

Dynamics of Bose-Einstein Condensates

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1 Main Result

Bosonic systems at very low temperature are characterized by the fact that a macroscopic fraction of the particles collapses into a single one-particle state. Although this phenomenon, known as Bose-Einstein condensation, was already predicted in the early days of quantum mechanics, the first empirical evidence for its existence was only obtained in 1995, in experiments performed by groups led by Cornell and Wieman at the University of Colorado at Boulder and by Ketterle at MIT (see [2, 4]). In these important experiments, atomic gases were initially trapped by magnetic fields and cooled down at very low temperatures. Then the magnetic traps were switched off and the consequent time evolution of the gas was observed; for sufficiently small temperatures, the gas moves as a single particle, a clear sign for the existence of condensation.

To describe these experiments from a theoretical point of view, we have, first of all, to give a precise definition of the meaning of Bose-Einstein condensation. A system of N bosons in three dimensions can be described by a normalized wave function ψ_N in the Hilbert space $L_s^2(\mathbb{R}^{3N})$, the subspace of $L^2(\mathbb{R}^{3N})$ consisting of permutation symmetric functions. For a given N -particle wave function $\psi_N \in L_s^2(\mathbb{R}^{3N})$, we define the density matrix $\gamma_N = |\psi_N\rangle\langle\psi_N|$ as the orthogonal projection onto ψ_N . Moreover, for $k = 1, \dots, N$, we define the k -particle marginal density $\gamma_N^{(k)}$ associated with ψ_N by taking the partial trace of γ_N over the degrees of freedom of the last $(N - k)$ particles. In other words, $\gamma_N^{(k)}$ is defined as the non-negative trace class operator on $L^2(\mathbb{R}^{3k})$ with kernel given by

$$\gamma_N^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) = \int d\mathbf{x}_{N-k} \psi_N(\mathbf{x}_k, \mathbf{x}_{N-k}) \overline{\psi_N}(\mathbf{x}'_k, \mathbf{x}_{N-k}). \quad (1.1)$$

Here we introduced the notation $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $\mathbf{x}_k = (x_1, x_2, \dots, x_k)$, $\mathbf{x}'_k = (x'_1, x'_2, \dots, x'_k)$, and $\mathbf{x}_{N-k} = (x_{k+1}, x_{k+2}, \dots, x_N)$. Note that, by definition, $\text{Tr} \gamma_N^{(k)} = 1$ for all N, k . In particular the one-particle density $\gamma_N^{(1)}$ is a non-negative trace class operator on $L^2(\mathbb{R}^3)$ with trace equal to one. The eigenvalues of $\gamma_N^{(1)}$ (which are all non-negative and sum up to one) can be interpreted as probabilities for finding particles in the state described by the corresponding eigenvector (a one-particle orbital). This observation justifies the following precise definition of complete Bose-Einstein condensation.

Definition 1.1. A sequence $\{\psi_N\}_{N \in \mathbb{N}}$ with $\psi_N \in L_s^2(\mathbb{R}^{3N})$ is said to exhibit complete Bose-Einstein condensation in $\varphi \in L^2(\mathbb{R}^3)$ if

$$\text{Tr} \left| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right| \rightarrow 0 \quad (1.2)$$

as $N \rightarrow \infty$ (recall that $\|A\|_1 = \text{Tr}|A| = \text{Tr}\sqrt{A^*A}$ defines the trace norm of the operator A).

Note that condensation is not a property of a single N -particle wave function ψ_N , but it is a property characterizing a sequence $\{\psi_N\}_{N \in \mathbb{N}}$ in the limit $N \rightarrow \infty$.

It is in general very difficult to verify that the condition (1.2) is satisfied for physically interesting wave functions of interacting systems. There exists, however, a class of interacting systems for which complete condensation of the ground state has been recently established.

In [12], Lieb, Yngvason, and Seiringer considered a trapped Bose gas consisting of N three-dimensional particles described by the Hamiltonian

$$H_N^{\text{trap}} = \sum_{j=1}^N (-\Delta_j + V_{\text{ext}}(x_j)) + \sum_{i < j}^N V_N(x_i - x_j), \quad (1.3)$$

where V_{ext} is an external confining potential with $\lim_{|x| \rightarrow \infty} V_{\text{ext}}(x) = \infty$, and $V_N(x) = N^2 V(Nx)$ is a spherically symmetric repulsive interaction potential, $V_N \geq 0$ (here and in the rest of these notes we use the notation $\nabla_j = \nabla_{x_j}$ and $\Delta_j = \Delta_{x_j}$). The potential V_N scales with N so that its scattering length is of the order $1/N$ (Gross-Pitaevskii scaling). Recall that if f denotes the spherical symmetric solution to the zero-energy scattering equation

$$\left(-\Delta + \frac{1}{2}V(x) \right) f = 0 \quad \text{with boundary condition } f(x) \rightarrow 1 \quad \text{as } |x| \rightarrow \infty, \quad (1.4)$$

the scattering length of V is defined by

$$a_0 = \lim_{|x| \rightarrow \infty} |x| - |x|f(x).$$

This limit can be proven to exist if V decays sufficiently fast at infinity. Another equivalent characterization of the scattering length is given by

$$8\pi a_0 = \int dx V(x)f(x). \quad (1.5)$$

Physically, the scattering length measures the effective range of the potential; two particles interacting through the potential V see each other as hard spheres with radius a_0 , when they are far apart. It is simple to check that, if f solves (1.4) then the rescaled function $f_N(x) = f(Nx)$ solves the zero energy scattering equation with rescaled potential V_N , that is

$$\left(-\Delta + \frac{1}{2}V_N\right) f_N = 0 \quad \text{with } f_N(x) \rightarrow 1 \quad \text{as } |x| \rightarrow \infty. \quad (1.6)$$

This implies immediately that the scattering length of V_N is given by $a = a_0/N$, where a_0 is the scattering length of the unscaled potential V . Note that, for $|x| \gg a$, $f_N(x) \simeq 1 - a/|x|$. For $|x| < a$, f_N remains bounded; for practical purposes, we can think of this function as $f_N(x) \simeq 1 - a/(|x| + a)$.

Letting $N \rightarrow \infty$, Lieb, Yngvason, and Seiringer showed that the ground state energy $E(N)$ of (1.3) divided by the number of particle N converges to

$$\lim_{N \rightarrow \infty, Na=a_0} \frac{E(N)}{N} = \min_{\varphi \in L^2(\mathbb{R}^3): \|\varphi\|=1} \mathcal{E}_{\text{GP}}(\varphi)$$

where \mathcal{E}_{GP} is the Gross-Pitaevskii energy functional

$$\mathcal{E}_{\text{GP}}(\varphi) = \int dx (|\nabla\varphi(x)|^2 + V_{\text{ext}}(x)|\varphi(x)|^2 + 4\pi a_0|\varphi(x)|^4). \quad (1.7)$$

Later, in [11], Lieb and Seiringer also proved that the ground state of the Hamiltonian (1.3) exhibits complete Bose-Einstein condensation into the minimizer of the Gross-Pitaevskii energy functional \mathcal{E}_{GP} . More precisely they showed that, if ψ_N is the ground state wave function of the Hamiltonian (1.3) and if $\gamma_N^{(1)}$ denotes the corresponding one-particle marginal, then

$$\gamma_N^{(1)} \rightarrow |\phi_{\text{GP}}\rangle\langle\phi_{\text{GP}}| \quad \text{as } N \rightarrow \infty, \quad (1.8)$$

where $\phi_{\text{GP}} \in L^2(\mathbb{R}^3)$ is the minimizer of the Gross-Pitaevskii energy functional (1.7).

To describe the experiments mentioned above, it is important to understand the time-evolution of the Bose-Einstein condensate after removing the external traps. Therefore, we define the translation invariant Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_j + \sum_{i<j}^N V_N(x_i - x_j) \quad (1.9)$$

and we consider solutions to the N -particle Schrödinger equation

$$i\partial_t\psi_{N,t} = H_N\psi_{N,t} \quad \Rightarrow \quad \psi_{N,t} = e^{-iH_N t} \quad (1.10)$$

with initial data exhibiting complete Bose-Einstein condensation. In a series of articles [6, 7, 8, 9], we prove that, for every fixed time $t \in \mathbb{R}$, the evolved N -particle wave function $\psi_{N,t}$ still exhibits complete Bose-Einstein condensation. Moreover we show that the time evolution of the condensate wave function evolves according to the one-particle time-dependent Gross-Pitaevskii equation associated with the energy functional \mathcal{E}_{GP} . Our main result is the following theorem.

Theorem 1.2. *Suppose that $V \geq 0$ is spherically symmetric and $V(x) \leq C\langle x \rangle^{-\sigma}$, for some $\sigma > 5$, and for all $x \in \mathbb{R}^3$. Assume that the family $\psi_N \in L_s^2(\mathbb{R}^{3N})$, with $\|\psi_N\| = 1$ for all N , has finite energy per particle, that is*

$$\langle \psi_N, H_N \psi_N \rangle \leq CN \quad (1.11)$$

and that it exhibits complete Bose-Einstein condensation in the sense that

$$\text{Tr} \left| \gamma_N^{(1)} - |\varphi\rangle\langle\varphi| \right| \rightarrow 0 \quad (1.12)$$

as $N \rightarrow \infty$ for some $\varphi \in L^2(\mathbb{R}^3)$. Then, for every $k \geq 1$ and $t \in \mathbb{R}$, we have

$$\text{Tr} \left| \gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \right| \rightarrow 0$$

as $N \rightarrow \infty$. Here φ_t is the solution of the nonlinear Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \quad (1.13)$$

with initial data $\varphi_{t=0} = \varphi$.

