lemma 3.9. *For any nonnegative function $f : \{0, \dots, N\} \to [0, \infty)$ we have*

$$\big\langle \Psi , \widehat{f} q_1 \Psi \big\rangle = \big\langle \Psi , \widehat{f}\, \widehat{m} \Psi \big\rangle, \tag{3.13}$$

$$\big\langle \Psi , \widehat{f} q_1 q_2 \Psi \big\rangle \leqslant \frac{N}{N-1} \big\langle \Psi , \widehat{f}\, \widehat{m}^2 \Psi \big\rangle. \tag{3.14}$$

Proof. The proof of (3.13) is an immediate consequence of (3.11). In order to prove (3.14) we write, using symmetry of Ψ as well as (3.11),

$$\begin{aligned} \big\langle \Psi , \widehat{f} q_1 q_2 \Psi \big\rangle &= \frac{1}{N(N-1)} \sum_{i \neq j} \big\langle \Psi , \widehat{f} q_i q_j \Psi \big\rangle \\ &\leqslant \frac{1}{N(N-1)} \sum_{i,j} \big\langle \Psi , \widehat{f} q_i q_j \Psi \big\rangle = \frac{N}{N-1} \big\langle \Psi , \widehat{f}\, \widehat{m}^2 \Psi \big\rangle, \end{aligned}$$

which is the claim. □

Next, we introduce the shift operation τ_n, $n \in \mathbb{Z}$, defined on functions f through

$$(\tau_n f)(k) := f(k+n). \tag{3.15}$$

Its usefulness for our purposes is encapsulated by the following lemma.

Lemma 3.10. *Let $r \geqslant 1$ and A be an operator on $\mathcal{H}^{(r)}$. Let Q_i, $i = 1, 2$, be two projectors of the form*

$$Q_i = \#_1 \cdots \#_r,$$

where each # stands for either p or q. Then

$$Q_1 A_{1\ldots r} \widehat{f} Q_2 = Q_1 \widehat{\tau_n f} A_{1\ldots r} Q_2,$$

where $n = n_2 - n_1$ and n_i is the number of factors q in Q_i.

Proof. Define

$$P_k^r := \sum_{\substack{a \in \{0,1\}^{N-r} \\ \sum_i a_i = k}} \prod_{i=r+1}^{N} p_i^{1-a_i} q_i^{a_i}.$$

Then,

$$Q_i \widehat{f} = \sum_k f(k)\, Q_i P_k = \sum_k f(k)\, Q_i P_{k-n_i}^r = \sum_k f(k+n_i)\, Q_i P_k^r.$$

The claim follows from the fact that P_k^r commutes with $A_{1\ldots r}$. $\square$

3.3.2. A bound on $\dot{\alpha}$. Let us abbreviate

$$W^\varphi := w * |\varphi|^2.$$

From (A3) and (A4) we find $W^\varphi \in L^\infty$ (see (3.20) below). Then $\mathrm{i}\partial_t \varphi = (h + W^\varphi)\varphi$, where $h + W^\varphi \in \mathcal{L}(X_1; X_1^*)$. Thus, for any $\psi \in X_1$ independent of t we have

$$\mathrm{i}\partial_t \langle \psi, p\,\psi \rangle = \langle \psi, [h + W^\varphi, p]\psi \rangle.$$

On the other hand, it is easy to see from (A3) and (A4) that $\widehat{m}\Psi \in \mathcal{Q}(H)$. Combining these observations, and noting that $\Psi \in \mathcal{Q}(H) \subset X$ by (A2), we see that α is differentiable in t with derivative

$$\dot{\alpha} = \mathrm{i}\big\langle \Psi, \big[H - H^\varphi, \widehat{m}\big]\Psi \big\rangle,$$

where $H^\varphi := \sum_i (h_i + W_i^\varphi)$. Thus,

$$\dot{\alpha} = \mathrm{i}\left\langle \Psi\,,\, \left[\frac{1}{N}\sum_{i<j} W_{ij} - \sum_i W_i^\varphi\,,\, \widehat{m}\right]\Psi \right\rangle.$$

By symmetry of Ψ and $\widehat{m}$ we get

$$\dot{\alpha} = \frac{\mathrm{i}}{2}\big\langle \Psi, \big[(N-1)W_{12} - N W_1^\varphi - N W_2^\varphi, \widehat{m}\big]\Psi \big\rangle. \tag{3.16}$$

In order to estimate the right-hand side, we introduce

$$\mathbb{1} = (p_1 + q_1)(p_2 + q_2)$$

on both sides of the commutator in (3.16). Of the sixteen resulting terms only three different types survive:

$$\tfrac{\mathrm{i}}{2}\big\langle\Psi\,,\,p_1p_2\big[(N-1)W_{12}-NW_1^{\varphi}-NW_2^{\varphi}\,,\widehat{m}\big]q_1p_2\Psi\big\rangle, \tag{I}$$

$$\tfrac{\mathrm{i}}{2}\big\langle\Psi\,,\,q_1p_2\big[(N-1)W_{12}-NW_1^{\varphi}-NW_2^{\varphi}\,,\widehat{m}\big]q_1q_2\Psi\big\rangle, \tag{II}$$

$$\tfrac{\mathrm{i}}{2}\big\langle\Psi\,,\,p_1p_2\big[(N-1)W_{12}-NW_1^{\varphi}-NW_2^{\varphi}\,,\widehat{m}\big]q_1q_2\Psi\big\rangle. \tag{III}$$

Indeed, Lemma 3.10 implies that terms with the same number of factors q on the left and on the right vanish. What remains is

$$\dot{\alpha}=2(\mathrm{I})+2(\mathrm{II})+(\mathrm{III})+\text{ complex conjugate.}$$

The remainder of the proof consists in estimating each term.

Term (I). First, we remark that

$$p_2W_{12}p_2=p_2W_1^{\varphi}. \tag{3.17}$$

This is easiest to see using operator kernels (we drop the trivial indices $x_3, y_3, \dots, x_N, y_N$):

$$\begin{aligned}(p_2W_{12}p_2)(x_1,x_2;y_1,y_2)&=\int \mathrm{d}z\varphi(x_2)\,\overline{\varphi}(z)\,w(x_1-z)\,\delta(x_1-y_1)\,\varphi(z)\,\overline{\varphi}(y_2)\\&=\varphi(x_2)\,\overline{\varphi}(y_2)\,\delta(x_1-y_1)\,(w*|\varphi|^2)(x_1).\end{aligned}$$

Therefore,

$$(\mathrm{I})=\frac{\mathrm{i}}{2}\big\langle\Psi\,,\,p_1p_2\big[(N-1)W_1^{\varphi}-NW_1^{\varphi}\,,\widehat{m}\big]q_1p_2\Psi\big\rangle=\frac{-\mathrm{i}}{2}\big\langle\Psi\,,\,p_1p_2\big[W_1^{\varphi}\,,\widehat{m}\big]q_1p_2\Psi\big\rangle.$$

Using Lemma 3.10 we find

$$(\mathrm{I})=\frac{-\mathrm{i}}{2}\big\langle\Psi\,,\,p_1p_2W_1^{\varphi}\big(\widehat{m}-\widehat{\tau_{-1}m}\big)q_1p_2\Psi\big\rangle=\frac{-\mathrm{i}}{2N}\big\langle\Psi\,,\,p_1p_2W_1^{\varphi}q_1p_2\Psi\big\rangle.$$

This gives

$$\big|(\mathrm{I})\big|\leqslant\frac{1}{2N}\,\|W^{\varphi}\|_{\infty}=\frac{1}{2N}\big\|w*|\varphi|^2\big\|_{\infty}.$$

By (A3), we may write

$$w=w^{(1)}+w^{(2)},\qquad w^{(i)}\in L^{p_i}. \tag{3.18}$$

By Young's inequality,

$$\big\|w^{(i)}*|\varphi|^2\big\|_{\infty}\leqslant\|w^{(i)}\|_{p_i}\|\varphi\|_{r_i}^2,$$

where r_1, r_2 are defined through

$$1=\frac{1}{p_i}+\frac{2}{r_i}. \tag{3.19}$$

Therefore,

$$\begin{aligned}\big\|w * |\varphi|^2\big\|_\infty &\leqslant \|w^{(1)}\|_{p_1}\|\varphi\|_{r_1}^2 + \|w^{(1)}\|_{p_2}\|\varphi\|_{r_2}^2 \\ &\leqslant \big(\|w^{(1)}\|_{p_1} + \|w^{(2)}\|_{p_2}\big)\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2.\end{aligned}$$

Taking the infimum over all decompositions (3.18) yields

$$\|W^\varphi\|_\infty = \big\|w * |\varphi|^2\big\|_\infty \leqslant \|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2. \tag{3.20}$$

Note that (A3) and (A4) imply

$$2 \leqslant r_i \leqslant q_1, \tag{3.21}$$

so that the right-hand side of (3.20) is finite. Summarizing,

$$\big|(\mathrm{I})\big| \leqslant \frac{1}{2N}\|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2. \tag{3.22}$$

Term (II). Applying Lemma 3.10 to (II) yields

$$\begin{aligned}(\mathrm{II}) &= \frac{\mathrm{i}}{2}\big\langle\Psi\,, q_1p_2\big((N-1)W_{12} - NW_2^\varphi\big)\big(\widehat{m} - \widehat{\tau_{-1}m}\big)q_1q_2\Psi\big\rangle \\ &= \frac{\mathrm{i}}{2}\Big\langle\Psi\ ,\ q_1p_2\Big(\frac{N-1}{N}W_{12} - W_2^\varphi\Big)q_1q_2\Psi\Big\rangle,\end{aligned}$$

so that

$$\big|(\mathrm{II})\big| \leqslant \frac{1}{2}\big|\big\langle\Psi\,, q_1p_2W_{12}q_1q_2\Psi\big\rangle\big| + \frac{1}{2}\big|\big\langle\Psi\,, q_1p_2W_2^\varphi q_1q_2\Psi\big\rangle\big|. \tag{3.23}$$

The second term of (3.23) is bounded by

$$\frac{1}{2}\|W^\varphi\|_\infty\,\|q_1\Psi\|^2 \leqslant \frac{1}{2}\|w\|_{L^{p_1}+L^{p_2}}\big(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\big)^2\alpha,$$

where we used the bound (3.20) as well as (3.12).

The first term of (3.23) is bounded using Cauchy-Schwarz by

$$\begin{aligned}&\frac{1}{2}\sqrt{\big\langle\Psi\,, q_1p_2W_{12}^2p_2q_1\Psi\big\rangle}\sqrt{\langle\Psi\,, q_1q_2\Psi\rangle} \\ &\quad= \frac{1}{2}\sqrt{\big\langle\Psi\,, q_1p_2\big(w^2 * |\varphi|^2\big)_1p_2q_1\Psi\big\rangle}\sqrt{\langle\Psi\,, q_1q_2\Psi\rangle}.\end{aligned}$$

This follows by applying (3.17) to W^2. Thus we get the bound

$$\frac{1}{2}\|q_1\Psi\|^2\sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty} = \frac{1}{2}\alpha\sqrt{\big\|w^2 * |\varphi|^2\big\|_\infty}.$$

We now proceed as above. Using the decomposition (3.18) we get

$$\big\|w^2 * |\varphi|^2\big\|_\infty \leqslant 2\big\|(w^{(1)})^2 * |\varphi|^2\big\|_\infty + 2\big\|(w^{(2)})^2 * |\varphi|^2\big\|_\infty.$$

Then Young's inequality gives

$$\big\|(w^{(i)})^2 * |\varphi|^2\big\|_\infty \leqslant \big\|w^{(i)}\big\|_{p_i}^2\|\varphi\|_{q_i}^2,$$

which implies that

$$\left\| w^2 * |\varphi|^2 \right\|_\infty \leqslant 2\|w\|^2_{L^{p_1}+L^{p_2}} \left(\|\varphi\|_{q_1} + \|\varphi\|_{q_2}\right)^2. \tag{3.24}$$

Putting all of this together we get

$$\left|(\mathrm{II})\right| \leqslant \frac{1}{2}\|w\|_{L^{p_1}+L^{p_2}} \left[\sqrt{2}\left(\|\varphi\|_{q_1} + \|\varphi\|_{q_2}\right) + \left(\|\varphi\|_{r_1} + \|\varphi\|_{r_2}\right)^2\right] \alpha.$$