In the rest of this article we present the main ideas of the proof of Theorem 1.2 under two additional assumptions:

- A) The interaction potential V is such that $\|\nabla^\alpha V\|_\infty < \infty$ for all $\alpha \in \mathbb{N}^2$ with $|\alpha| \leq 2$.
- B) The initial data ψ_N is such that there exists a constant $C > 0$ and, for every $k \in \mathbb{N}$, $N_0 = N_0(k)$ such that

$$\langle \psi_N, H_N^k \psi_N \rangle \leq C^k N^k \quad (1.14)$$

for all $N > N_0$.

Both assumptions can then be relaxed by appropriate approximation arguments (see [9, Section 9 and Appendix B]). Note also that the condition of spherical symmetry of the potential can be relaxed to the condition $V(-x) = V(x)$ (see [9]).

2 Strategy of the Proof

The main idea for proving Theorem 1.2 is to study the time-evolution of the marginal densities $\gamma_{N,t}^{(k)}$ associated with the solution $\psi_{N,t} = e^{-iH_N t} \psi_N$ of the N -particle Schrödinger equation, in the limit of large N . From (1.10), it follows that the densities $\gamma_{N,t}^{(k)}$, $k = 1, \dots, N$, solve a hierarchy of N coupled equations usually known as the BBGKY hierarchy:

$$\begin{aligned} i\partial_t \gamma_{N,t}^{(k)} &= \sum_{j=1}^k \left[-\Delta_j, \gamma_{N,t}^{(k)} \right] + \sum_{i < j}^k \left[V_N(x_i - x_j), \gamma_{N,t}^{(k)} \right] \\ &+ (N - k) \sum_{j=1}^k \text{Tr}_{k+1} \left[V_N(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right], \end{aligned} \quad (2.1)$$

where Tr_{k+1} denotes the partial trace over the degrees of freedom of the $(k+1)$ -th particle. In particular we will be interested in the behavior of solutions of this hierarchy for fixed k and in the limit $N \rightarrow \infty$. More precisely, the proof of Theorem 1.2 is divided into three steps.

Step 1. Compactness of $\gamma_{N,t}^{(k)}$. Recall that, for $k = 1, \dots, N$, the k -particle density $\gamma_{N,t}^{(k)}$ is defined as a non-negative operator in $\mathcal{L}_k^1 = \mathcal{L}^1(L^2(\mathbb{R}^{3k}))$ (the space of trace class operators on $L^2(\mathbb{R}^{3k})$) with trace equal to one, and with kernel given by

$$\gamma_{N,t}^{(k)}(\mathbf{x}_k; \mathbf{x}'_k) = \int d\mathbf{x}_{N-k} \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) \overline{\psi}_N(\mathbf{x}'_k, \mathbf{x}_{N-k}).$$

For fixed $t \in \mathbb{R}$ and $k \geq 1$, it follows by standard abstract arguments (Banach-Alaouglu Theorem) that the sequence $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ is compact with respect to the weak* topology of \mathcal{L}_k^1 . Note here that \mathcal{L}_k^1 has a weak* topology because $\mathcal{L}_k^1 = \mathcal{K}_k^*$, where $\mathcal{K}_k = \mathcal{K}(L^2(\mathbb{R}^{3k}))$ is the space of compact operators on $L^2(\mathbb{R}^{3k})$. To make sure that we can find subsequences of $\gamma_{N,t}^{(k)}$ which converge for all times in a certain interval, we fix $T > 0$ and consider the space $C([0, T], \mathcal{L}_k^1)$ of all functions of $t \in [0, T]$ with values in \mathcal{L}_k^1 which are continuous with respect to the weak* topology on \mathcal{L}_k^1 . Since \mathcal{K}_k is separable, it follows that the weak* topology on the unit ball of \mathcal{L}_k^1 is metrizable. We prove therefore the equicontinuity of the densities $\gamma_{N,t}^{(k)}$, and we obtain the compactness of the sequences $\{\gamma_{N,t}^{(k)}\}_{N \geq k}$ in $C([0, T], \mathcal{L}_k^1)$ by the Arzela-Ascoli Theorem.

Step 2. Convergence to an infinite hierarchy. From Step 1 it follows that, as $N \rightarrow \infty$, the family of marginal densities $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ has at least one limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ in $\bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ with respect to the product topology. Next, we derive evolution equations for the limiting densities $\gamma_{\infty,t}^{(k)}$. Starting from the BBGKY hierarchy (2.1) for the family $\Gamma_{N,t}$, we prove that any limit point $\Gamma_{\infty,t}$ satisfies the infinite hierarchy of equations

$$i\partial_t \gamma_{\infty,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{\infty,t}^{(k)} \right] + 8\pi a_0 \sum_{j=1}^k \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)} \right] \quad (2.2)$$

for $k \geq 1$. The δ -function in the last term on r.h.s. of this hierarchy originates from the N -dependent potential in the last term on the r.h.s. of the BBGKY hierarchy (2.1). Note however that, formally,

$$(N-k)V_N(x_j - x_{k+1}) \simeq N^3 V(N(x_j - x_{k+1})) \simeq b_0 \delta(x_j - x_{k+1}) \quad (2.3)$$

as $N \rightarrow \infty$. Here we defined $b_0 = \int dx V(x)$. The emergence of a different coupling constant, proportional to the scattering length, in front of the interaction term on the r.h.s. of (2.2) is a subtle consequence of the correlation structure developed by the solution to the N -particle Schrödinger equation and inherited by its marginal densities. This short scale correlation structure, which, as we will see, can be described in good approximation by the solution f_N of the zero-energy scattering equation (1.6), is characterized by exactly the same length-scale of the order $1/N$ which characterizes the interaction potential. For this reason, before taking the limit $N \rightarrow \infty$ in the potential (as done in (2.3)), we need to multiply it with f_N . This leads, by (1.5), to

$$(N-k)V_N(x_j - x_{k+1})f_N(x_j - x_{k+1}) \simeq N^3 V(N(x_j - x_{k+1}))f(N(x_j - x_{k+1})) \simeq 8\pi a_0 \delta(x_j - x_{k+1}), \quad (2.4)$$

and thus to the correct coupling constant. We will discuss this important part of the proof in more details in Section 5.

It is worth noticing that the infinite hierarchy (2.2) has a factorized solution. In fact, it is simple to see that the infinite family

$$\gamma_t^{(k)} = |\varphi_t\rangle \langle \varphi_t|^{\otimes k} \quad \text{for } k \geq 1 \quad (2.5)$$

solves (2.2) if and only if φ_t is a solution to the Gross-Pitaevskii equation (1.13).

Step 3. Uniqueness of the solution to the infinite hierarchy. To conclude the proof of Theorem 1.2, we show that the infinite hierarchy (2.2) has a unique solution. This implies immediately that the densities $\gamma_{N,t}^{(k)}$ converge; in fact, a compact sequence with at most one limit point is always convergent. Moreover, since we know that the factorized densities (2.5) are a solution, it also follows that, for any $k \geq 1$,

$$\gamma_{N,t}^{(k)} \rightarrow |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{as } N \rightarrow \infty$$

with respect to the weak* topology of \mathcal{L}_k^1 (since the limit is a projection, convergence in the norm-topology follows automatically from the weak* convergence).

Similar strategies have been used to obtain rigorous derivations of the nonlinear Hartree equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + (v * |\varphi_t|^2)\varphi_t \quad (2.6)$$

for the dynamics of initially factorized wave functions in a bosonic mean field model described by the Hamiltonian

$$H_N^{\text{mf}} = \sum_{j=1}^N -\Delta_j + \frac{1}{N} \sum_{i<j}^N v(x_i - x_j). \quad (2.7)$$

In this context, the approach outlined above was introduced by Spohn in [14], who applied it to derive (2.6) in the case of a bounded potential v . In [10], Erdős and Yau extended Spohn's result to the case of a Coulomb interaction $v(x) = \pm 1/|x|$ (partial results for the Coulomb case, in particular the convergence to the infinite hierarchy, were also obtained by Bardos, Golse, and Mauser, see [3]). More recently, Adami, Golse, and Teta used the same approach in [1] for one-dimensional systems with dynamics generated by a Hamiltonian of the form (2.7) with an N -dependent pair potential $v_N(x) = N^\beta V(N^\beta x)$, $\beta < 1$. In the limit $N \rightarrow \infty$, they obtain the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + b_0|\varphi_t|^2\varphi_t \quad \text{with } b_0 = \int V(x)dx.$$

Notice that the Hamiltonian (1.9) has the same form as the mean field Hamiltonian (2.7), with an N -dependent pair potential $v_N(x) = N^3V(Nx)$. Of course, one may also ask what happens if we consider the mean field Hamiltonian (2.7) with the N -dependent potential $v_N(x) = N^{3\beta}V(N^\beta x)$, for $\beta \neq 1$. If $\beta < 1$, the short scale structure developed by the solution of the Schrödinger equation is still characterized by the length scale $1/N$ (because the scattering length of $N^{3\beta-1}V(N^\beta x)$ is still of order $1/N$); but this time the potential varies on much larger scales, of the order $N^{-\beta} \gg N^{-1}$. For this reason, if $\beta < 1$, the scattering length does not appear in the effective macroscopic equation ($8\pi a_0$ is replaced by $b_0 = \int dx V(x)$).