Term (III). The final term (III) is equal to

$$\begin{aligned}
\frac{\mathrm{i}}{2}\left\langle \Psi\,,\, p_1 p_2 \left[(N-1) W_{12}\,,\, \widehat{m}\right] q_1 q_2 \Psi\right\rangle &= \frac{\mathrm{i}}{2}\left\langle \Psi\,,\, p_1 p_2 (N-1) W_{12} \left(\widehat{m} - \widehat{\tau_{-2} m}\right) q_1 q_2 \Psi\right\rangle \\
&= \mathrm{i}\frac{N-1}{N}\left\langle \Psi\,,\, p_1 p_2 W_{12} q_1 q_2 \Psi\right\rangle,
\end{aligned}$$

where we used Lemma 3.10. Next, we note that, on the range of q_1, the operator $\widehat{n}^{-1}$ is well-defined and bounded. Thus (III) is equal to

$$\mathrm{i}\frac{N-1}{N}\left\langle \Psi\,,\, p_1 p_2 W_{12}\, \widehat{n}\, \widehat{n}^{-1} q_1 q_2 \Psi\right\rangle = \mathrm{i}\frac{N-1}{N}\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, W_{12}\, \widehat{n}^{-1} q_1 q_2 \Psi\right\rangle,$$

where we used Lemma 3.10 again. We now use Cauchy-Schwarz to get

$$\begin{aligned}
\left|(\mathrm{III})\right| &\leqslant \sqrt{\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, W_{12}^2\, \widehat{\tau_2 n}\, p_1 p_2 \Psi\right\rangle} \sqrt{\left\langle \Psi\,,\, \widehat{n}^{-2} q_1 q_2 \Psi\right\rangle} \\
&= \sqrt{\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, \left(w^2 * |\varphi|^2\right)_1 \widehat{\tau_2 n}\, p_1 p_2 \Psi\right\rangle} \sqrt{\left\langle \Psi\,,\, \widehat{m}^{-1} q_1 q_2 \Psi\right\rangle} \\
&\leqslant \sqrt{\left\| w^2 * |\varphi|^2 \right\|_\infty}\, \|\widehat{\tau_2 n}\Psi\| \sqrt{\frac{N}{N-1}} \sqrt{\langle \Psi\,,\, \widehat{m}\Psi\rangle} \\
&= \sqrt{\left\| w^2 * |\varphi|^2 \right\|_\infty} \sqrt{\frac{N}{N-1}} \sqrt{\left\langle \Psi\,,\, \widehat{\tau_2 m}\Psi\right\rangle} \sqrt{\alpha} \\
&= \sqrt{\left\| w^2 * |\varphi|^2 \right\|_\infty} \sqrt{\frac{N}{N-1}} \sqrt{\left\langle \Psi\,,\, \widehat{m}\Psi\right\rangle + \frac{2}{N}}\, \sqrt{\alpha} \\
&\leqslant \sqrt{\left\| w^2 * |\varphi|^2 \right\|_\infty} \sqrt{\frac{N}{N-1}} \left(\alpha + \sqrt{\frac{2\alpha}{N}}\right) \\
&\leqslant \sqrt{\left\| w^2 * |\varphi|^2 \right\|_\infty} \sqrt{\frac{N}{N-1}}\, 2\left(\alpha + \frac{1}{N}\right).
\end{aligned}$$

Using the estimate (3.24) we get finally

$$\left|(\mathrm{III})\right| \leqslant 2\sqrt{2}\|w\|_{L^{p_1}+L^{p_2}} \left(\|\varphi\|_{q_1} + \|\varphi\|_{q_2}\right) \sqrt{\frac{N}{N-1}} \left(\alpha + \frac{1}{N}\right).$$

Conclusion of the proof. We have shown that the estimate (3.2) holds with

$$\begin{aligned}
B_N(t) &= 2\|w\|_{L^{p_1}+L^{p_2}} \left[\left(\|\varphi(t)\|_{r_1} + \|\varphi(t)\|_{r_2}\right)^2 + 6\left(\|\varphi(t)\|_{q_1} + \|\varphi(t)\|_{q_2}\right)\right], \\
A_N(t) &= \frac{B_N(t)}{N}.
\end{aligned}$$

Using L^2-norm conservation $\|\varphi(t)\| = 1$ and interpolation we find $\|\varphi(t)\|_{r_i}^2 \leqslant \|\varphi(t)\|_{q_i}$. Thus,

$$B_N(t) \leqslant 16\|w\|_{L^{p_1}+L^{p_2}} \big(\|\varphi(t)\|_{q_1} + \|\varphi(t)\|_{q_2}\big).$$

The claim now follows from the Grönwall estimate (3.3).

4. Convergence for Stronger Singularities

In this section we extend the results of the Sect. 3 to more singular interaction potentials. We consider the case $w \in L^{p_0} + L^\infty$, where

$$\frac{1}{p_0} = \frac{1}{2} + \frac{1}{d}. \tag{4.1}$$

For example in three dimensions $p_0 = 6/5$, which corresponds to singularities up to, but not including, the type $|x|^{-5/2}$. Of course, there are other restrictions on the interaction potential which ensure the stability of the N-body Hamiltonian and the well-posedness of the Hartree equation. In practice, it is often these latter restrictions that determine the class of allowed singularities.

In the words of [11] (p. 169), it is "venerable physical folklore" that an N-body Hamiltonian of the form (3.4), with $h = -\Delta$ and $w(x) = |x|^{-\zeta}$ for $\zeta < 2$, produces reasonable quantum dynamics in three dimensions. Mathematically, this means that such a Hamiltonian is self-adjoint; this is a well-known result (see e.g. [11]). The corresponding Hartree equation is known to be globally well-posed (see [5]). This section answers (affirmatively) the question whether, in the case of such singular interaction potentials, the mean-field limit of the N-body dynamics is governed by the Hartree equation.

4.1. Outline and main result. As in Sect. 3, we need to control expressions of the form $\|w^2 * |\varphi|^2\|_\infty$. The situation is considerably more involved when w^2 is not locally integrable. An important step in dealing with such potentials in our proof is to express w as the divergence of a vector field $\xi \in L^2$. This approach requires the control of not only $\alpha = \|q_1\Psi\|^2$ but also $\|\nabla_1 q_1 \Psi\|^2$, which arises from integrating by parts in expressions containing the factor $\nabla \cdot \xi$. As it turns out, β, defined through

$$\beta_N(t) := \langle \Psi_N , \widehat{n}\, \Psi_N \rangle\big|_t, \tag{4.2}$$

does the trick. This follows from an estimate exploiting conservation of energy (see Lemma 4.6 below). The inequality $m \leqslant n$ and the representation (3.12) yield

$$\alpha \leqslant \beta. \tag{4.3}$$

We consider a Hamiltonian of the form (3.4) and make the following assumptions.

(B1) The one-particle Hamiltonian h is self-adjoint and bounded from below. Without loss of generality we assume that $h \geqslant 0$. We also assume that there are constants $\kappa_1, \kappa_2 > 0$ such that

$$-\Delta \leqslant \kappa_1 h + \kappa_2,$$

as an inequality of forms on $\mathcal{H}^{(1)}$.

(B2) The Hamiltonian (3.4) is self-adjoint and bounded from below. We also assume that $\mathcal{Q}(H_N) \subset X_N$, where X_N is defined as in Assumption (A1).

(B3) There is a constant $\kappa_3 \in (0, 1)$ such that

$$0 \leqslant (1 - \kappa_3)(h_1 + h_2) + W_{12},$$

as an inequality of forms on $\mathcal{H}^{(2)}$.

(B4) The interaction potential w is a real and even function satisfying $w \in L^p + L^\infty$, where $p_0 < p \leqslant 2$.

(B5) The solution $\varphi(\cdot)$ of (1.3) satisfies

$$\varphi(\cdot) \in C(\mathbb{R}; X_1^2 \cap L^\infty) \cap C^1(\mathbb{R}; L^2),$$

where $X_1^2 := \mathcal{Q}(h^2) \subset L^2$ is equipped with the norm

$$\|\varphi\|_{X_1^2} := \left\|(1 + h^2)^{1/2}\varphi\right\|.$$

Next, we define the microscopic energy per particle

$$E_N^\Psi(t) := \frac{1}{N}\langle \Psi_N \,, H_N \,\Psi_N\rangle\big|_t,$$

as well as the Hartree energy

$$E^\varphi(t) := \left[\langle \varphi \,, h\,\varphi\rangle + \frac{1}{2}\int \mathrm{d}x \; \mathrm{d}y w(x-y)|\varphi(x)|^2|\varphi(y)|^2\right]\Bigg|_t.$$

By spectral calculus, $E_N^\Psi(t)$ is independent of t. Also, invoking Assumption (B5) to differentiate $E^\varphi(t)$ with respect to t shows that $E^\varphi(t)$ is conserved as well. Summarizing,

$$E_N^\Psi(t) = E_N^\Psi(0), \qquad E^\varphi(t) = E^\varphi(0), \qquad t \in \mathbb{R}.$$

We may now state the main result of this section.

Theorem 4.1. *Let $\Psi_{N,0} \in \mathcal{Q}(H_N)$ and assume that Assumptions (B1) – (B5) hold. Then there is a constant K, depending only on d, h, w and p, such that*

$$\beta_N(t) \leqslant \left(\beta_N(0) + E_N^\Psi - E^\varphi + \frac{1}{N^\eta}\right)\mathrm{e}^{K\phi(t)},$$

where

$$\eta := \frac{p/p_0 - 1}{2p/p_0 - p/2 - 1} \tag{4.4}$$

and

$$\phi(t) := \int_0^t \mathrm{d}s\Big(1 + \|\varphi(s)\|^3_{X_1^2 \cap L^\infty}\Big).$$

Remark 4.2. We have convergence to the mean-field limit whenever $\lim_N E_N^\Psi = E^\varphi$ and $\lim_N \beta_N(0) = 0$. For instance if we start in a fully factorized state, $\Psi_{N,0} = \varphi_0^{\otimes N}$, then $\beta_N(0) = 0$ and

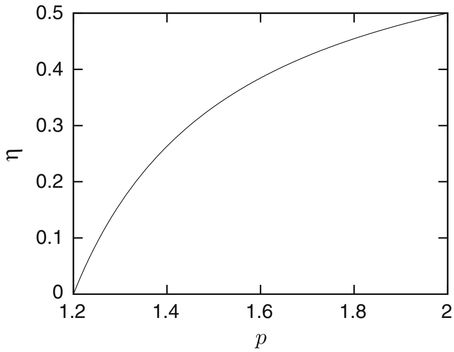
$$E_N^\Psi - E^\varphi = \frac{1}{N}\langle \varphi_0 \otimes \varphi_0\,,\, W_{12}\,\varphi_0 \otimes \varphi_0 \rangle,$$

so that Theorem 4.1 yields

$$E_N^{(1)}(t) \leqslant \beta_N(t) \lesssim \frac{1}{N^\eta}\mathrm{e}^{K\phi(t)},$$

and the analogue of Corollary 3.2 holds.

Remark 4.3. The following graph shows the dependence of η on p for $d = 3$, i.e. $p_0 = 6/5$.



Remark 4.4. Theorem 4.1 remains valid for a large class of time-dependent one-particle Hamiltonians $h(t)$. See Sect. 4.4 below for a full discussion.

Remark 4.5. In three dimensions Assumption (B1) and Sobolev's inequality imply that $\|\varphi\|_\infty \lesssim \|\varphi\|_{X_1^2}$, so that Assumption (B5) is equivalent to $\varphi \in C(\mathbb{R}; X_1^2) \cap C^1(\mathbb{R}; L^2)$.

4.2. Example: nonrelativistic particles with interaction potential of critical type. Consider nonrelativistic particles in $\mathbb{R}^3$ with one-particle Hamiltonian $h = -\Delta$. The interaction potential is given by $w(x) = \lambda|x|^{-2}$. This corresponds to a critical nonlinearity of the Hartree equation. We require that $\lambda > -1/2$, which ensures that the N-body Hamiltonian is stable and the Hartree equation has global solutions. To see this, recall Hardy's inequality in three dimensions,

$$\langle \varphi\,,\, |x|^{-2}\varphi \rangle \leqslant 4\langle \varphi\,,\, -\Delta\varphi \rangle. \tag{4.5}$$

One easily infers that Assumptions (B1) – (B3) hold. Moreover, Assumption (B4) holds for any $p < 3/2$.