Theorem 2.1. *Suppose that $V \geq 0$ satisfies the same assumption as in Theorem 1.2, and assume that $0 < \beta \leq 1$. Let $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$, for some $\varphi \in H^1(\mathbb{R}^3)$ and $\psi_{N,t} = e^{-iH_{\beta,N}t}\psi_N$ with the mean-field Hamiltonian*

$$H_{\beta,N} = \sum_{j=1}^N -\Delta_j + \frac{1}{N} \sum_{i<j}^N N^{3\beta}V(N^\beta(x_i - x_j)).$$

Then, for every fixed $k \geq 1$ and $t \in \mathbb{R}$, we have

$$\gamma_{N,t}^{(k)} \rightarrow |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$$

as $N \rightarrow \infty$, where φ_t is the solution to the nonlinear Schrödinger equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + \sigma |\varphi_t|^2 \varphi_t$$

with initial data $\varphi_{t=0} = \varphi$ and with

$$\sigma = \begin{cases} 8\pi a_0 & \text{if } \beta = 1 \\ b_0 & \text{if } 0 < \beta < 1 \end{cases} .$$

3 Uniqueness of the Infinite Hierarchy

In this section we discuss the main ideas used to prove the uniqueness of the solution to the infinite hierarchy (Step 3 in the strategy outlined in Section 2). It is in this part of the proof that we use Feynman diagrams.

First of all, we need to specify in which class of densities $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1}$ we want to prove the uniqueness of the solution to the infinite hierarchy (2.2). Clearly, the proof of the uniqueness is simpler if we can restrict our attention to smaller classes. But of course the class of densities for which we prove uniqueness cannot be too small because, to prove Theorem 1.2, we need to make sure that any limit point of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ is in the class for which we have uniqueness.

In Section 4, we are going to prove that (under the additional assumptions (A) and (B) listed at the end of Section 1) an arbitrary limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ of the sequence of marginal densities $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ is such that

$$\text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{\infty,t}^{(k)} \leq C^k \quad (3.1)$$

for all $k \geq 1$. For this reason, it is enough to prove the uniqueness of the solution to the infinite hierarchy in the class of densities satisfying (3.1). In [6], we prove the following theorem.

Theorem 3.1. *Fix $T > 0$ and $\Gamma = \{\gamma^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} \mathcal{L}_k^1$, with $\gamma^{(k)} \geq 0$ for all $k \in \mathbb{N}$. Then there exists at most one solution $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \bigoplus C([0, T], \mathcal{L}_k)$ of the integral equation*

$$\gamma_t^{(k)} = \mathcal{U}^{(k)}(t) \gamma_0^{(k)} - 8i\pi a_0 \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_s^{(k)} \right] \quad (3.2)$$

with $\Gamma_{t=0} = \Gamma$, such that $\gamma_t^{(k)} \geq 0$ is symmetric with respect to permutations, and with

$$\|\gamma_t^{(k)}\|_{\mathcal{H}_k} := \text{Tr} \left| (1 - \Delta_1)^{1/2} \dots (1 - \Delta_k)^{1/2} \gamma_t^{(k)} (1 - \Delta_k)^{1/2} \dots (1 - \Delta_1)^{1/2} \right| \leq C^k \quad (3.3)$$

for all $k \geq 1$ and all $t \in [0, T]$. In (3.2),

$$\mathcal{U}^{(k)}(t) \gamma^{(k)} = e^{it \sum_{j=1}^k \Delta_j} \gamma^{(k)} e^{-it \sum_{j=1}^k \Delta_j} \quad (3.4)$$

is the free evolution of the k -particle operator $\gamma^{(k)}$, and Tr_{k+1} denotes the partial trace over the $(k+1)$ -th particle.

Remarks.

- 1) The hierarchy (3.2) is equivalent to the hierarchy (2.2), rewritten in integral form.

2) A k -particle operator $\gamma^{(k)}$ is said to be symmetric w.r.t. permutations if

$$\Theta_\sigma \gamma^{(k)} \Theta_{\sigma^{-1}} = \gamma^{(k)} \quad (3.5)$$

for all permutations $\sigma \in \mathcal{S}_k$, where Θ_σ is the unitary operator on $L^2(\mathbb{R}^{3k})$ defined by

$$(\Theta_\sigma \psi)(x_1, \dots, x_k) = \psi(x_{\sigma(1)}, \dots, x_{\sigma(k)}). \quad (3.6)$$

3) For a non-negative density $\gamma^{(k)}$, we have

$$\begin{aligned} \|\gamma^{(k)}\|_{\mathcal{H}_k} &= \text{Tr} \left| (1 - \Delta_1)^{1/2} \dots (1 - \Delta_k)^{1/2} \gamma^{(k)} (1 - \Delta_k)^{1/2} \dots (1 - \Delta_1)^{1/2} \right| \\ &= \text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma^{(k)} \end{aligned} \quad (3.7)$$

and therefore limit points $\gamma_{\infty, t}^{(k)}$ of the sequence $\gamma_{N, t}^{(k)}$ satisfy (3.3) because of (3.1).

From (3.2), we obtain

$$\gamma_t = \mathcal{U}^{(k)}(t) \gamma_0 + \int_0^t ds \mathcal{U}^{(k)}(t-s) B^{(k)} \gamma_s^{(k+1)}, \quad (3.8)$$

where the collision operator $B^{(k)}$ is defined by

$$B^{(k)} \gamma^{(k+1)} = -8i\pi a_0 \sum_{j=1}^k \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma^{(k+1)} \right]. \quad (3.9)$$

(Note that $B^{(k)}$ maps $(k+1)$ -particle operators into k -particle operators). On kernels in momentum space $B^{(k)}$ acts according to

$$\begin{aligned} (B^{(k)} \gamma^{(k+1)})(\mathbf{p}_k; \mathbf{p}'_k) &= (-i) \sum_{j=1}^k \int dq_{k+1} dq'_{k+1} \left(\gamma^{(k+1)}(p_1, \dots, p_j - q_{k+1} + q'_{k+1}, \dots, p_k, q_{k+1}; \mathbf{p}'_k, q'_{k+1}) \right. \\ &\quad \left. - \gamma^{(k+1)}(\mathbf{p}_k, q_{k+1}; p'_1, \dots, p'_j + q_{k+1} - q'_{k+1}, \dots, p'_k, q'_{k+1}) \right) \\ &= (-i) \sum_{j=1}^k \int d\mathbf{q}_{k+1} d\mathbf{q}'_{k+1} \left(\prod_{\ell \neq j}^k \delta(p_\ell - q_\ell) \delta(p'_\ell - q'_\ell) \right) \gamma^{(k+1)}(\mathbf{q}_{k+1}; \mathbf{q}'_{k+1}) \\ &\quad \times [\delta(p'_j - q'_j) \delta(p_j - (q_j + q_{k+1} - q'_{k+1})) - \delta(p_j - q_j) \delta(p'_j - (q'_j + q'_{k+1} - q_{k+1}))]. \end{aligned} \quad (3.10)$$

Iterating (3.8) n times we obtain the Duhamel series

$$\gamma_t^{(k)} = \mathcal{U}^{(k)}(t) \gamma_0^{(k)} + \sum_{m=1}^{n-1} \xi_{m, t}^{(k)} + \eta_{n, t}^{(k)} \quad (3.11)$$

with

$$\begin{aligned} \xi_{m, t}^{(k)} &= \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) B^{(k+1)} \dots B^{(k+m-1)} \mathcal{U}^{(k+m)}(s_m) \gamma_0^{(k+m)} \\ &= \sum_{j_1=1}^k \sum_{j_2=1}^{k+1} \dots \sum_{j_m=1}^{k+m} \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1) \text{Tr}_{k+1} \left[\delta(x_{j_1} - x_{k+1}), \right. \\ &\quad \left. \mathcal{U}^{(k+1)}(s_1-s_2) \text{Tr}_{k+2} \left[\delta(x_{j_2} - x_{k+2}), \dots \text{Tr}_{k+m} \left[\delta(x_{j_m} - x_{k+m}), \mathcal{U}^{(k+m)}(s_m) \gamma_0^{(k+m)} \right] \dots \right] \right] \end{aligned} \quad (3.12)$$

and the error term

$$\mu_{n,t}^{(k)} = \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) B^{(k+1)} \dots B^{(k+n-1)} \gamma_{s_n}^{(k+n)}. \quad (3.13)$$

Note that the error term (3.13) has exactly the same form as the fully expanded terms in (3.12), with the only difference that the last free evolution is replaced by the full evolution $\gamma_{s_n}^{(k+n)}$.

To prove the uniqueness of the infinite hierarchy, we show the convergence of the series (3.11). The main problem here is that the delta function in the collision operator $B^{(k)}$ cannot be controlled by the kinetic energy (in the sense that, in three dimensions, the operator inequality $\delta(x) \leq C(1-\Delta)$ does not hold true). For this reason, the a-priori estimates (3.3) are not sufficient to show that (3.13) converges to zero, as $n \rightarrow \infty$ (for more regular interactions the a-priori bounds are enough; see Appendix A for a proof of the uniqueness of the infinite hierarchy in the case of bounded potentials and in the case of a Coulomb potential). For this reason, we have to make use of the smoothing effects of the free evolutions $\mathcal{U}^{(k+j)}(s_j - s_{j+1})$ in (3.13). To this end, we rewrite each term in the series (3.11) as a sum of contributions associated with suitable Feynman graphs, and then we prove the convergence of the Duhamel expansion by controlling each contribution separately.