In order to verify Assumption (B5) we refer to [5], where local well-posedness is proven. Global existence follows by standard methods using conservation of the mass

$\|\varphi\|^2$, conservation of the energy E^φ, and Hardy's inequality (4.5). Together they yield an a-priori bound on $\|\varphi\|_{X_1}$, from which an a-priori bound for $\|\varphi\|_{X_1^2}$ may be inferred; see [5] for details.

We conclude: For any $\eta < 1/3$ there is a continuous function $\phi(t)$ such that Theorem 4.1 holds.

4.3. Proof of Theorem 4.1.

4.3.1. An energy estimate. In the first step of our proof we exploit conservation of energy to derive an estimate on $\|\nabla_1 q_1 \Psi\|$.

Lemma 4.6. *Assume that Assumptions (B1) – (B5) hold. Then*

$$\|\nabla_1 q_1 \Psi\|^2 \lesssim E^\Psi - E^\varphi + \big(1 + \|\varphi\|^2_{X_1^2 \cap L^\infty}\big)\bigg(\beta + \frac{1}{\sqrt{N}}\bigg).$$

Proof. Write

$$E^\varphi = \langle \varphi\,, h\varphi\rangle + \frac{1}{2}\langle \varphi\,, W^\varphi \varphi\rangle, \tag{4.6}$$

as well as

$$E^\Psi = \langle \Psi\,, h_1 \Psi\rangle + \frac{N-1}{2N}\langle \Psi\,, W_{12}\Psi\rangle. \tag{4.7}$$

Inserting

$$\mathbb{1} = p_1 p_2 + (\mathbb{1} - p_1 p_2)$$

in front of every Ψ in (4.7) and multiplying everything out yields

$$\begin{aligned}
&\big\langle \Psi\,, (\mathbb{1} - p_1 p_2) h_1 (\mathbb{1} - p_1 p_2)\Psi\big\rangle \\
&\quad = E^\Psi - \langle \Psi\,, p_1 p_2 h_1 p_1 p_2 \Psi\rangle \\
&\qquad - \frac{N-1}{2N}\langle \Psi\,, p_1 p_2 W_{12} p_1 p_2 \Psi\rangle \\
&\qquad - \big\langle \Psi\,, (\mathbb{1} - p_1 p_2) h_1 p_1 p_2 \Psi\big\rangle - \big\langle \Psi\,, p_1 p_2 h_1 (\mathbb{1} - p_1 p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle \Psi\,, (\mathbb{1} - p_1 p_2) W_{12} p_1 p_2 \Psi\big\rangle - \frac{N-1}{2N}\big\langle \Psi\,, p_1 p_2 W_{12} (\mathbb{1} - p_1 p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle \Psi\,, (\mathbb{1} - p_1 p_2) W_{12} (\mathbb{1} - p_1 p_2)\Psi\big\rangle.
\end{aligned}$$

We want to find an upper bound for the left-hand side. In order to control the last term on the right-hand side for negative interaction potentials, we need to use some of the kinetic energy on the left-hand side. To this end, we split the left-hand side by multiplying it with $1 = \kappa_3 + (1 - \kappa_3)$. Thus, using (4.6), we get

$$
\begin{aligned}
&\kappa_3\big\langle\Psi\,,(\mathbb{1} - p_1p_2)h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\quad = E^\Psi - E^\varphi \\
&\qquad - \langle\Psi\,, p_1p_2h_1p_1p_2\Psi\rangle + \langle\varphi\,, h\varphi\rangle \\
&\qquad - \frac{N-1}{2N}\langle\Psi\,, p_1p_2W_{12}p_1p_2\Psi\rangle + \frac{1}{2}\langle\varphi\,, W^\varphi\varphi\rangle \\
&\qquad - \big\langle\Psi\,,(\mathbb{1} - p_1p_2)h_1p_1p_2\Psi\big\rangle - \big\langle\Psi\,, p_1p_2h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle\Psi\,,(\mathbb{1} - p_1p_2)W_{12}p_1p_2\Psi\big\rangle - \frac{N-1}{2N}\big\langle\Psi\,, p_1p_2W_{12}(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad - \frac{N-1}{2N}\big\langle\Psi\,,(\mathbb{1} - p_1p_2)W_{12}(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\qquad - (1 - \kappa_3)\big\langle\Psi\,,(\mathbb{1} - p_1p_2)h_1(\mathbb{1} - p_1p_2)\Psi\big\rangle.
\end{aligned}
\tag{4.8}
$$

The rest of the proof consists in estimating each line on the right-hand side of (4.8) separately. There is nothing to be done with the first line.

Lines 6–7. The last two lines of (4.8) are equal to

$$
\begin{aligned}
&-\frac{N-1}{2N}\Big\langle\Psi\,,\ (\mathbb{1} - p_1p_2)W_{12}(\mathbb{1} - p_1p_2)\Psi\Big\rangle \\
&\quad - \frac{1}{2}(1 - \kappa_3)\big\langle\Psi\,,(\mathbb{1} - p_1p_2)(h_1 + h_2)(\mathbb{1} - p_1p_2)\Psi\big\rangle \\
&\leqslant -\frac{N-1}{2N}\Big\langle\Psi\,,\ (\mathbb{1} - p_1p_2)\big[(1 - \kappa_3)(h_1 + h_2) + W_{12}\big](\mathbb{1} - p_1p_2)\Psi\Big\rangle \leqslant 0,
\end{aligned}
$$

where in the last step we used Assumption (B3).

Line 2. The second line on the right-hand side of (4.8) is bounded in absolute value by

$$
\begin{aligned}
\big|\langle\varphi\,, h\varphi\rangle - \langle\Psi\,, p_1p_2h_1p_1p_2\Psi\rangle\big| &= \langle\varphi\,, h\varphi\rangle\big|\langle\Psi\,,(\mathbb{1} - p_1p_2)\Psi\rangle\big| \\
&= \langle\varphi\,, h\varphi\rangle\big|\langle\Psi\,,(q_1p_2 + p_1q_2 + q_1q_2)\Psi\rangle\big| \\
&\leqslant 3\,\alpha\,\langle\varphi\,, h\varphi\rangle \\
&\leqslant 3\,\beta\,\langle\varphi\,, h\varphi\rangle,
\end{aligned}
$$

where in the last step we used (4.3).

Line 3. The third line on the right-hand side of (4.8) is bounded in absolute value by

$$
\begin{aligned}
&\left|\frac{1}{2}\langle\varphi\,, W^\varphi\varphi\rangle - \frac{N-1}{2N}\langle\Psi\,, p_1p_2W_{12}p_1p_2\Psi\rangle\right| \\
&\quad = \frac{1}{2}\big|\langle\varphi\,, W^\varphi\varphi\rangle\big|\left|1 - \frac{N-1}{N}\langle\Psi\,, p_1p_2\Psi\rangle\right| \\
&\quad \leqslant \frac{1}{2}\|W^\varphi\|_\infty\left|\big\langle\Psi\,,(q_1p_2 + p_1q_2 + q_1q_2)\Psi\big\rangle + \frac{1}{N}\langle\Psi\,, p_1p_2\Psi\rangle\right| \\
&\quad \leqslant \frac{3}{2}\|W^\varphi\|_\infty\left(\alpha + \frac{1}{N}\right) \\
&\quad \leqslant \frac{3}{2}\|W^\varphi\|_\infty\left(\beta + \frac{1}{N}\right).
\end{aligned}
$$

As in (3.20), one finds that

$$\|W^\varphi\|_\infty \leqslant \|w\|_{L^1+L^\infty}\|\varphi\|^2_{L^2\cap L^\infty}.$$

Line 4. The fourth line on the right-hand side of (4.8) is bounded in absolute value by

$$\begin{aligned}\big|\big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\big\rangle\big| &= \big|\big\langle\Psi\,,(q_1p_2+p_1q_2+q_1q_2)h_1p_1p_2\Psi\big\rangle\big|\\ &= \big|\big\langle\Psi\,,q_1h_1p_1p_2\Psi\big\rangle\big|\\ &= \big|\big\langle\Psi\,,q_1\,\widehat{n}^{-1/2}\,\widehat{n}^{1/2}\,h_1p_1p_2\Psi\big\rangle\big|\\ &= \big|\big\langle\Psi\,,q_1\,\widehat{n}^{-1/2}\,h_1\,\widehat{\tau_1 n}^{1/2}\,p_1p_2\Psi\big\rangle\big|,\end{aligned}$$

where in the last step we used Lemma 3.10. Using Cauchy-Schwarz, we thus get

$$\begin{aligned}\big|\big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\big\rangle\big| &\leqslant \sqrt{\big\langle\Psi\,,q_1\widehat{n}^{-1}\Psi\big\rangle}\sqrt{\big\langle\Psi\,,p_1p_2\,\widehat{\tau_1 n}^{1/2}\,h_1^2\,\widehat{\tau_1 n}^{1/2}\,p_1p_2\Psi\big\rangle}\\ &= \sqrt{\langle\Psi\,,\widehat{n}\,\Psi\rangle}\sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\big\langle\Psi\,,\widehat{\tau_1 n}\;p_1p_2\Psi\big\rangle},\end{aligned}$$

where in the second step we used Lemma 3.9. Using

$$(\tau_1 n)(k)=\sqrt{\frac{k+1}{N}}\leqslant n(k)+\frac{1}{\sqrt{N}}$$

we find

$$\begin{aligned}\big|\big\langle\Psi\,,(\mathbb{1}-p_1p_2)h_1p_1p_2\Psi\big\rangle\big| &\leqslant \sqrt{\beta}\sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\langle\Psi\,,\widehat{n}\,\Psi\rangle+\frac{1}{\sqrt{N}}}\\ &= \sqrt{\langle\varphi\,,h^2\varphi\rangle}\sqrt{\beta}\left(\sqrt{\beta}+\frac{1}{N^{1/4}}\right)\\ &\leqslant 2\sqrt{\langle\varphi\,,h^2\varphi\rangle}\left(\beta+\frac{1}{\sqrt{N}}\right).\end{aligned}$$

Line 5. Finally, we turn our attention to the fifth line on the right-hand side of (4.8), which is bounded in absolute value by

$$\big|\big\langle\Psi\,,p_1p_2W_{12}(\mathbb{1}-p_1p_2)\Psi\big\rangle\big| = \big|\big\langle\Psi\,,p_1p_2W_{12}(p_1q_2+q_1p_2+q_1q_2\Psi\big\rangle\big| \leqslant 2(\mathrm{a})+(\mathrm{b}),$$

where

$$(\mathrm{a}) := \big|\big\langle\Psi\,,p_1p_2W_{12}q_1p_2\Psi\big\rangle\big|,\qquad (\mathrm{b}) := \big|\big\langle\Psi\,,p_1p_2W_{12}q_1q_2\Psi\big\rangle\big|.$$

One finds, using (3.17), Lemma 3.10 and Lemma 3.9,

$$\begin{aligned}(\mathrm{a}) &= \big|\big\langle\Psi\,,p_1p_2W_1^\varphi q_1\Psi\big\rangle\big|\\ &= \big|\big\langle\Psi\,,p_1p_2W_1^\varphi\,\widehat{n}^{1/2}\,\widehat{n}^{-1/2}\,q_1\Psi\big\rangle\big|\\ &= \big|\big\langle\Psi\,,p_1p_2\,\widehat{\tau_1 n}^{1/2}\,W_1^\varphi\,\widehat{n}^{-1/2}\,q_1\Psi\big\rangle\big|\\ &\leqslant \|W^\varphi\|_\infty\sqrt{\big\langle\Psi\,,\widehat{\tau_1 n}\,\Psi\big\rangle}\sqrt{\big\langle\Psi\,,\widehat{n}^{-1}\,q_1\Psi\big\rangle}\\ &\leqslant \|W^\varphi\|_\infty\sqrt{\big\langle\Psi\,,\widehat{n}\,\Psi\big\rangle+\frac{1}{\sqrt{N}}}\sqrt{\big\langle\Psi\,,\widehat{n}\,\Psi\big\rangle}\\ &\leqslant 2\|W^\varphi\|_\infty\left(\beta+\frac{1}{\sqrt{N}}\right).\end{aligned}$$

The estimation of (b) requires a little more effort. We start by splitting

$$w = w^{(p)} + w^{(\infty)}, \qquad w^{(p)} \in L^p,\ w^{(\infty)} \in L^\infty.$$

This yields (b) $\leqslant$ (b)$^{(p)}$ + (b)$^{(\infty)}$ in self-explanatory notation. Let us first concentrate on (b)$^{(\infty)}$:

$$\begin{aligned}
(\mathrm{b})^{(\infty)} &= \left|\left\langle \Psi\,,\, p_1 p_2 W_{12}^{(\infty)} q_1 q_2 \Psi \right\rangle\right| \\
&= \left|\left\langle \Psi\,,\, p_1 p_2 W_{12}^{(\infty)} \widehat{n}\,\widehat{n}^{-1}\, q_1 q_2 \Psi \right\rangle\right| \\
&= \left|\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, W_{12}^{(\infty)}\, \widehat{n}^{-1}\, q_1 q_2 \Psi \right\rangle\right| \\
&\leqslant \| W^{(\infty)} \|_\infty \sqrt{\left\langle \Psi\,,\, \widehat{\tau_2 n}^2 \Psi \right\rangle}\sqrt{\left\langle \Psi\,,\, \widehat{n}^{-2}\, q_1 q_2 \Psi \right\rangle} \\
&\leqslant \| w^{(\infty)} \|_\infty \sqrt{\alpha + \frac{2}{N}}\,\sqrt{\alpha} \\
&\leqslant 2 \| w^{(\infty)} \|_\infty \left(\beta + \frac{2}{N} \right).
\end{aligned}$$

Let us now consider (b)$^{(p)}$. In order to deal with the singularities in $w^{(p)}$, we write it as the divergence of a vector field ξ,

$$w^{(p)} = \nabla \cdot \xi. \tag{4.9}$$

This is nothing but a problem of electrostatics, which is solved by

$$\xi = C\,\frac{x}{|x|^d} * w^{(p)},$$

with some constant C depending on d. By the Hardy-Littlewood-Sobolev inequality, we find

$$\|\xi\|_q \lesssim \left\| w^{(p)} \right\|_p, \qquad \frac{1}{q} = \frac{1}{p} - \frac{1}{d}. \tag{4.10}$$

Thus if $p \geqslant p_0$ then $q \geqslant 2$. Denote by X_{12} multiplication by $\xi(x_1 - x_2)$. For the following it is convenient to write $\nabla \cdot \xi = \nabla^\rho \xi^\rho$, where a summation over $\rho = 1, \ldots, d$ is implied.

Recalling Lemma 3.10, we therefore get

$$\begin{aligned}
(\mathrm{b})^{(p)} &= \left|\left\langle \Psi\,,\, p_1 p_2 W_{12}^{(p)} \widehat{n}\,\widehat{n}^{-1} q_1 q_2 \Psi \right\rangle\right| \\
&= \left|\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, W_{12}^{(p)}\, \widehat{n}^{-1} q_1 q_2 \Psi \right\rangle\right| \\
&= \left|\left\langle \Psi\,,\, p_1 p_2\, \widehat{\tau_2 n}\, (\nabla_1^\rho X^\rho)_{12}\, \widehat{n}^{-1} q_1 q_2 \Psi \right\rangle\right|.
\end{aligned}$$

Integrating by parts yields

$$\begin{aligned}
(\mathrm{b})^{(p)} \leqslant\ & \left|\left\langle \nabla_1^\rho \widehat{\tau_2 n}\, p_1 p_2 \Psi\,,\, X_{12}^\rho\, \widehat{n}^{-1} q_1 q_2 \Psi \right\rangle\right| \\
&+ \left|\left\langle \widehat{\tau_2 n}\, p_1 p_2 \Psi\,,\, X_{12}^\rho \nabla_1^\rho\, \widehat{n}^{-1} q_1 q_2 \Psi \right\rangle\right|.
\end{aligned} \tag{4.11}$$

Let us begin by estimating the first term. Recalling that $p = |\varphi\rangle\langle\varphi|$, we find that the first term on the right-hand side of (4.11) is equal to

$$\begin{aligned}
&\left|\left\langle X_{12}^{\rho}\, p_2 (\nabla^{\rho} p)_1 \widehat{\tau_2 n}\, \Psi\,,\, \widehat{n}^{-1} q_1 q_2 \Psi\right\rangle\right| \\
&\leqslant \sqrt{\left\langle (\nabla^{\rho} p)_1 \widehat{\tau_2 n}\, \Psi\,,\, p_2 X_{12}^{\rho} X_{12}^{\sigma}\, p_2 (\nabla^{\sigma} p)_1 \widehat{\tau_2 n}\, \Psi\right\rangle}\, \left\| \widehat{n}^{-1} q_1 q_2 \Psi \right\| \\
&\leqslant \sqrt{\left\| |\varphi|^2 * \xi^2 \right\|_{\infty}}\, \|\nabla\varphi\|\, \left\|\widehat{\tau_2 n}\, \Psi\right\|\, \left\|\widehat{n}^{-1} q_1 q_2 \Psi\right\| \\
&\lesssim \|\xi\|_q\, \|\varphi\|_{L^2 \cap L^\infty}\, \|\varphi\|_{X_1} \sqrt{\alpha + \frac{2}{N}}\, \sqrt{\alpha},
\end{aligned}$$

where we used Young's inequality, Assumption (B1), and Lemma 3.9. Recalling that $\beta \leqslant \alpha$, we conclude that the first term on the right-hand side of (4.11) is bounded by

$$C\, \|\varphi\|_{X_1 \cap L^\infty}^2 \left(\beta + \frac{1}{N}\right).$$

Next, we estimate the second term on the right-hand side of (4.11). It is equal to

$$\begin{aligned}
\left|\left\langle X_{12}^{\rho}\, p_1 p_2\, \widehat{\tau_2 n}\, \Psi\,,\, \nabla_1^{\rho}\, \widehat{n}^{-1} q_1 q_2 \Psi\right\rangle\right| &\leqslant \sqrt{\left\langle \widehat{\tau_2 n}\, \Psi\,,\, p_1 p_2 X_{12}^2 p_1 p_2\, \widehat{\tau_2 n}\, \Psi\right\rangle}\, \left\|\nabla_1 \widehat{n}^{-1}\, q_1 q_2 \Psi\right\| \\
&\leqslant \sqrt{\left\| |\varphi|^2 * \xi^2 \right\|_{\infty}}\, \left\|\widehat{\tau_2 n}\, \Psi\right\|\, \left\|\nabla_1 \widehat{n}^{-1}\, q_1 q_2 \Psi\right\| \\
&\leqslant \|\xi\|_q\, \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\alpha + \frac{2}{N}}\, \left\|\nabla_1 \widehat{n}^{-1}\, q_1 q_2 \Psi\right\|.
\end{aligned}$$

We estimate $\left\|\nabla_1 \widehat{n}^{-1}\, q_1 q_2 \Psi\right\|$ by introducing $\mathbb{1} = p_1 + q_1$ on the left. The term arising from p_1 is bounded by

$$\begin{aligned}
\left\| p_1 \nabla_1 \widehat{n}^{-1}\, q_1 q_2 \Psi\right\| &= \left\| p_1 q_2\, \widehat{\tau_1 n}^{-1}\, \nabla_1 q_1 \Psi\right\| \\
&\leqslant \sqrt{\left\langle \nabla_1 q_1 \Psi\,,\, q_2\, \widehat{\tau_1 n}^{-2}\, \nabla_1 q_1 \Psi\right\rangle} \\
&= \sqrt{\left\langle \nabla_1 q_1 \Psi\;,\; \frac{1}{N-1} \sum_{i=2}^{N} q_i\, \widehat{\tau_1 n}^{-2}\, \nabla_1 q_1 \Psi\right\rangle} \\
&\leqslant \sqrt{\left\langle \nabla_1 q_1 \Psi\;,\; \frac{1}{N} \sum_{i=1}^{N} q_i\, \widehat{\tau_1 n}^{-2}\, \nabla_1 q_1 \Psi\right\rangle} \\
&= \sqrt{\left\langle \nabla_1 q_1 \Psi\,,\, \widehat{n}^2\, \widehat{\tau_1 n}^{-2}\, \nabla_1 q_1 \Psi\right\rangle} \\
&\leqslant \|\nabla_1 q_1 \Psi\|.
\end{aligned}$$

The term arising from q_1 in the above splitting is dealt with in exactly the same way. Thus we have proven that the second term on the right-hand side of (4.11) is bounded by

$$C \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\beta + \frac{1}{N}}\, \|\nabla_1 q_1 \Psi\|.$$

Summarizing, we have

$$(\mathrm{b})^{(p)} \lesssim \|\varphi\|^2_{X_1\cap L^\infty}\left(\beta + \frac{1}{N}\right) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1 q_1 \Psi\|.$$

Conclusion of the proof. Putting all the estimates of the right-hand side of (4.8) together, we find

$$\begin{aligned}&\left\langle \Psi\,,(\mathbb{1} - p_1p_2)h_1(\mathbb{1} - p_1p_2)\Psi\right\rangle \\ &\quad\lesssim E^\Psi - E^\varphi + \left(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\right)\left(\beta + \frac{1}{\sqrt{N}}\right) + \|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1 q_1\Psi\|.\end{aligned} \tag{4.12}$$

Next, from $\mathbb{1} - p_1p_2 = p_1q_2 + q_1$ we deduce

$$\begin{aligned}\|\sqrt{h_1}q_1\Psi\| &= \left\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi - \sqrt{h_1}p_1q_2\Psi\right\| \\ &\leqslant \left\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi\right\| + \|\sqrt{h_1}p_1q_2\Psi\|.\end{aligned}$$

Now, recalling that $p = |\varphi\rangle\langle\varphi|$, we find

$$\|\sqrt{h_1}p_1q_2\Psi\| \leqslant \|\sqrt{h_1}p_1\|\|q_2\Psi\| \leqslant \|\varphi\|_{X_1}\sqrt{\beta}.$$

Therefore,

$$\|\sqrt{h_1}q_1\Psi\|^2 \lesssim \left\|\sqrt{h_1}(\mathbb{1} - p_1p_2)\Psi\right\|^2 + \|\varphi\|^2_{X_1}\beta.$$

Plugging in (4.13) yields

$$\begin{aligned}\left\|\sqrt{h_1}q_1\Psi\right\|^2 \lesssim{}& E^\Psi - E^\varphi + \left(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\right)\left(\beta + \frac{1}{\sqrt{N}}\right) \\ &+\|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\nabla_1 q_1\Psi\|.\end{aligned}$$

Next, we observe that Assumption (B1) implies

$$\|\nabla_1 q_1\Psi\| \lesssim \left\|\sqrt{h_1}q_1\Psi\right\| + \sqrt{\beta},$$

so that we get

$$\begin{aligned}\left\|\sqrt{h_1}q_1\Psi\right\|^2 \lesssim{}& E^\Psi - E^\varphi + \left(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\right)\left(\beta + \frac{1}{\sqrt{N}}\right) \\ &+\|\varphi\|_{L^2\cap L^\infty}\sqrt{\beta + \frac{1}{N}}\,\|\sqrt{h_1}q_1\Psi\|.\end{aligned}$$

Now we claim that

$$\left\|\sqrt{h_1}q_1\Psi\right\|^2 \lesssim E^\Psi - E^\varphi + \left(1 + \|\varphi\|^2_{X_1^2\cap L^\infty}\right)\left(\beta + \frac{1}{\sqrt{N}}\right). \tag{4.13}$$

This follows from the general estimate

$$x^2 \leqslant C(R + ax) \quad\Longrightarrow\quad x^2 \leqslant 2CR + C^2a^2,$$

which itself follows from the elementary inequality

$$C(R + ax) \leqslant CR + \frac{1}{2}C^2a^2 + \frac{1}{2}x^2.$$

The claim of the lemma now follows from (4.13) by using Assumption (B1). $\square$