In Sections 3.1 we introduce the graphs and we prove that the terms in (3.12), and (3.13) can be expressed as sums of appropriate contributions associated with the graphs (known as the *amplitudes* of the graphs). Then in Section 3.2, we show how to bound these amplitudes, and we show how to conclude, with this information, the proof of Theorem 3.1. We only explain the main ideas of our analysis; more details can be found in [6, Section 9].

Notation. In the rest of this section, we will mostly work with kernels in momentum space. We use the convention that p, q, r always refer to three dimensional Fourier variables, while x, y, z are reserved for configuration space variables. With this convention, the usual hat indicating the Fourier transform will be omitted (as in (3.10)). For example, the kernel of a two-particle density matrix $\gamma_0^{(2)}$ in position space is $\gamma_0^{(2)}(x_1, x_2; x'_1, x'_2)$; in momentum space it is given by the Fourier transform

$$\gamma_0^{(2)}(q_1, q_2; q'_1, q'_2) = \int dx_1 dx_2 dx'_1 dx'_2 \gamma_0^{(2)}(x_1, x_2; x'_1, x'_2) e^{-i(x_1 \cdot p_1 + x_2 \cdot p_2)} e^{i(x'_1 \cdot p'_1 + x'_2 \cdot p'_2)},$$

with the slight abuse of notation of omitting the hat on left hand side. Furthermore, to avoid (2π) -factors in the Fourier transform, we make the convention that the integration measure for the three dimensional momentum variables p, q, r are always divided by $(2\pi)^3$, i.e.

$$dp := \frac{d_{\text{Leb}} p}{(2\pi)^3} \quad \text{for all three dimensional momentum variables}$$

where d_{Leb} denotes the usual Lebesgue measure. We will also use delta functions in momentum space, $\delta(p)$, and they will correspond to the measure dp above, i.e.

$$\int f(p) \delta(p - q) dp = f(q)$$

for smooth functions. Delta functions in position space, $\delta(x)$, remain subordinated to the usual Lebesgue measure. Similar convention is used for the frequency variables (dual variables to the time) that will always be denoted by α :

$$d\alpha := \frac{d_{\text{Leb}} \alpha}{2\pi} \quad \text{for all one dimensional frequency variables}$$

and to the delta functions involving α -variables.

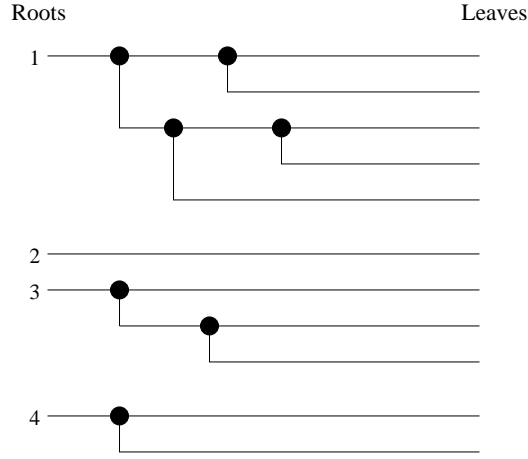


Figure 2: Example of forest in $\mathcal{G}_{n,k}$ with $n = 7$ and $k = 4$

numbers. They are given by the closed formula

$$C_n = \frac{1}{n+1} \binom{2n}{n},$$

and can be estimated by $C_n \leq 4^n$.

For $k \geq 1$, $n \geq 1$, we consider forests consisting of k rooted, marked, binary trees, G_1, G_2, \dots, G_k , so that the total number of (internal) vertices is n . We assume that the trees, i.e. their roots, are labeled; permutations of the trees result in inequivalent forests. The set of such forests will be denoted by $\mathcal{G}_{n,k}$. In Fig. 2, we draw an example of a graph in $\mathcal{G}_{7,4}$.

Note that the number of inequivalent forests in $\mathcal{G}_{n,k}$ is given by

$$\sum_{(n_1, \dots, n_k): \sum_{i=1}^k n_i = n} C_{n_1} C_{n_2} \dots C_{n_k}$$

where the summation runs over all k -tuples of nonnegative integers that add up to n . This number can be bounded by

$$|\mathcal{G}_{n,k}| \leq 4^n \cdot \binom{n+k-1}{k-1} \leq 2^{3n+k}. \quad (3.14)$$

Again, for $G \in \mathcal{G}_{n,k}$, we will denote by $V(G)$ the set of the vertices of G , by $E(G)$ the set of edges, by $\text{Int}(G)$, and $\text{Ext}(G)$ the sets of internal and, respectively, external edges. Moreover, $R(G)$ and $L(G)$ will be used for the set of roots (there are k roots in each forest), and for the set of leaves (there are $n+k$ leaves) of G , respectively. The vertices in $V(G)$ are again partially ordered by their succession towards the roots: for any $v, v' \in V(G)$ within the same tree we have $v \prec v'$ if v lies on the (unique) route from v' to the root of the tree. There is no order relation between vertices in different trees.

3.1.2 Quantum (Feynman) Graphs

We construct quantum Feynman graphs starting from the classical graphs. For any $G \in \mathcal{G}_{n,k}$ and $\sigma = \{\sigma_v \in \{\pm 1\} : v \in V(G)\}$ we define a Feynman graph, $\Gamma = \Gamma(G, \sigma)$, as follows: We double each edge of G and equip them with an opposite orientation (arrows). An edge is called outward

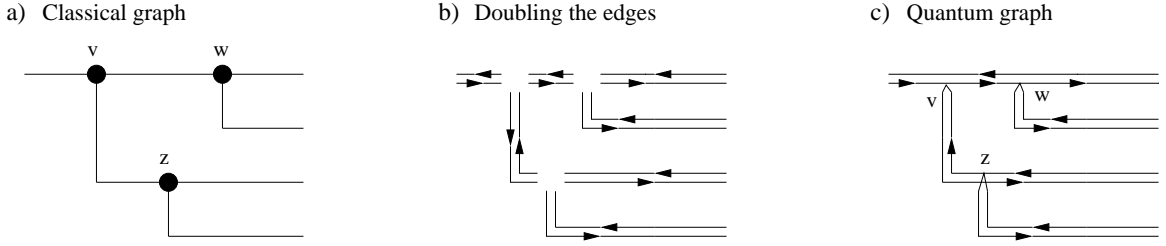


Figure 3: From $\mathcal{G}_{n,k}$ to $\mathcal{F}_{n,k}$

if its orientation points away from the root, otherwise it is called inward. At any vertex of G we define the new vertex of the six edges of Γ involved as follows. For $\sigma_v = 1$, the outward father-edge is joined with both edges of the unmarked son-edge and with the outward edge of the marked son-edge; this creates a vertex of Γ with four edges. The inward father-edge is joined with the inward edge of the marked son-edge and we consider it as a simple continuation, removing the (virtual) vertex. Analogously, if $\sigma_v = -1$, the inward father-edge is joined with both edges of the unmarked son-edge and with the inward edge of the marked son-edge. The outward father-edge is joined with the outward edge of the marked son-edge (and we consider it as a simple continuation). In Fig. 3 we illustrate this procedure with an example: given the graph $G \in \mathcal{G}_{3,1}$ in a), we first double each edge of G and equip the new edges with opposite orientation in b). Then we define the new vertices: for example, if $(\sigma_v, \sigma_w, \sigma_z) = (1, 1, -1)$ we obtain the Feynman graph in drawn in c). We denote by $\mathcal{F}_{n,k}$ the set of all quantum Feynman graphs constructed from classical graphs in $\mathcal{G}_{n,k}$. Note that graphs in $\mathcal{F}_{n,k}$ which are topologically equivalent are identified and counted only once (taking into account however that, as for classical graphs, the roots are ordered, and permutation of the roots leads to a different graph). In particular, this implies that the representation of $\Gamma \in \mathcal{F}_{n,k}$ as $\Gamma = \Gamma(G, \sigma)$, for some $G \in \mathcal{G}_{n,k}$ is, in general, not unique. The ambiguity comes from the fact that although the vertices of each component of G are partially ordered (and so are the vertices of each component of Γ), the order $v \prec v'$ in the classical graph is lost in the graph Γ if v and v' are assigned to different components of Γ . Therefore two different G or σ may lead to identical Feynman graphs (see Fig. 4: the Feynman graphs a) and b) are the same element of $\mathcal{F}_{3,1}$, but they are obtained from two different classical graphs in c) and d)).