4.3.2. A bound on $\dot{\beta}$. We start exactly as in Sect. 3. Assumptions (B1) – (B5) imply that β is differentiable in t with derivative

$$\begin{aligned}\dot{\beta} &= \frac{\mathrm{i}}{2}\big\langle \Psi\,,\big[(N-1)W_{12} - NW_1^{\varphi} - NW_2^{\varphi}\,,\widehat{n}\big]\Psi\big\rangle \\ &= 2(\mathrm{I}) + 2(\mathrm{II}) + (\mathrm{III}) + \text{ complex conjugate},\end{aligned} \tag{4.14}$$

where

$$\begin{aligned}(\mathrm{I}) &:= \frac{\mathrm{i}}{2}\big\langle \Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^{\varphi} - NW_2^{\varphi}\,,\widehat{n}\big]q_1p_2\Psi\big\rangle,\\ (\mathrm{II}) &:= \frac{\mathrm{i}}{2}\big\langle \Psi\,, q_1p_2\big[(N-1)W_{12} - NW_1^{\varphi} - NW_2^{\varphi}\,,\widehat{n}\big]q_1q_2\Psi\big\rangle,\\ (\mathrm{III}) &:= \frac{\mathrm{i}}{2}\big\langle \Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^{\varphi} - NW_2^{\varphi}\,,\widehat{n}\big]q_1q_2\Psi\big\rangle.\end{aligned}$$

Term (I). Using (3.17) we find

$$\begin{aligned}2\big|(\mathrm{I})\big| &= \big|\big\langle \Psi\,, p_1p_2\big[(N-1)W_{12} - NW_1^{\varphi} - NW_2^{\varphi}\,,\widehat{n}\big]q_1p_2\Psi\big\rangle\big|\\ &= \big|\big\langle \Psi\,, p_1p_2\big[W_1^{\varphi}\,,\widehat{n}\big]q_1p_2\Psi\big\rangle\big|\\ &= \big|\big\langle \Psi\,, p_1p_2W_1^{\varphi}\big(\widehat{n} - \widehat{\tau_{-1}n}\big)q_1p_2\Psi\big\rangle\big|,\end{aligned}$$

where we used Lemma 3.10. Define

$$\mu(k) := N\big(n(k) - (\tau_{-1}n)(k)\big) = \frac{\sqrt{N}}{\sqrt{k} + \sqrt{k-1}} \leqslant n^{-1}(k), \qquad k = 1, \ldots, N. \tag{4.15}$$

Thus,

$$\begin{aligned}\big|(\mathrm{I})\big| &= \frac{1}{N}\big|\big\langle \Psi\,, p_1p_2W_1^{\varphi}\,\widehat{\mu}\,q_1p_2\Psi\big\rangle\big|\\ &\leqslant \frac{1}{N}\|W^{\varphi}\|_{\infty}\sqrt{\big\langle \Psi\,, \widehat{\mu}^2\,q_1\Psi\big\rangle}\\ &\leqslant \frac{1}{N}\|W^{\varphi}\|_{\infty}\sqrt{\big\langle \Psi\,, \widehat{n}^{-2}\,q_1\Psi\big\rangle}\\ &\lesssim \frac{1}{N}\|\varphi\|^2_{L^2\cap L^{\infty}},\end{aligned}$$

by (3.13).

Term (II). Using Lemma 3.10 we find

$$2|(\mathrm{II})| = \big|\big\langle \Psi\,, q_1p_2\big[(N-1)W_{12} - NW_2^{\varphi}\,,\widehat{n}\big]q_1q_2\Psi\big\rangle\big| \tag{4.16}$$

$$= \left|\left\langle \Psi\ ,\ q_1p_2\left(\frac{N-1}{N}W_{12} - W_2^{\varphi}\right)\widehat{\mu}\,q_1q_2\Psi\right\rangle\right| \tag{4.17}$$

$$\leqslant \underbrace{\big|\big\langle \Psi\,, q_1p_2W_{12}\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|}_{=:(\mathrm{a})} + \underbrace{\big|\big\langle \Psi\,, q_1p_2W_2^{\varphi}\,\widehat{\mu}\,q_1q_2\Psi\big\rangle\big|}_{=:(\mathrm{b})}. \tag{4.18}$$

One immediately finds

$$(\mathrm{b}) \leqslant \|W^{\varphi}\|_{\infty} \|q_1 \Psi\| \sqrt{\langle \Psi , \widehat{\mu}^2 q_1 q_2 \Psi \rangle} \lesssim \|\varphi\|_{L^2 \cap L^\infty}^2 \beta.$$

In (a) we split

$$w = w^{(p)} + w^{(\infty)}, \qquad w^{(p)} \in L^p, w^{(\infty)} \in L^\infty,$$

with a resulting splitting (a) $\leqslant$ (a)$^{(p)}$ + (a)$^{(\infty)}$. The easy part is

$$(\mathrm{a})^{(\infty)} \leqslant \|w^{(\infty)}\|_\infty \|q_1 \Psi\|^2 \lesssim \beta.$$

In order to deal with (a)$^{(p)}$ we write $w^{(p)} = \nabla \cdot \xi$ as the divergence of a vector field ξ, exactly as in the proof of Lemma 4.6; see (4.9) and the remarks after it. We integrate by parts to find

$$\begin{aligned} (\mathrm{a})^{(p)} &= \left|\left\langle \Psi , q_1 p_2 (\nabla_1^\rho X^\rho)_{12}\, \widehat{\mu}\, q_1 q_2 \Psi \right\rangle\right| \\ &\leqslant \left|\left\langle \nabla_1^\rho q_1 p_2 \Psi , X_{12}^\rho\, \widehat{\mu}\, q_1 q_2 \Psi \right\rangle\right| + \left|\left\langle q_1 p_2 \Psi , X_{12}^\rho \nabla_1^\rho\, \widehat{\mu}\, q_1 q_2 \Psi \right\rangle\right|. \end{aligned} \tag{4.19}$$

The first term of (4.19) is equal to

$$\begin{aligned} \left|\left\langle X_{12}^\rho p_2 \nabla_1^\rho q_1 \Psi , \widehat{\mu}\, q_1 q_2 \Psi \right\rangle\right| &\leqslant \sqrt{\left\langle \nabla_1^\rho q_1 \Psi , p_2 X_{12}^\rho X_{12}^\sigma p_2 \nabla_1^\sigma q_1 \Psi \right\rangle} \sqrt{\left\langle \Psi , \widehat{\mu}^2\, q_1 q_2 \Psi \right\rangle} \\ &\lesssim \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\, \|\nabla_1 q_1 \Psi\| \sqrt{\left\langle \Psi , \widehat{n}^{-2}\, q_1 q_2 \Psi \right\rangle} \\ &\leqslant \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\, \|\nabla_1 q_1 \Psi\| \sqrt{\frac{N}{N-1} \left\langle \Psi , \widehat{n}^2 \Psi \right\rangle} \\ &\lesssim \|\xi\|_q \|\varphi\|_{L^2 \cap L^\infty} \|\nabla_1 q_1 \Psi\| \sqrt{\beta} \\ &\lesssim \|\nabla_1 q_1 \Psi\|^2 \|\varphi\|_{L^2 \cap L^\infty} + \beta \|\varphi\|_{L^2 \cap L^\infty}, \end{aligned}$$

where in the second step we used (4.15), in the third Lemma 3.9, and in the last (4.3), Young's inequality, and (4.10). The second term of (4.19) is equal to

$$\begin{aligned} &\left|\left\langle q_1 p_2 \Psi , X_{12}^\rho (p_1 + q_1) \nabla_1^\rho\, \widehat{\mu}\, q_1 q_2 \Psi \right\rangle\right| \\ &\quad \leqslant \left|\left\langle q_1 p_2 \Psi , X_{12}^\rho p_1\, \widehat{\tau_1 \mu}\, \nabla_1^\rho q_1 q_2 \Psi \right\rangle\right| + \left|\left\langle q_1 p_2 \Psi , X_{12}^\rho q_1\, \widehat{\mu}\, \nabla_1^\rho q_1 q_2 \Psi \right\rangle\right|, \end{aligned} \tag{4.20}$$

where we used Lemma 3.10. We estimate the first term of (4.20). The second term is dealt with in exactly the same way. We find

$$
\begin{aligned}
&\big|\big\langle p_1 X^{\rho}_{12} q_1 p_2 \Psi \,,\, \widehat{\tau_1 \mu}\, \nabla^{\rho}_1 q_1 q_2 \Psi\big\rangle\big| \\
&\leqslant \sqrt{\big\langle \Psi \,,\, q_1 p_2 X^2_{12} p_2 q_1 \Psi\big\rangle}\sqrt{\big\langle \nabla_1 q_1 \Psi \,,\, q_2\, \widehat{\tau_1 \mu}^2\, q_2 \nabla_1 q_1 \Psi\big\rangle} \\
&\leqslant \sqrt{\|\xi^2 * |\varphi|^2\|_\infty}\, \|q_1 \Psi\| \sqrt{\big\langle \nabla_1 q_1 \Psi \,,\, \widehat{n}^{-2}\, q_2 \nabla_1 q_1 \Psi\big\rangle} \\
&\lesssim \|\xi\|_q\, \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\alpha} \sqrt{\frac{1}{N-1} \sum_{i=2}^N \big\langle \nabla_1 q_1 \Psi \,,\, \widehat{n}^{-2}\, q_i \nabla_1 q_1 \Psi\big\rangle} \\
&\lesssim \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\beta} \sqrt{\frac{1}{N-1} \sum_{i=1}^N \big\langle \nabla_1 q_1 \Psi \,,\, \widehat{n}^{-2}\, q_i \nabla_1 q_1 \Psi\big\rangle} \\
&= \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\beta} \sqrt{\frac{N}{N-1} \big\langle \nabla_1 q_1 \Psi \,,\, \widehat{n}^{-2}\, \widehat{n}^2\, \nabla_1 q_1 \Psi\big\rangle} \\
&\lesssim \|\varphi\|_{L^2 \cap L^\infty} \sqrt{\beta}\, \|\nabla_1 q_1 \Psi\| \\
&\leqslant \beta\, \|\varphi\|_{L^2 \cap L^\infty} + \|\nabla_1 q_1 \Psi\|^2\, \|\varphi\|_{L^2 \cap L^\infty}.
\end{aligned}
$$

In summary, we have proven that

$$
\big|(\mathrm{II})\big| \lesssim \beta\, \|\varphi\|_{L^2 \cap L^\infty} + \|\nabla_1 q_1 \Psi\|^2\, \|\varphi\|_{L^2 \cap L^\infty}.
$$

Term (III). Using Lemma 3.10 we find

$$
\begin{aligned}
2|(\mathrm{III})| &= (N-1)\big|\big\langle \Psi \,,\, p_1 p_2 \big[W_{12} \,,\, \widehat{n}\big] q_1 q_2 \Psi\big\rangle\big| \\
&= (N-1)\big|\big\langle \Psi \,,\, p_1 p_2 W_{12} \big(\widehat{n} - \widehat{\tau_{-2} n}\big) q_1 q_2 \Psi\big\rangle\big|.
\end{aligned}
$$

Defining

$$
\nu(k) := N\big(n(k) - (\tau_{-2} n)(k)\big) = \frac{\sqrt{N}}{\sqrt{k} + \sqrt{k-2}} \leqslant n^{-1}(k), \qquad k = 2, \dots, N, \tag{4.21}
$$

we have

$$
2\big|(\mathrm{III})\big| \leqslant \big|\big\langle \Psi \,,\, p_1 p_2 W_{12}\, \widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big|.
$$

As usual we start by splitting

$$
w = w^{(p)} + w^{(\infty)}, \qquad w^{(p)} \in L^p, w^{(\infty)} \in L^\infty,
$$

with the induced splitting (III) = $(\mathrm{III})^{(p)} + (\mathrm{III})^{(\infty)}$. Thus, using Lemma 3.10, we find

$$\begin{aligned}
2\big|(\mathrm{III})^{(\infty)}\big| &= \big|\big\langle \Psi\,,\, p_1 p_2 W_{12}^{(\infty)}\,\widehat{n}^{1/2}\,\widehat{n}^{-1/2}\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big| \\
&= \big|\big\langle \Psi\,,\, p_1 p_2\,\widehat{\tau_2 n}^{1/2}\, W_{12}^{(\infty)}\,\widehat{n}^{-1/2}\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big| \\
&\leqslant \|w^{(\infty)}\|_\infty \sqrt{\big\langle \Psi\,,\, \widehat{\tau_2 n}\,\Psi\big\rangle}\sqrt{\big\langle \Psi\,,\, \widehat{n}^{-1}\,\widehat{\nu}^2\, q_1 q_2 \Psi\big\rangle} \\
&\lesssim \sqrt{\beta + \sqrt{\frac{2}{N}}}\,\sqrt{\big\langle \Psi\,,\, \widehat{n}^{-3}\, q_1 q_2 \Psi\big\rangle} \\
&\leqslant \sqrt{\beta + \sqrt{\frac{2}{N}}}\,\sqrt{\frac{N}{N-1}\beta} \\
&\lesssim \beta + \frac{1}{\sqrt{N}},
\end{aligned}$$

where in the fifth step we used Lemma 3.9.