By construction, graphs in $\mathcal{F}_{n,k}$ have n vertices, $2k + 3n$ edges, $2k$ roots, $2(n + k)$ leaves, and thus $4k + 2n$ external edges (trivial edges, which are at the same time roots and leaves are counted twice). The set of vertices of Γ is denoted by $V(\Gamma)$, the set of edges by $E(\Gamma)$, the set of roots by $R(\Gamma)$, the set of leaves by $L(\Gamma)$, the external edges (roots and leaves) are $\text{Ext}(\Gamma)$ and the internal edges are denoted by $\text{Int}(\Gamma)$. The vertices of Γ , $V(\Gamma)$, have four adjacent edges, two incoming and two outgoing. An edge e is called outgoing w.r.t. an adjacent vertex v if the arrow of e points away from v , incoming otherwise (note that the concept of incoming/outgoing is relative to the adjacent vertex and it does not coincide with the concept of inward/outward which is solely a property of the edge). For $e \in E(\Gamma)$ and $v \in V(\Gamma)$, the notation $e \in v$ indicates that the edge e is adjacent to the vertex v . For $e \in E(\Gamma)$, we also introduce the notation $\tau_e = 1$ if e is outward and $\tau_e = -1$ if e is inward. Due to the fact that they are ordered in the classical graphs, roots can be labeled. Since roots are paired (the natural pairing is inherited by the classical through the doubling), we will label every pair of roots by a map $\pi_1 : R(\Gamma) \rightarrow \{1, \dots, k\}$ (the label 1 applies to the two roots forming the first pair from the top, and so on). Similarly to the classical graphs, the fact that each component of Γ has a root induces a partial ordering among the vertices of Γ ; this will be denoted by \prec . From

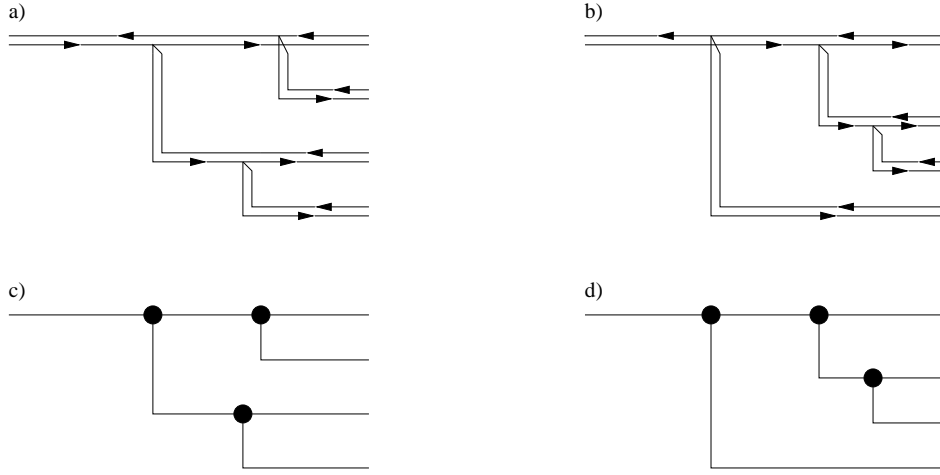


Figure 4: The graphs a) and b) are the same element of $\mathcal{F}_{3,1}$, but c) and d) are different elements of $\mathcal{G}_{3,1}$

(3.14), and from the construction of graphs in $\mathcal{F}_{n,k}$, it is clear that

$$|\mathcal{F}_{n,k}| \leq 2^n |\mathcal{G}_{n,k}| \leq 2^{4n+k}. \quad (3.15)$$

3.1.3 Amplitudes of Feynman Graphs

Each Feynman graph $\Gamma \in \mathcal{F}_{n,k}$ represents a map acting on density matrices; it encodes how the initial density matrix changes as the system undergoes a specific sequence of collisions. In this section we describe the kernel of this map, commonly known as the *amplitude* of the Feynman graph.

Given an arbitrary quantity x_e defined for $e \in E(\Gamma)$, and a vertex $v \in V(\Gamma)$, we will use the notation $\sum_{e \in v} \pm x_e$ to indicate that x_e is summed with a plus sign if the edge e is incoming (w.r.t v) while it is summed with a minus sign if e is outgoing.

For any $\Gamma \in \mathcal{F}_{n,k}$, we choose a family $\boldsymbol{\eta} = \{\eta_e\}_{e \in E(\Gamma)}$, with the property $\eta_e > 0$ for all $e \in E(\Gamma)$, and such that, at every vertex $v \in V(\Gamma)$,

$$\sum_{e \in v} \pm \tau_e \eta_e = 0. \quad (3.16)$$

(Recall that $\tau_e = 1$ for outward and $\tau_e = -1$ for inward edges.) It is easy to check that (3.16) is equivalent to the requirement that the η associated with any father-edge equals the sum of the η associated to its son-edges. In particular, the values of η on each of the $2(n+k)$ leaves uniquely determine η_e for all edges $e \in E(\Gamma)$ (and $\eta_e > 0$ is guaranteed for all $e \in E(\Gamma)$ if $\eta_e > 0$ for all leaves). For a given $\Gamma \in \mathcal{F}_{n,k}$, and a given family $\boldsymbol{\eta}$, we define the operator $K_{\Gamma,t,\boldsymbol{\eta}}$ (the amplitude of Γ at time t , and with regularization $\boldsymbol{\eta}$) through the kernel

$$\begin{aligned} & K_{\Gamma,t,\boldsymbol{\eta}}(\mathbf{q}_k, \mathbf{q}'_k; \mathbf{r}_{n+k}, \mathbf{r}'_{n+k}) \\ &= \frac{1}{(n+k)!} \sum_{\pi_2 \in S_{n+k}} \int \int_{\mathbb{R}} \prod_{e \in E(\Gamma)} d\alpha_e dp_e \prod_{e \in R(\Gamma)} \delta(p_e - q_{\pi_1(e)}^{\#e}) \prod_{e \in L(\Gamma)} \delta(p_e - r_{\pi_2(e)}^{\#e}) \\ & \times e^{-it \sum_{e \in R(\Gamma)} \tau_e (\alpha_e + i\tau_e \eta_e)} \prod_{e \in E(\Gamma)} \frac{1}{\alpha_e - p_e^2 + i\tau_e \eta_e} \prod_{v \in V(\Gamma)} \delta\left(\sum_{e \in v} \pm \alpha_e\right) \delta\left(\sum_{e \in v} \pm p_e\right), \end{aligned} \quad (3.17)$$

where $q_j^{\sharp e} = q_j$ if e points away from the root and $q_j^{\sharp e} = q_j'$ if e points toward the root and similar notation is used for the r variables. Here the map π_1 labeling the roots is fixed, since Γ is considered as a graph with labeled roots. The map $\pi_2 : L(\Gamma) \rightarrow \{1, \dots, n+k\}$, on the other hand, labels the leaves of Γ in such a way that the two elements of a leaf pair receives the same label. Since there is no natural ordering among the leaves, we sum over all possible labeling π_2 , and we divide the result by the number of labeling $(n+k)!$. Notice that $K_{\Gamma,t,\eta}$ maps operators on $L_s^2(\mathbb{R}^{3(n+k)})$ into operators on $L_s^2(\mathbb{R}^{3k})$ by the formula

$$\left(K_{\Gamma,t,\eta} \gamma^{(n+k)} \right) (\mathbf{q}_k; \mathbf{q}'_k) = \int K_{\Gamma,t,\eta}(\mathbf{q}_k, \mathbf{q}'_k; \mathbf{r}_{n+k}, \mathbf{r}'_{n+k}) \gamma^{(n+k)}(\mathbf{r}_{n+k}; \mathbf{r}'_{n+k}) d\mathbf{r}_{n+k} d\mathbf{r}'_{n+k}$$

where $\gamma^{(n+k)}$ is an operator on $L_s^2(\mathbb{R}^{3(n+k)})$ with the kernel $\gamma^{(n+k)}(\mathbf{r}_{n+k}; \mathbf{r}'_{n+k})$ in Fourier space (in our application, the density $\gamma^{(n+k)}$ will be symmetric w.r.t. permutations of the $n+k$ particles, and thus the sum over π_2 will disappear).

We will represent the fully expanded terms (3.12) in the Duhamel expansion (3.11) as a sum of contributions associated with Feynman graphs. More precisely, we will show in the next subsection that the term (3.12) can be rewritten as the sum of $K_{\Gamma,t,\eta} \gamma_0^{(k+m)}$ over all $\Gamma \in \mathcal{F}_{m,k}$ independently of the choice of η .

On the intuitive level, it is possible to recognize the origin of some of the factors in the formula (3.17) for the kernel $K_{\Gamma,t,\eta}$. The appearance of the one-dimensional variables α_e and the propagators $(\alpha_e - p_e^2 + i\tau_e \eta_e)^{-1}$, for example, derives from the free evolution $e^{-it\tau_e p_e^2}$, expressed as

$$e^{-it\tau_e p_e^2} = (i\tau_e) \int_{\mathbb{R}} d\alpha_e \frac{e^{-it\tau_e(\alpha_e + i\tau_e \eta_e)}}{\alpha_e - p_e^2 + i\tau_e \eta_e}. \quad (3.18)$$

The presence of the factor $\delta(\sum_{e \in v} \pm p_e)$ (conservation of momentum at every vertex), on the other hand, is due to the translation invariance of the interaction, and it just reproduces the non-trivial delta-function in the kernel of the operators $B^{(k)}$ in momentum space (see the two delta-function with four momenta in their arguments in the last line of (3.10)). Finally, one can understand the presence of the factors $\delta(\sum_{e \in v} \pm \alpha_e)$ as the result of the integration over the constrained time-variables, after all the free evolutions $e^{\pm it p_e^2}$ have been rewritten in terms of resolvents according to (3.18) (but there are linear constraints among the times, e.g. the time arguments of the free evolutions in (3.12) sum up to t).