In order to estimate $(\mathrm{III})^{(p)}$ we introduce a splitting of $w^{(p)}$ into "singular" and "regular" parts,

$$w^{(p)} = w^{(p,1)} + w^{(p,2)} := w^{(p)}\,\mathbb{1}_{\{|w^{(p)}|>a\}} + w^{(p)}\,\mathbb{1}_{\{|w^{(p)}|\leqslant a\}}, \tag{4.22}$$

where a is a positive (N-dependent) constant we choose later. For future reference we record the estimates

$$\|w^{(p,1)}\|_{p_0} \leqslant a^{1-p/p_0}\,\|w^{(p)}\|_p^{p/p_0}, \tag{4.23a}$$
$$\|w^{(p,2)}\|_2 \leqslant a^{1-p/2}\,\|w^{(p)}\|_p^{p/2}. \tag{4.23b}$$

The proof of (4.23) is elementary; for instance (4.23a) follows from

$$\begin{aligned}
\|w^{(p,1)}\|_{p_0}^{p_0} &= \int \mathrm{d}x \big|w^{(p)}\big|^p \big|w^{(p)}\big|^{p_0-p}\,\mathbb{1}_{\{|w^{(p)}|>a\}} \\
&\leqslant a^{p_0-p}\int \mathrm{d}x\big|w^{(p)}\big|^p\,\mathbb{1}_{\{|w^{(p)}|>a\}} \leqslant a^{p_0-p}\int \mathrm{d}x\big|w^{(p)}\big|^p.
\end{aligned}$$

Let us start with $(\mathrm{III})^{(p,1)}$. As in (4.9), we use the representation

$$w^{(p,1)} = \nabla\cdot\xi.$$

Then (4.10) and (4.23a) imply that

$$\|\xi\|_2 \lesssim \|w^{(p,1)}\|_{p_0} \lesssim a^{1-p/p_0}. \tag{4.24}$$

Integrating by parts, we find

$$\begin{aligned}
2\big|(\mathrm{III})^{(p,1)}\big| &= \big|\big\langle \Psi\,,\, p_1 p_2 W_{12}^{(p,1)}\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big| \\
&= \big|\big\langle \Psi\,,\, p_1 p_2 (\nabla_1^\rho X_{12}^\rho)\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big| \\
&\leqslant \big|\big\langle \nabla_1^\rho p_1 p_2 \Psi\,,\, X_{12}^\rho\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big| + \big|\big\langle p_1 p_2 \Psi\,,\, X_{12}^\rho \nabla_1^\rho\,\widehat{\nu}\, q_1 q_2 \Psi\big\rangle\big|.
\end{aligned} \tag{4.25}$$

Using $\|\nabla p\| = \|\nabla\varphi\|$ and Lemma 3.9 we find that the first term of (4.25) is bounded by

$$\begin{aligned}\sqrt{\langle \nabla_1^\rho p_1\Psi\,,\, p_2 X_{12}^\rho X_{12}^\sigma p_2 \nabla_1^\sigma p_1\Psi\rangle}\sqrt{\langle\Psi\,,\,\widehat{\nu}^2 q_1 q_2\Psi\rangle} &\lesssim \|\nabla p\|\,\|\varphi\|_\infty \|\xi\|_2\sqrt{\alpha}\\ &\leqslant \|\nabla\varphi\|\,\|\varphi\|_\infty\, a^{1-p/p_0}\sqrt{\beta}\\ &\leqslant \|\nabla\varphi\|\,\|\varphi\|_\infty\big(\beta + a^{2-2p/p_0}\big),\end{aligned}$$

where in the second step we used the estimate (4.24). Next, using Lemma 3.10, we find that the second term of (4.25) is equal to

$$\begin{aligned}&\big|\langle p_1 p_2\Psi\,,\, X_{12}^\rho(p_1+q_1)\nabla_1^\rho\,\widehat{\nu}\, q_1 q_2\Psi\rangle\big|\\ &\quad\leqslant \big|\langle p_1 p_2\Psi\,,\, X_{12}^\rho p_1\,\widehat{\tau_1\nu}\,\nabla_1^\rho q_1 q_2\Psi\rangle\big| + \big|\langle p_1 p_2\Psi\,,\, X_{12}^\rho q_1\,\widehat{\nu}\,\nabla_1^\rho q_1 q_2\Psi\rangle\big|.\end{aligned}$$

We estimate the first term (the second is dealt with in exactly the same way):

$$\begin{aligned}\big|\langle p_1 p_2\Psi\,,\, X_{12}^\rho p_1\,\widehat{\tau_1\nu}\,\nabla_1^\rho q_1 q_2\Psi\rangle\big| &\leqslant \sqrt{\langle\Psi\,,\, p_1 p_2 X_{12}^2 p_1 p_2\Psi\rangle}\sqrt{\langle\nabla_1 q_1\Psi\,,\,\widehat{\tau_1\nu}^2\, q_2\nabla_1 q_1\Psi\rangle}\\ &\leqslant \sqrt{\|p_2 X_{12}^2 p_2\|}\sqrt{\frac{1}{N-1}\sum_{i=2}^N\langle\nabla_1 q_1\Psi\,,\,\widehat{n}^{-2}\, q_i\nabla_1 q_1\Psi\rangle}\\ &\leqslant \|\xi\|_2\,\|\varphi\|_\infty\sqrt{\frac{1}{N-1}\sum_{i=1}^N\langle\nabla_1 q_1\Psi\,,\,\widehat{n}^{-2}\, q_i\nabla_1 q_1\Psi\rangle}\\ &\lesssim a^{1-p/p_0}\|\varphi\|_\infty\sqrt{\frac{N}{N-1}\langle\nabla_1 q_1\Psi\,,\,\nabla_1 q_1\Psi\rangle}\\ &\leqslant \|\varphi\|_\infty\big(a^{2-2p/p_0} + \|\nabla_1 q_1\Psi\|^2\big).\end{aligned}$$

Summarizing,

$$\big|(\mathrm{III})^{(p,1)}\big| \lesssim \|\varphi\|_\infty\Big(\beta\|\varphi\|_{X_1} + \|\nabla_1 q_1\Psi\|^2 + a^{2-2p/p_0}\|\varphi\|_{X_1}\Big).$$

Finally, we estimate

$$(\mathrm{III})^{(p,2)} = \big|\langle\Psi\,,\, p_1 p_2 W_{12}^{(p,2)}\,\widehat{\nu}\, q_1 q_2\Psi\rangle\big| = \big|\langle\Psi\,,\, p_1 p_2 W_{12}^{(p,2)}\,\widehat{\nu}\,(\widehat{\chi^{(1)}} + \widehat{\chi^{(2)}}) q_1 q_2\Psi\rangle\big|, \tag{4.26}$$

where

$$1 = \chi^{(1)} + \chi^{(2)}, \qquad \chi^{(1)}, \chi^{(2)} \in \{0,1\}^{\{0,\dots,N\}},$$

is some partition of the unity to be chosen later. The need for this partitioning will soon become clear. In order to bound the term with $\chi^{(1)}$, we note that the operator norm of $p_1 p_2 W_{12}^{(p,2)} q_1 q_2$ on the full space $L^2(\mathbb{R}^{dN})$ is much larger than on its symmetric subspace. Thus, as a first step, we symmetrize the operator $p_1 p_2 W_{12}^{(p,2)} q_1 q_2$ in coordinate

2. We get the bound

$$\begin{aligned}
&\left|\left\langle\Psi\,,\, p_1 p_2 W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(1)}}\, q_1 q_2 \Psi\right\rangle\right| \\
&\quad = \frac{1}{N-1}\left|\left\langle\Psi\,,\, \sum_{i=2}^{N} p_1 p_i W_{1i}^{(p,2)}\, q_i q_1\, \widehat{\chi^{(1)}}\,\widehat{\nu}\, q_1 \Psi\right\rangle\right| \\
&\quad \leqslant \frac{1}{N-1}\left\|\widehat{\nu}\, q_1 \Psi\right\| \sqrt{\sum_{i,j=2}^{N} \left\langle\Psi\,,\, p_1 p_i W_{1i}^{(p,2)} q_1 q_i\, \widehat{\chi^{(1)}}\, q_1 q_j W_{1j}^{(p-2)}\, p_j p_1 \Psi\right\rangle}.
\end{aligned}$$

Using

$$\left\|\widehat{\nu}\, q_1 \Psi\right\| \leqslant \|\widehat{n}^{-1} q_1 \Psi\| \leqslant 1$$

we find

$$\left|\left\langle\Psi\,,\, p_1 p_2 W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(1)}}\, q_1 q_2 \Psi\right\rangle\right| \leqslant \frac{1}{N-1}\sqrt{A+B}, \tag{4.27}$$

where

$$\begin{aligned}
A &:= \sum_{2\leqslant i\neq j\leqslant N} \left\langle\Psi\,,\, p_1 p_i W_{1i}^{(p,2)} q_1 q_i\, \widehat{\chi^{(1)}}\, q_j W_{1j}^{(p,2)}\, p_j p_1 \Psi\right\rangle, \\
B &:= \sum_{i=2}^{N} \left\langle\Psi\,,\, p_1 p_i W_{1i}^{(p,2)} q_1 q_i\, \widehat{\chi^{(1)}}\, W_{1i}^{(p,2)}\, p_i p_1 \Psi\right\rangle.
\end{aligned}$$

The easy part is

$$\begin{aligned}
B &\leqslant \sum_{i=2}^{N} \left\langle\Psi\,,\, p_1 p_i \left(W_{1i}^{(p,2)}\right)^2 p_i p_1 \Psi\right\rangle \\
&\leqslant \sum_{i=2}^{N} \left\|\left(w^{(p,2)}\right)^2 * |\varphi|^2\right\|_\infty \langle\Psi\,,\, p_1 p_i \Psi\rangle \\
&\leqslant (N-1)\|\varphi\|_\infty^2 \|w^{(p,2)}\|_2^2 \\
&\lesssim N\, a^{2-p}\, \|\varphi\|_\infty^2 .
\end{aligned}$$

Let us therefore concentrate on

$$\begin{aligned}
A &= \sum_{2\leqslant i\neq j\leqslant N} \left\langle\Psi\,,\, p_1 p_i W_{1i}^{(p,2)} q_1 q_i\, \widehat{\chi^{(1)}}\;\widehat{\chi^{(1)}}\, q_j W_{1j}^{(p,2)}\, p_j p_1 \Psi\right\rangle \\
&= \sum_{2\leqslant i\neq j\leqslant N} \left\langle\Psi\,,\, p_1 p_i q_j\, \widehat{\tau_2\chi^{(1)}}\, W_{1i}^{(p,2)} q_1 W_{1j}^{(p,2)}\, \widehat{\tau_2\chi^{(1)}}\, q_i p_j p_1 \Psi\right\rangle \\
&= A_1 + A_2,
\end{aligned}$$

with $A = A_1 + A_2$ arising from the splitting $q_1 = \mathbb{1} - p_1$. We start with

$$\begin{aligned}|A_1| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big|\big\langle \Psi\,,\, p_1 p_i q_j\, \widehat{\tau_2\chi^{(1)}}\, W_{1i}^{(p,2)} W_{1j}^{(p,2)}\, \widehat{\tau_2\chi^{(1)}}\, q_i p_j p_1 \Psi\big\rangle\big| \\ &= \sum_{2\leqslant i\neq j\leqslant N} \big|\big\langle \Psi\,,\, p_1 p_i q_j\, \widehat{\tau_2\chi^{(1)}}\, \sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\, \widehat{\tau_2\chi^{(1)}}\, q_i p_j p_1 \Psi\big\rangle\big| \\ &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big\langle \Psi\,,\, \widehat{\tau_2\chi^{(1)}}\, q_j p_1 p_i \big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big| p_1 p_i q_j\, \widehat{\tau_2\chi^{(1)}}\, \Psi\big\rangle,\end{aligned}$$

by Cauchy-Schwarz and symmetry of Ψ. Here $\sqrt{\cdot}$ is any complex square root.