The fact that (3.18) holds true independently of $\eta_e > 0$ already suggests that the kernel (3.17) is actually independent of the choice of the family $\eta = \{\eta_e\}_{e \in E(\Gamma)}$. This fact can be proven rigorously by noticing that, because of the condition that at each vertex the η associated with the father-edge equals the sum of the η 's associated with the son-edges, the only independent η 's are those associated with the leaves of Γ . It is moreover clear that, for every fixed $\bar{e} \in L(\Gamma)$, $K_{\Gamma,t,\eta}$, as a function of $\eta_{\bar{e}}$, has an analytic extension in the whole half plane $\text{Re } \eta_{\bar{e}} > 0$. It is therefore sufficient to show that $K_{\Gamma,t,\eta}$ is constant in a small neighborhood of a given value $\eta_{\bar{e}}$ with $\text{Re } \eta_{\bar{e}} > 0$ (while all the other $\eta_e > 0$, $\bar{e} \neq e \in L(\Gamma)$, are kept constant). After replacing $\eta_{\bar{e}}$ by $\eta_{\bar{e}} + \xi$, we can shift the α_e variables as follows. For $e \in E(\Gamma)$ on the route from \bar{e} to the unique root connected to \bar{e} , we shift $\alpha_e \rightarrow \tilde{\alpha}_e = \alpha_e + i\tau_e \xi$, while for all other $e \in E(\Gamma)$ we leave $\tilde{\alpha}_e = \alpha_e$. Here we assume that $|\text{Re } \xi| < \min_{e \in E(\Gamma)} \text{Re } \eta_e$ to avoid deforming the α_e integral contour through the pole at $\alpha_e = p_e^2 - i\tau_e \eta_e$. Then we can see that the integral remains unchanged. This follows from observing that for all v

$$\sum_{e \in v} \pm \alpha_e = \sum_{e \in v} \pm \tilde{\alpha}_e$$

thanks to the definition of τ_e and the sign convention of the summation. This proves the independence of (3.17) from the family $\boldsymbol{\eta}$. In particular we can use the simpler notation $K_{\Gamma,t}$.

For a given $\Gamma \in \mathcal{F}_{n,k}$, we denote by $R_1(\Gamma)$ the set of trivial roots of Γ (a trivial root is a root which is also a leaf). Moreover we denote by $R_2(\Gamma) = R(\Gamma) \setminus R_1(\Gamma)$, $L_2(\Gamma) = L(\Gamma) \setminus R_1(\Gamma)$ and $E_2(\Gamma) = E(\Gamma) \setminus R_1(\Gamma)$ the sets of non-trivial roots, of non-trivial leaves, and, respectively, of non-trivial edges. Note that, on the r.h.s. of (3.17), the integration over the frequency variables α_e , for $e \in R_1(\Gamma)$, reduces exactly to an integral like the one on the r.h.s. of (3.18). One can prove that these integrals are the only ones in (3.17) which are not absolutely convergent. In these notes we neglect this side issue of non absolute convergence of these special α -integrals.

Note that in (3.17) there are $|R_2| + |L_2| + |V| = 4k + 3n - 2k_1$ momentum delta-functions involving p_e variables and only $|E_2| = 2k + 3n - k_1$ momentum integration variables. Together with the k_1 direct delta-functions related to the roots in $R_1(\Gamma)$, we see that the kernel $K_{\Gamma,t,\boldsymbol{\eta}}$ contains $2k$ delta-functions among its $2n + 4k$ variables. This corresponds to the $2k$ momentum conservation in each of the $2k$ components of Γ . It can easily be seen that all the p_e momenta can indeed be uniquely expressed through the external momenta $\mathbf{r}_{n+k}, \mathbf{r}'_{n+k}, \mathbf{q}_k, \mathbf{q}'_k$. In particular, the dp_e integrations are all well defined and they correspond to substituting the appropriate linear combinations of the external momenta into p_e .

The amplitudes $K_{\Gamma,t}$ will describe the terms (3.12) of the summation in (3.11). The input of the error term (3.13) is somewhat different; it involves the density matrix $\gamma^{(k+n)}$ at an intermediate time s_n and the last free evolution is absent. We thus introduce a slight modification of the amplitude $K_{\Gamma,t}$ to represent this term. We define the operator $L_{\Gamma,t}$, for $\Gamma \in \mathcal{F}_{n,k}$, $n, k \geq 1$, through

$$\begin{aligned} L_{\Gamma,t}(\mathbf{q}_k, \mathbf{q}'_k; \mathbf{r}_{n+k}, \mathbf{r}'_{n+k}) &:= \frac{1}{(n+k)!} \sum_{\pi_2 \in S_{n+k}} \sum_{\bar{v} \in M(\Gamma)} \sigma_{\bar{v}} \int \int_{\mathbb{R}} \prod_{\substack{e \in E(\Gamma) \\ e \notin S_{\bar{v}}}} d\alpha_e \prod_{e \in E(\Gamma)} dp_e \\ &\times \prod_{e \in R(\Gamma)} \delta(p_e - q_{\pi_1(e)}^{\#e}) \prod_{e \in L(\Gamma)} \delta(p_e - r_{\pi_2(e)}^{\#e}) \prod_{v \in V(\Gamma)} \delta\left(\sum_{e \in v} \pm p_e\right) \\ &\times \exp\left(-it \sum_{e \in R(\Gamma)} \tau_e(\alpha_e + i\tau_e \eta_e)\right) \prod_{\substack{e \in E(\Gamma) \\ e \notin S_{\bar{v}}}} \frac{1}{\alpha_e - p_e^2 + i\tau_e \eta_e} \prod_{\bar{v} \neq v \in V(\Gamma)} \delta\left(\sum_{e \in v} \pm \alpha_e\right), \end{aligned} \quad (3.19)$$

where $M(\Gamma) \subset V(\Gamma)$ is the set of maximal vertices of Γ , that is the set of all $v \in V(\Gamma)$ so that there exists no \tilde{v} with $\tilde{v} \succ v$ (recall that \prec was the partial order on $V(\Gamma)$ induced by the distance to the root). Moreover, for a vertex $v \in V(\Gamma)$, we denote by S_v the set of son-edges of v (clearly, $R(\Gamma) \cap S_v = \emptyset$, for any $v \in V(\Gamma)$), and we set

$$\sigma_v = \sum_{e \in S_v} \tau_e,$$

i.e., $\sigma_v = 1$ if of the four edges adjacent to v , three are outward and one is inward, $\sigma_v = -1$ otherwise.

In other words, $L_{\Gamma,t}$ is defined so that there are no propagators associated with the son-edges of a $\bar{v} \in M(\Gamma)$. The variables $\boldsymbol{\eta} = \{\eta_e\}_{e \in E(\Gamma)}$ are chosen as in (3.16): although η_e , for $e \in S_{\bar{v}}$, does not appear directly in (3.19), the value of the η -variable associated to the father-edge of \bar{v} depends on it. Analogously to $K_{\Gamma,t}$, it can be proven that $L_{\Gamma,t}$ is independent of the choice of $\boldsymbol{\eta}$.

With these definition of the amplitudes $K_{\Gamma,t}$ and $L_{\Gamma,t}$, we have the following theorem.

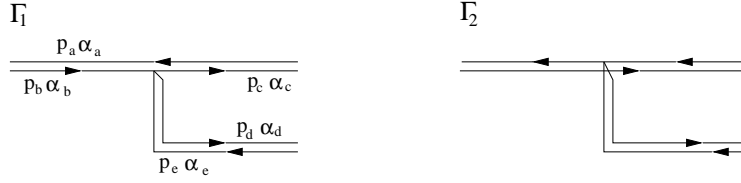


Figure 5: The two Feynman graphs in $\mathcal{F}_{1,1}$

Theorem 3.2. Fix $k, n \geq 1$. Then, for any $\gamma_0^{(k+n)}$ that is symmetric with respect to permutations (in the sense of (3.5)), we have

$$\begin{aligned} & \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}_0^{(k)}(t-s_1) B^{(k)} \dots \mathcal{U}_0^{(k+n-1)}(s_{n-1}-s_n) B^{(k+n-1)} \mathcal{U}_0^{(k+n)}(s_n) \gamma_0^{(k+n)} \\ &= \sum_{\Gamma \in \mathcal{F}_{n,k}} K_{\Gamma,t} \gamma_0^{(k+n)}. \end{aligned} \quad (3.20)$$

For $n = 0, k \geq 1$ we have

$$\mathcal{U}_0^{(k)}(t) \gamma_0^{(k)} = \sum_{\Gamma \in \mathcal{F}_{0,k}} K_{\Gamma,t} \gamma_0^{(k)} \quad (3.21)$$

where the summation is only for the trivial graph. Moreover, for any fixed $k, n \geq 1$, if $\gamma_t^{(k+n)} \in C([0, T]; \mathcal{H}_k)$ is symmetric with respect to permutations for all $t \in [0, T]$, we have

$$\begin{aligned} & \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}_0^{(k)}(t-s_1) B^{(k)} \dots \mathcal{U}_0^{(k+n-1)}(s_{n-1}-s_n) B^{(k+n-1)} \gamma_{s_n}^{(k+n)} \\ &= -i \sum_{\Gamma \in \mathcal{F}_{n,k}} \int_0^t ds L_{\Gamma,t-s} \gamma_s^{(k+n)} \end{aligned} \quad (3.22)$$

for all $t \in [0, T]$.