In order to estimate this we claim that, for $i \neq j$,

$$\Big\| p_1 p_i \big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big| p_1 p_i \Big\| \leqslant \big\| \big|w^{(p,2)}\big| * |\varphi|^2 \big\|_\infty^2. \tag{4.28}$$

Indeed, by (3.17), we have

$$\begin{aligned} p_1 p_i \big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big| p_1 p_i &= p_1 p_i \big|W_{1i}^{(p,2)}\big| p_i \big|W_{1j}^{(p,2)}\big| p_1 \\ &= p_1 p_i \big(\big|w^{(p,2)}\big| * |\varphi|^2\big)_1 \big|W_{1j}^{(p,2)}\big| p_1. \end{aligned}$$

The operator $p_1 \big(\big|w^{(p,2)}\big| * |\varphi|^2\big)_1 \big|W_{1j}^{(p,2)}\big| p_1$ is equal to $f_j\, p_1$, where

$$f(x_j) = \int \mathrm{d}x_1 \overline{\varphi(x_1)} \big(\big|w^{(p,2)}\big| * |\varphi|^2\big)(x_1) \big|w^{(p,2)}(x_1 - x_j)\big| \varphi(x_1).$$

Thus,

$$\|f\|_\infty \leqslant \big\| \big|w^{(p,2)}\big| * |\varphi|^2 \big\|_\infty^2,$$

from which (4.28) follows immediately.

Using (4.28), we get

$$\begin{aligned} |A_1| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big\| \big|w^{(p,2)}\big| * |\varphi|^2 \big\|_\infty^2 \big\| \widehat{\tau_2\chi^{(1)}} q_1 \Psi \big\|^2 \\ &\leqslant N^2 \|w^{(p)}\|_p^2\, \|\varphi\|_{L^2\cap L^\infty}^4 \big\langle \Psi\,,\, \widehat{\tau_2\chi^{(1)}}\, q_1 \Psi \big\rangle \\ &\lesssim N^2\, \|\varphi\|_{L^2\cap L^\infty}^4 \big\langle \Psi\,,\, \widehat{\tau_2\chi^{(1)}}\, \widehat{n}^2\, \Psi \big\rangle. \end{aligned}$$

Now let us choose

$$\chi^{(1)}(k) := \mathbb{1}_{\{k\leqslant N^{1-\delta}\}} \tag{4.29}$$

for some $\delta \in (0, 1)$. Then

$$(\tau_2\chi^{(1)})\, n^2 \leqslant N^{-\delta}$$

implies

$$|A_1| \lesssim \|\varphi\|_{L^2\cap L^\infty}^4\, N^{2-\delta}.$$

Similarly, we find

$$\begin{aligned}|A_2| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \left|\left\langle\Psi\,,\, q_j\,\widehat{\tau_2\chi^{(1)}}\,p_i\,p_1\,W_{1i}^{(p,2)}\,p_1\,W_{1j}^{(p,2)}\,p_1\,p_j\,\widehat{\tau_2\chi^{(1)}}\,q_i\,\Psi\right\rangle\right| \\ &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \left\|w^{(p,2)} * |\varphi|^2\right\|_\infty^2 \langle\Psi\,,\,\widehat{\tau_2\chi^{(1)}}\,q_1\Psi\rangle \\ &\lesssim N^2\|\varphi\|^4_{L^2\cap L^\infty} N^{-\delta} \\ &= \|\varphi\|^4_{L^2\cap L^\infty} N^{2-\delta}.\end{aligned}$$

Thus we have proven

$$|A| \lesssim \|\varphi\|^4_{L^2\cap L^\infty} N^{2-\delta}.$$

Going back to (4.27), we see that

$$\left|\left\langle\Psi\,,\,p_1p_2W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(1)}}\,q_1q_2\Psi\right\rangle\right| \lesssim \|\varphi\|^2_{L^2\cap L^\infty} N^{-\delta/2} + \|\varphi\|_\infty N^{-1/2}\,a^{1-p/2}.$$

What remains is to estimate is the term of $(\mathrm{III})^{(p,2)}$ containing $\chi^{(2)}$,

$$\begin{aligned}&\left|\left\langle\Psi\,,\,p_1p_2W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(2)}}\,q_1q_2\Psi\right\rangle\right| \\ &= \frac{1}{N-1}\left|\left\langle\Psi\,,\,\sum_{i=2}^N p_1p_i\,W_{1i}^{(p,2)}\,q_iq_1\,\widehat{\chi^{(2)}}\,\widehat{\nu}^{1/2}\,\widehat{\nu}^{1/2}\,q_1\Psi\right\rangle\right| \\ &\leqslant \frac{1}{N-1}\left\|\widehat{\nu}^{1/2}\,q_1\Psi\right\|\sqrt{\sum_{i,j=2}^N \left\langle\Psi\,,\,p_1p_i\,W_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\,q_1q_j\,W_{1j}^{(p-2)}\,p_jp_1\Psi\right\rangle}.\end{aligned}$$

Using

$$\left\|\widehat{\nu}^{1/2}\,q_1\Psi\right\| \leqslant \sqrt{\langle\Psi\,,\,\widehat{n}^{-1}\,\widehat{n}^2\,\Psi\rangle} = \sqrt{\beta}$$

we find

$$\left|\left\langle\Psi\,,\,p_1p_2W_{12}^{(p,2)}\,\widehat{\nu}\,\widehat{\chi^{(2)}}\,q_1q_2\Psi\right\rangle\right| \leqslant \frac{\sqrt{\beta}}{N-1}\sqrt{A+B}, \tag{4.30}$$

where

$$\begin{aligned}A &:= \sum_{2\leqslant i\neq j\leqslant N} \left\langle\Psi\,,\,p_1p_i\,W_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\,q_j\,W_{1j}^{(p,2)}\,p_jp_1\Psi\right\rangle, \\ B &:= \sum_{i=2}^N \left\langle\Psi\,,\,p_1p_i\,W_{1i}^{(p,2)}q_1q_i\,\widehat{\chi^{(2)}}\,\widehat{\nu}\,W_{1i}^{(p,2)}\,p_ip_1\Psi\right\rangle.\end{aligned}$$

Since

$$\chi^{(2)}(k) = \mathbb{1}_{\{k>N^{1-\delta}\}}$$

we find

$$\chi^{(2)}\,\nu \leqslant \chi^{(2)}\,n^{-1} \leqslant N^{\delta/2}.$$

Thus, $\|q_1 q_i \widehat{\chi^{(2)}}\,\widehat{\nu}\| \leqslant N^{\delta/2}$ and we get

$$
\begin{aligned}
B &\leqslant N^{\delta/2} \sum_{i=2}^{N} \big\langle \Psi\,,\, p_1 p_i \big(W_{1i}^{(p,2)}\big)^2 p_i p_1 \Psi \big\rangle \leqslant N^{1+\delta/2} \,\Big\| \big(w^{(p,2)}\big)^2 * |\varphi|^2 \Big\|_\infty \\
&\leqslant N^{1+\delta/2} \,\|w^{(p,2)}\|_2^2 \,\|\varphi\|_\infty^2 \lesssim N^{1+\delta/2}\, a^{2-p}\, \|\varphi\|_\infty^2,
\end{aligned}
$$

by (4.23b).

Next, using Lemma 3.10, we find

$$
\begin{aligned}
A &= \sum_{2\leqslant i\neq j\leqslant N} \big\langle \Psi\,,\, p_1 p_i q_j W_{1i}^{(p,2)} \widehat{\chi^{(2)}}\,\widehat{\nu}^{1/2} q_1 \widehat{\chi^{(2)}}\,\widehat{\nu}^{1/2}\, W_{1j}^{(p,2)} q_i p_j p_1 \Psi \big\rangle \\
&= \sum_{2\leqslant i\neq j\leqslant N} \big\langle \Psi\,,\, p_1 p_i q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, W_{1i}^{(p,2)} q_1 W_{1j}^{(p,2)}\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_i p_j p_1 \Psi \big\rangle \\
&= A_1 + A_2,
\end{aligned}
$$

where, as above, the splitting $A = A_1 + A_2$ arises from writing $q_1 = \mathbb{1} - p_1$. Thus,

$$
\begin{aligned}
|A_1| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \Big|\big\langle \Psi\,,\, p_1 p_i q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, W_{1i}^{(p,2)} W_{1j}^{(p,2)}\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_i p_j p_1 \Psi \big\rangle\Big| \\
&= \sum_{2\leqslant i\neq j\leqslant N} \Big|\big\langle \Psi p_1 p_i q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2} \sqrt{W_{1i}^{(p,2)}}\sqrt{W_{1j}^{(p,2)}}\sqrt{W_{1i}^{(p,2)}} \\
&\qquad \times \sqrt{W_{1j}^{(p,2)}}\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_i p_j p_1 \Psi \big\rangle\Big| \\
&\leqslant \sum_{2\leqslant i\neq j\leqslant N} \big\langle \Psi\,,\, q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, p_1 p_i \big|W_{1i}^{(p,2)}\big|\big|W_{1j}^{(p,2)}\big| p_i p_1\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_j \Psi \big\rangle,
\end{aligned}
$$

by Cauchy-Schwarz and symmetry of Ψ. Using (4.28) we get

$$
\begin{aligned}
|A_1| &\leqslant N^2 \,\Big\| \big|w^{(p,2)}\big| * |\varphi|^2 \Big\|_\infty^2 \big\langle \Psi\,,\, \widehat{\tau_2\nu}\, q_1 \Psi \big\rangle \\
&\leqslant N^2 \|w^{(p,2)}\|_p^2 \,\|\varphi\|_{L^2\cap L^\infty}^4 \,\langle \Psi\,,\, \widehat{n}\,\Psi \rangle \\
&\lesssim N^2\, \|\varphi\|_{L^2\cap L^\infty}^4 \beta.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
|A_2| &\leqslant \sum_{2\leqslant i\neq j\leqslant N} \Big|\big\langle \Psi\,,\, p_i q_j\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, p_1 W_{1i}^{(p,2)} p_1 W_{1j}^{(p,2)} p_1\, \widehat{\tau_2\chi^{(2)}}\, \widehat{\tau_2\nu}^{1/2}\, q_i p_j \Psi \big\rangle\Big| \\
&\leqslant \sum_{2\leqslant i\neq j\leqslant N} \Big\| w^{(p,2)} * |\varphi|^2 \Big\|_\infty^2 \big\langle \Psi\,,\, \widehat{\tau_2\nu}\, q_1 \Psi \big\rangle \\
&\leqslant N^2 \|w^{(p)}\|_p^2 \,\|\varphi\|_{L^2\cap L^\infty}^4 \,\langle \Psi\,,\, \widehat{n}\,\Psi \rangle \\
&\lesssim N^2\, \|\varphi\|_{L^2\cap L^\infty}^4\, \beta.
\end{aligned}
$$

Plugging all this back into (4.30), we find that

$$
\Big|\big\langle \Psi\,,\, p_1 p_2 W_{12}^{(p,2)}\, \widehat{\nu}\, \widehat{\chi^{(2)}}\, q_1 q_2 \Psi \big\rangle\Big| \lesssim \beta\big(\|\varphi\|_{L^2\cap L^\infty}^2 + \|\varphi\|_\infty\big) + \|\varphi\|_\infty a^{2-p} N^{\delta/2-1}.
$$

Summarizing:

$$\left|(\mathrm{III})^{(p,2)}\right| \lesssim \left(1+\|\varphi\|^2_{L^2\cap L^\infty}\right)\left(\beta + a^{2-p}\,N^{\delta/2-1} + N^{-\delta/2} + N^{-1/2}a^{1-p/2}\right),$$

from which we deduce

$$\begin{aligned}\left|(\mathrm{III})^{(p)}\right| &\lesssim \|\varphi\|_\infty \|\nabla_1 q_1 \Psi\|^2 \\ &\quad + \left(1+\|\varphi\|_{X_1\cap L^\infty}\right)\left(\beta + a^{2-p}\,N^{\delta/2-1} + N^{-\delta/2} + N^{-1/2}a^{1-p/2} + a^{2-2p/p_0}\right).\end{aligned}$$

Let us set $a \equiv a_N = N^\zeta$ and optimize in δ and ζ. This yields the relations

$$\zeta(2-p)+\delta = 1, \qquad -\frac{\delta}{2} = 2\zeta\left(1-\frac{p}{p_0}\right),$$

which imply

$$\frac{\delta}{2} = \frac{p/p_0 - 1}{2p/p_0 - p/2 - 1},$$

with $\delta \leqslant 1$. Thus,

$$\left|(\mathrm{III})^{(p)}\right| \lesssim \|\varphi\|_\infty \|\nabla_1 q_1 \Psi\|^2 + \left(1+\|\varphi\|_{X_1\cap L^\infty}\right)\left(\beta + N^{-\eta}\right),$$

where $\eta = \delta/2$ satisfies (4.4).