The precise proof of Theorem 3.2 can be found in [6, Section 9]; here we only show it in the case $n = 1, k = 1$. Already this very simple case is useful to understand how the structure of the operators $K_{\Gamma,t}$ emerges from the Duhamel expansion. We thus consider (3.20) for $n = 1, k = 1$, i.e.,

$$\int_0^t ds \mathcal{U}_0^{(1)}(t-s) B^{(1)} \mathcal{U}_0^{(2)}(s) \gamma_0^{(2)} = K_{\Gamma_1,t} \gamma_0^{(2)} + K_{\Gamma_2,t} \gamma_0^{(2)}, \quad (3.23)$$

where Γ_1 and Γ_2 are the two elements of $\mathcal{F}_{1,1}$ drawn in Figure 5.

By definition of the map $B^{(1)}$, the l.h.s. of (3.23) is given by

$$-i \int_0^t ds \mathcal{U}_0^{(1)}(t-s) \text{Tr}_2 \delta(x_1 - x_2) \mathcal{U}_0^{(2)}(s) \gamma_0^{(2)} + i \int_0^t ds \mathcal{U}_0^{(1)}(t-s) \text{Tr}_2 \mathcal{U}_0^{(2)}(s) \gamma_0^{(2)} \delta(x_1 - x_2). \quad (3.24)$$

We now show that the first term coincides with the contribution of the Feynman diagram Γ_1 (analogously one can prove that the second term equals the contribution of Γ_2).

Recall that $K_{\Gamma_1,t} \in \mathcal{F}_{1,1}$ maps operators on $L_s^2(\mathbb{R}^3 \times \mathbb{R}^3)$ into operators on $L_s^2(\mathbb{R}^3)$. In momentum space, the kernel of $\gamma_0^{(2)}$ has four variables, $\gamma_0^{(2)}(p_c, p_d; p_a, p_e)$. These are the momentum variables on the right hand side of Feynman graph Γ_1 (here c, d, a, e label the leave-edges). The resulting

operator, $K_{\Gamma,t}\gamma_0^{(2)}$, acts on $L_s^2(\mathbb{R}^3)$, and its kernel has two variables, $(p_b; p_a)$ represented on the l.h.s. of the Feynman graph (a, b label the roots of the graph).

The pairs of variables, $(p_c; p_a)$ and $(p_d; p_e)$, in the argument of $\gamma_0^{(2)}$ correspond to the input and output of the first and the second variable of the $L_s^2(\mathbb{R}^3 \times \mathbb{R}^3)$ space. Similarly, p_b is the input and p_a is the output variable of the resulting operator $K_{\Gamma,t}\gamma_0^{(2)}$: arrows in the Feynman graph pointing away from the roots indicate input-variables, arrows pointing towards the roots indicate output-variables of the corresponding density matrix.

For any kernel $\gamma^{(2)}(p_1, p_2; p'_1, p'_2)$, the free time evolution in momentum space acts as follows

$$\left(\mathcal{U}_0^{(2)}(s)\gamma^{(2)}\right)(p_1, p_2; p'_1, p'_2) = e^{-is(p_1^2+p_2^2)} e^{is([p'_1]^2+[p'_2]^2)} \gamma_0^{(2)}(p_1, p_2; p'_1, p'_2).$$

The multiplication by $\delta(x_1 - x_2)$ corresponds to convolution with $\delta(p_1 + p_2)$ in Fourier space,

$$\left(\delta(x_1 - x_2)\gamma^{(2)}\right)(p_1, p_2, p'_1, p'_2) = \int dr \gamma^{(2)}(r, p_1 - r + p_2; p'_1, p'_2),$$

thus after taking the partial trace, we have

$$\left[\text{Tr}_2\left(\delta(x_1 - x_2)\gamma^{(2)}\right)\right](p_1; p'_1) = \int drdq \gamma^{(2)}(r, p_1 - r + q; p'_1, q).$$

Applying these elementary steps for the first term of (3.24), we get

$$\begin{aligned} & \left[-i \int_0^t ds \mathcal{U}_0^{(1)}(t-s) \text{Tr}_2 \delta(x_1 - x_2) \mathcal{U}_0^{(2)}(s) \gamma_0^{(2)} \right] (p_b; p_a) \\ &= -i \int_0^t ds e^{-i(t-s)p_b^2} e^{i(t-s)p_a^2} \int dqdr \left(\mathcal{U}_0^{(2)}(s)\gamma_0^{(2)}\right)(r, p_b - r + q; p_a, q) \\ &= -i \int_0^t ds e^{-i(t-s)p_b^2} e^{i(t-s)p_a^2} \int dp_c dp_d dp_e \delta(p_b + p_e - p_c - p_d) \left(\mathcal{U}_0^{(2)}(s)\gamma_0^{(2)}\right)(p_c, p_d; p_a, p_e). \end{aligned} \tag{3.25}$$

In the last step we changed variables, which now correspond to the variables in the Feynman graph. In particular, the vertex involves a delta function expressing the Kirchoff law (conservation of momentum at the vertex).

Now we show how the time integrals of the propagators can be expressed in terms of auxiliary α -integrals and resolvents. Neglecting the momentum integrations, the last term in (3.25) contains the following propagators:

$$\Pi := \int_0^t ds e^{-i(t-s)p_b^2} e^{i(t-s)p_a^2} e^{-is(p_c^2+p_d^2)} e^{is(p_a^2+p_e^2)}.$$

Using the identity (3.18) for the propagator of each momentum variable, we obtain

$$\Pi = i \int_0^t ds \int_{\mathbb{R}} \frac{d\alpha_a d\alpha_b d\alpha_c d\alpha_d d\alpha_e e^{it(\alpha_a - i\eta_a) - i(t-s)(\alpha_b + i\eta_b) - is(\alpha_c + i\eta_c) - is(\alpha_d + i\eta_d) + is(\alpha_e - i\eta_e)}}{(\alpha_a - p_a^2 - i\eta_a)(\alpha_b - p_b^2 + i\eta_b)(\alpha_c - p_c^2 + i\eta_c)(\alpha_d - p_d^2 + i\eta_d)(\alpha_e - p_e^2 - i\eta_e)}$$

(In our example, $\tau_b = \tau_c = \tau_d = 1$ and $\tau_a = \tau_e = -1$ by the definition of τ). Notice that the time integration can be extended to $s \in (-\infty, \infty)$, since all η 's are positive and by residue calculation

$$\int_{\mathbb{R}} \frac{d\alpha e^{-is(\alpha+i\eta)}}{\alpha - p^2 + i\eta} = 0$$

if $s < 0$ and $\eta > 0$.

Using that $\eta_b = \eta_c + \eta_d + \eta_e$ and performing the ds integration, we obtain the delta function in the α variables:

$$\Pi = i \int_{\mathbb{R}} \frac{e^{it(\alpha_a - i\eta_a)} e^{-it(\alpha_b + i\eta_b)} d\alpha_a d\alpha_b d\alpha_c d\alpha_d d\alpha_e \delta(\alpha_b - \alpha_c - \alpha_d + \alpha_e)}{(\alpha_a - p_a^2 - i\eta_a)(\alpha_b - p_b^2 + i\eta_b)(\alpha_c - p_c^2 + i\eta_c)(\alpha_d - p_d^2 + i\eta_d)(\alpha_e - p_e^2 - i\eta_e)}$$

(recall that the δ -function in the α -variables is defined w.r.t. to the measure $d\alpha = d_{\text{Leb}}\alpha/2\pi$).

Combining this formula with (3.25), we arrive at

$$\begin{aligned} & \left[-i \int_0^t ds \mathcal{U}_0^{(1)}(t-s) \text{Tr}_2 \delta(x_1 - x_2) \mathcal{U}_0^{(2)}(s) \gamma_0^{(2)} \right] (p_b; p_a) \\ &= \int dp_c dp_d dp_e \delta(p_b + p_e - p_c - p_d) \gamma_0^{(2)}(p_c, p_d; p_a, p_e) \\ & \quad \times \int e^{it(\alpha_a - i\eta_a)} e^{-it(\alpha_b + i\eta_b)} \left[\prod_{j=a,b,c,d,e} \frac{d\alpha_j}{\alpha_j - p_j^2 + i\tau_j \eta_j} \right] \delta(\alpha_b + \alpha_e - \alpha_c - \alpha_d) \end{aligned} \quad (3.26)$$

which is exactly the action of the kernel $K_{\Gamma,1,t}$ (as defined in (3.17)) on $\gamma_0^{(2)}$.

3.2 Bounds for Amplitudes of Feynman Graphs

For brevity, we introduce the notation

$$\langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle := \int d\mathbf{q}_k d\mathbf{q}'_k d\mathbf{r}_{n+k} d\mathbf{r}'_{n+k} J^{(k)}(\mathbf{q}_k; \mathbf{q}'_k) K_{\Gamma,t}(\mathbf{q}_k, \mathbf{q}'_k; \mathbf{r}_{n+k}, \mathbf{r}'_{n+k}) \gamma^{(n+k)}(\mathbf{r}_{n+k}, \mathbf{r}'_{n+k})$$

for an operator $J^{(k)} \in \mathcal{K}_k$ with kernel $J^{(k)}(\mathbf{q}_k; \mathbf{q}'_k)$ expressed in momentum space. We also define $\langle J^{(k)}, L_{\Gamma,t} \gamma^{(n+k)} \rangle$ similarly. In the next theorem we show how to bound $\langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle$ and $\langle J^{(k)}, L_{\Gamma,t} \gamma^{(n+k)} \rangle$ (for $\Gamma \in \mathcal{F}_{n,k}$ and for an observable $J^{(k)}$ decaying sufficiently fast in momentum space) in terms of the \mathcal{H}_{n+k} -norm of $\gamma^{(n+k)}$. By Theorem 3.2, and by the a-priori estimates (3.3), this will allow us to control the terms (3.12) and (3.13) in the Duhamel expansion (3.11).