Conclusion of the proof. We have shown that

$$\dot{\beta} \lesssim \|\varphi\|_{L^2\cap L^\infty}\|\nabla_1 q_1 \Psi\|^2 + \left(1+\|\varphi\|_{X_1\cap L^\infty}\right)\left(\beta + N^{-\eta}\right).$$

Using Lemma 4.6 we find

$$\dot{\beta} \lesssim \left(1+\|\varphi\|^3_{X_1^2\cap L^\infty}\right)\left(\beta + E^\Psi - E^\varphi + \frac{1}{N^\eta}\right). \tag{4.31}$$

The claim then follows from the Grönwall estimate (3.3).

4.4. A remark on time-dependent external potentials. Theorem 4.1 can be extended to time-dependent external potentials $h(t)$ without too much sweat. The only complication is that energy is no longer conserved. We overcome this problem by observing that, while the energies $E^\Psi(t)$ and $E^\varphi(t)$ exhibit large variations in t, their difference remains small. In the following we estimate the quantity $E^\Psi(t) - E^\varphi(t)$ by controlling its time derivative.

We need the following assumptions, which replace Assumptions (B1) – (B3).

(B1') The Hamiltonian $h(t)$ is self-adjoint and bounded from below. We assume that there is an operator $h_0 \geqslant 0$ that such that $0 \leqslant h(t) \leqslant h_0$ for all t. We define the Hilbert space $X_N = \mathcal{Q}\big(\sum_i (h_0)_i\big)$ as in (A1), and the space $X_1^2 = \mathcal{Q}(h_0^2)$ as in (B5) using h_0. We also assume that there are time-independent constants $\kappa_1, \kappa_2 > 0$ such that

$$-\Delta \leqslant \kappa_1\, h(t) + \kappa_2$$

for all t.

We make the following assumptions on the differentiability of $h(t)$. The map $t \mapsto \langle \psi\,, h(t)\psi \rangle$ is continuously differentiable for all $\psi \in X_1$, with derivative $\langle \psi\,, \dot{h}(t)\psi \rangle$ for some self-adjoint operator $\dot{h}(t)$. Moreover, we assume that the quantities

$$\langle \varphi(t)\,, \dot{h}(t)^2 \varphi(t) \rangle, \qquad \left\| (\mathbb{1} + h(t))^{-1/2}\, \dot{h}(t)\, (\mathbb{1} + h(t))^{-1/2} \right\|$$

are continuous and finite for all t.

(B2') The Hamiltonian $H_N(t)$ is self-adjoint and bounded from below. We assume that $\mathcal{Q}(H_N(t)) \subset X_N$ for all t. We also assume that the N-body propagator $U_N(t,s)$, defined by

$$\mathrm{i}\partial_t U_N(t,s) = H_N(t) U_N(t,s), \qquad U_N(s,s) = \mathbb{1},$$

exists and satisfies $U_N(t,0)\Psi_{N,0} \in \mathcal{Q}(H_N(t))$ for all t.

(B3') There is a time-independent constant $\kappa_3 \in (0,1)$ such that

$$0 \leqslant (1-\kappa_3)(h_1(t) + h_2(t)) + W_{12}$$

for all t.

Theorem 4.7. *Assume that Assumptions (B1') – (B3'), (B4), and (B5) hold. Then there is a continuous nonnegative function ϕ, independent of N and $\Psi_{N,0}$, such that*

$$\beta_N(t) \leqslant \phi(t)\left(\beta_N(0) + E_N^{\Psi}(0) - E^{\varphi}(0) + \frac{1}{N^{\eta}}\right),$$

with η defined in (4.4).

Proof. We start by deriving an upper bound on the energy difference $\mathcal{E}(t) := E^{\Psi}(t) - E^{\varphi}(t)$. Assumptions (B1') and (B2') and the fundamental theorem of calculus imply

$$\mathcal{E}(t) = \mathcal{E}(0) + \int_0^t \mathrm{d}s\, \Big(\underbrace{\langle \Psi(s)\,, \dot{h}_1(s)\Psi(s)\rangle - \langle \varphi(s)\,, \dot{h}(s)\varphi(s)\rangle}_{=:\, G(s)} \Big).$$

By inserting $\mathbb{1} = p_1(s) + q_1(s)$ on both sides of $\dot{h}_1(s)$ we get (omitting the time argument s)

$$G = \langle \Psi\,, p_1 \dot{h}_1 p_1 \Psi \rangle - \langle \varphi\,, \dot{h}\varphi \rangle + 2\,\mathrm{Re}\langle \Psi\,, p_1 \dot{h}_1 q_1 \Psi \rangle + \langle \Psi\,, q_1 \dot{h}_1 q_1 \Psi \rangle. \qquad (4.32)$$

The first two terms of (4.32) are equal to

$$\big(\langle \Psi\,, p_1 \Psi \rangle - 1\big) \langle \varphi\,, \dot{h}\varphi \rangle = \alpha \langle \varphi\,, \dot{h}\varphi \rangle \leqslant \beta |\langle \varphi\,, \dot{h}\varphi \rangle|.$$

The third term of (4.32) is bounded, using Lemmas 3.9 and 3.10, by

$$\begin{aligned}
2\big|\langle \Psi\,, p_1 \dot{h}_1\, \widehat{n}^{1/2}\ \widehat{n}^{-1/2} q_1 \Psi \rangle\big| &= 2\big|\langle \dot{h}_1 p_1\, \widehat{\tau_1 n}^{1/2}\, \Psi\,, \widehat{n}^{-1/2}\, q_1 \Psi \rangle\big| \\
&\leqslant \sqrt{\big\langle \widehat{\tau_1 n}^{1/2}\, \Psi\,, p_1 \dot{h}_1^2 p_1\, \widehat{\tau_1 n}^{1/2}\, \Psi \big\rangle}\, \big\| \widehat{n}^{-1/2}\, q_1 \Psi \big\| \\
&\leqslant \sqrt{|\langle \varphi\,, \dot{h}^2 \varphi \rangle|}\, \sqrt{\big\langle \Psi\,, \widehat{\tau_1 n}\, \Psi \big\rangle}\, \sqrt{\big\langle \Psi\,, \widehat{n}^{-1}\, q_1 \Psi \big\rangle} \\
&\leqslant \sqrt{|\langle \varphi\,, \dot{h}^2 \varphi \rangle|}\, \sqrt{\beta + \frac{1}{\sqrt{N}}}\, \sqrt{\beta}, \\
&\lesssim \sqrt{|\langle \varphi\,, \dot{h}^2 \varphi \rangle|} \left(\beta + \frac{1}{\sqrt{N}} \right).
\end{aligned}$$

The last term of (4.32) is equal to

$$\begin{aligned}&\big\langle \Psi\,, q_1(\mathbb{1}+h_1)^{1/2}(\mathbb{1}+h)^{-1/2}\dot{h}_1(\mathbb{1}+h_1)^{-1/2}(\mathbb{1}+h)^{1/2}q_1\Psi\big\rangle\\ &\quad\leqslant \big\|(\mathbb{1}+h)^{-1/2}\dot{h}(\mathbb{1}+h)^{-1/2}\big\|\,\big\|(\mathbb{1}+h_1)^{1/2}q_1\Psi\big\|^2.\end{aligned}$$

Thus, using Assumption (B1') we conclude that

$$G(t)\leqslant C(t)\bigg(\beta(t)+\frac{1}{\sqrt{N}}+\big\|h_1(t)^{1/2}q_1(t)\Psi(t)\big\|^2\bigg) \tag{4.33}$$

for all t. Here, and in the following, $C(t)$ denotes some continuous nonnegative function that does not depend on N.

Next, we observe that, under Assumptions (B1') – (B3'), the proof of Lemma 4.6 remains valid for time-dependent one-particle Hamiltonians. Thus, (4.13) implies

$$\big\|h_1(t)^{1/2}q_1(t)\Psi(t)\big\|^2\lesssim \mathcal{E}(t)+\big(1+\|\varphi(t)\|^2_{X_1^2\cap L^\infty}\big)\bigg(\beta(t)+\frac{1}{\sqrt{N}}\bigg).$$

Plugging this into (4.33) yields

$$G(t)\leqslant C(t)\bigg(\beta(t)+\frac{1}{\sqrt{N}}+\mathcal{E}(t)\bigg).$$

Therefore,

$$\mathcal{E}(t)\leqslant \mathcal{E}(0)+\int_0^t \mathrm{d}s\, C(s)\bigg(\beta(s)+\mathcal{E}(s)+\frac{1}{\sqrt{N}}\bigg). \tag{4.34}$$

Next, we observe that, under Assumptions (B1') – (B3'), the derivation of the estimate (4.31) in the proof of Theorem 4.1 remains valid for time-dependent one-particle Hamiltonians. Therefore,

$$\beta(t)\leqslant \beta(0)+\int_0^t \mathrm{d}s\, C(s)\bigg(\beta(s)+\mathcal{E}(s)+\frac{1}{N^\eta}\bigg). \tag{4.35}$$

Applying Grönwall's lemma to the sum of (4.34) and (4.35) yields

$$\beta(t)+\mathcal{E}(t)\leqslant \big(\beta(0)+\mathcal{E}(0)\big)\,\mathrm{e}^{\int_0^t C}+\frac{1}{N^\eta}\int_0^t \mathrm{d}s\, C(s)\,\mathrm{e}^{\int_0^t C}.$$

Plugging this back into (4.35) yields

$$\beta(t)\leqslant C(t)\bigg(\beta(0)+\mathcal{E}(0)+\frac{1}{N^\eta}\bigg),$$

which is the claim.

Acknowledgements. We would like to thank J. Fröhlich and E. Lenzmann for helpful and stimulating discussions. We also gratefully acknowledge discussions with A. Michelangeli which led to Lemma 2.1.

References

1. Elgart, A., Schlein, B.: Mean field dynamics of boson stars. Comm. Pure Appl. Math. **60**(4), 500–545 (2007)
2. Erdős, L., Schlein, B.: *Quantum dynamics with mean field interactions: a new approach.* http://arXiv.org/abs/0804.3774v1[math.ph], 2008
3. Erdős, L., Yau, H.-T.: Derivation of the nonlinear Schrödinger equation with Coulomb potential. Adv. Theor. Math. Phys. **5**, 1169–1205 (2001)
4. Fröhlich, J., Knowles, A., Schwarz, S.: On the mean-field limit of bosons with Coulomb two-body interaction. Commun. Math. Phys. **288**, 1023–1059 (2009)
5. Ginibre, J., Velo, G.: On a class of non linear Schrödinger equations with non local interaction. Math. Z. **170**, 109–136 (1980)
6. Hepp, K.: The classical limit for quantum mechanical correlation functions. Commun. Math. Phys. **35**, 265–277 (1974)
7. Lenzmann, E.: Well-posedness for semi-relativistic Hartree equations of critical type. Math. Phys. Anal. Geom. **10**(1), 43–64 (2007)
8. Lieb, E., Yau, H.-T.: The Chandrasekhar theory of stellar collapse as the limit of quantum mechanics. Commun. Math. Phys. **112**(1), 147–174 (1987)
9. Lieb, E.H., Seiringer, R.: Proof of Bose-Einstein condensation for dilute trapped gases. Phys. Rev. Lett. **88**(17), 170409 (2002)
10. Pickl, P.: *A simple derivation of mean field limits for quantum systems.* To appear
11. Reed, M., Simon, B.: *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness.* New York: Academic Press, 1975
12. Rodnianski, I., Schlein, B.: *Quantum fluctuations and rate of convergence towards mean field dynamics.* http://arXiv.org/abs/0711.3087v1[math.ph], 2007
13. Spohn, H.: Kinetic equations from Hamiltonian dynamics: Markovian limits. Rev. Mod. Phys. **53**(3), 569–615 (1980)

Communicated by H.-T. Yau