Theorem 3.3. *Fix $k \geq 1$. For any $n \geq 1$, suppose $\gamma^{(n+k)}$ is non-negative and symmetric with respect to permutations (in the sense of (3.5)). Assume $0 < t \leq 1$. Choose $J^{(k)} \in \mathcal{K}_k$, symmetric with respect to permutations and with*

$$|J^{(k)}(\mathbf{p}_k; \mathbf{p}'_k)| \leq C \prod_{j=1}^k \frac{1}{\langle p_j \rangle^3 \langle p'_j \rangle^3}. \quad (3.27)$$

Then we have

$$\left| \langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle \right| \leq C^n \text{Tr} (1 - \Delta_1) \dots (1 - \Delta_{n+k}) \gamma^{(n+k)} \quad (3.28)$$

for every $n \geq 0$. Moreover for every $n \geq 10 + k/2$, we have

$$\left| \langle J^{(k)}, L_{\Gamma,t} \gamma^{(n+k)} \rangle \right| \leq C^n t^{\frac{n}{4}} \text{Tr} (1 - \Delta_1) \dots (1 - \Delta_{n+k}) \gamma^{(n+k)}. \quad (3.29)$$

Note that the constant C in (3.27) depends on k (which is fixed), and so do the constants on the r.h.s. of (3.28) and (3.29). The restriction $t \leq 1$ plays no significant role in the theorem; it simplifies the proof in a trivial manner. It is also possible to obtain a t -power in (3.28) but it is not needed. In fact, according to Theorem 3.2, (3.28) will be applied to control the fully expanded terms (3.12) in the Duhamel series (3.11). For the proof of the uniqueness of the solution to the infinite hierarchy

(3.2), it will be sufficient to show that these terms are finite. On the other hand, (3.29) will be applied to control the last term (3.13) in (3.11), involving a density matrix at an intermediate time s_n . In this case it is not enough to show the finiteness of the contributions; we also need to prove that they are small (for sufficiently small t). Note also that the power $n/4$ in (3.29) is not optimal and we do not aim at the optimal t -dependence. Naively $L_{\Gamma,t}$ contains an n -fold time integration, so it should behave as t^n , but we remark that part of the time integration is used to fight against the singularity of the interaction (we use the smoothing effect of the free Schrödinger evolution). In this sense, the estimates (3.28), (3.29) can be viewed as Strichartz type inequalities in the many particle setting. Recall that the Strichartz inequality states that

$$\int_0^t \|e^{is\Delta} f\|_p^r ds \leq C \|f\|_2^r, \quad f \in L^2(\mathbb{R}^3),$$

for r, p satisfying $\frac{2}{r} + \frac{3}{p} = \frac{3}{2}$ and $2 \leq r \leq \infty$. This inequality implies that

$$\int_0^t \|e^{is\Delta} f\|_p ds \leq C t^{1-\frac{1}{r}} \|f\|_2,$$

which means that the free evolution smoothes out possible singularities of f at the expense of reducing the t -power.

Another form of the Strichartz inequality asserts that

$$\left\| \int_0^t ds e^{i(t-s)\Delta} f_s \right\|_{L_t^r L_x^p} \leq C \|f_t\|_{L_t^{r'} L_x^{p'}}, \quad f_t = f_t(x),$$

where $L_t^r L_x^p$ denotes the space $L^r(\mathbb{R}; L^p(\mathbb{R}^3))$ and the positive exponents p, r, p', r' satisfy

$$\frac{1}{p} + \frac{2}{3r} = \frac{1}{2}, \quad r \geq 2; \quad \frac{1}{p'} + \frac{2}{3r'} = \frac{7}{6}, \quad r' \leq 2. \quad (3.30)$$

Once again, this estimate quantifies the smoothing effect of the free evolution operator. The price of reducing the t -power is now expressed in terms of the change from the L^r norm to the $L^{r'}$ norm in the t variable.

The kernels $K_{\Gamma,t}$ and $L_{\Gamma,t}$, though defined in Green function form, actually have representations in terms of n -fold time integrations like the formulae appearing in (3.12) and (3.13) (with the operators $B^{(k+j)}$ defined in (3.9)). If we replace the δ -function (which came from the two-body interaction) in the definition of $B^{(k+j)}$ by a smooth function, the correct t dependence in (3.29) would be t^n (at least for small t). The estimate (3.29) states that the δ interaction is allowed if we give up some power in t — in the same spirit as in the Strichartz inequality.

Each integration step on the left hand side of (3.12) and (3.13) actually involves a time integration and a space integration via the partial trace in $B^{(k+j)}$. It would therefore be natural to perform an iterative estimate involving subsequent one-particle space-time dispersive bounds. Unfortunately, we were unable to find an appropriate one-particle scheme to implement this approach. Our method is much more complicated and it involves tracking several singularity structures of the density matrices in the integration step.

One reason to use the Feynman diagram representation is to obtain estimates with correct n dependence. From the summation in the definition of $B^{(m)}$ (see (3.9)), the number of terms on the l.h.s of (3.13) is $2^n k(k+1) \cdots (n+k-1) \sim n!$. This factorial can be exactly compensated by the multiple time integration,

$$\int_0^t ds_1 \int_0^{s_1} ds_2 \cdots \int_0^{s_{n-1}} ds_n = \frac{t^n}{n!}, \quad (3.31)$$

but only if the L^1 -norm is used in time. Higher L^r -norms (in the time integration) result in a partial loss of the $1/n!$ in (3.31) and thus the summation over n will not converge for any t .

For this reason, we developed a new method, based on the expansions (3.12) and (3.13) in terms of Feynman graphs. Our graphical representation, among its other merits, reduces the number of terms in the expansion from $n!$ to C^n (see (3.15)). This combinatorial reduction stems from the recombination of several contributions (in particular this is the reason why Feynman graphs are only partially ordered, while times in (3.12) and (3.13) are totally ordered; we present a simple example showing how the resummation of different contributions to (3.12) and (3.13) leads to the removal of the ordering in the Feynman graphs in Appendix B). The dispersive properties of $e^{it\Delta}$ are now captured by the decay properties of the integrands in the kernels $K_{\Gamma,t}$, $L_{\Gamma,t}$ (see (3.17), (3.19)). These multiple integrations can be successively performed yielding the bounds (3.28) and (3.29). Our representation treats all smoothing effects simultaneously and thus exploits an additional decay which we were not able to obtain with one-particle methods. We do not know if it is possible to design a one-particle inequality similar to the Strichartz inequality to give a short proof for the estimates (3.28) and (3.29). We however refer to a recent work by Klainerman and Machedon, see [13], where this attractive idea was implemented to prove uniqueness of the infinite hierarchy in a different class of densities. Unfortunately, it is not clear whether the a-priori bounds used in [13] are satisfied by limit points of the sequence of marginal densities $\gamma_{N,t}^{(k)}$.

Before discussing the main ideas used in the proof of Theorem 3.3, we show how it can be applied, together with Theorem 3.2, to prove Theorem 3.1.

Proof of Theorem 3.1. Suppose that $\Gamma_{1,t} = \{\gamma_{1,t}^{(k)}\}_{k \geq 1}$ and $\Gamma_{2,t} = \{\gamma_{2,t}^{(k)}\}_{k \geq 1}$ are two solutions in $\bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ of the infinite hierarchy (3.2), such that, for $j = 1, 2$, $\gamma_{j,t}^{(k)}$ is non-negative, symmetric w.r.t. permutations and satisfies $\|\gamma_{j,t}^{(k)}\|_{\mathcal{H}_k} \leq C^k$ (see (3.3) for the definition of the norm $\|\cdot\|_{\mathcal{H}_k}$), for all $k \geq 1$ and $t \in [0, T]$, and such that $\gamma_{1,0}^{(k)} = \gamma_{2,0}^{(k)}$, for all $k \geq 1$. We want to prove that $\Gamma_{1,t} = \Gamma_{2,t}$, for every $t \in [0, T]$. To this end we will prove that, for every fixed $k \geq 1$, $\gamma_{1,t}^{(k)} = \gamma_{2,t}^{(k)}$ for every $t \in [0, T]$ (as elements of \mathcal{H}_k). By a simple approximation argument it is then sufficient to prove that

$$\text{Tr } J^{(k)} \left(\gamma_{1,t}^{(k)} - \gamma_{2,t}^{(k)} \right) = 0 \quad (3.32)$$

for all $J^{(k)}$ in a dense subset of the dual space of \mathcal{H}_k . Since we assumed $\gamma_{1,t}^{(k)}$ and $\gamma_{2,t}^{(k)}$ to be symmetric w.r.t. permutations, it is enough to consider permutation symmetric observables $J^{(k)}$. We will show (3.32) for all permutation symmetric $J^{(k)}$ with kernel $J^{(k)}(\mathbf{p}_k; \mathbf{p}'_k)$ (in momentum space) satisfying

$$|J^{(k)}(\mathbf{p}_k; \mathbf{p}'_k)| \leq C \prod_{j=1}^k \frac{1}{\langle p_j \rangle^3 \langle p'_j \rangle^3}.$$

For fixed $k \geq 1$ we can expand $\gamma_{j,t}^{(k)}$ in a Duhamel-type expansion as in (3.11). With Theorem 3.2 we can identify each term in the expansion (3.11) as the sum of contributions of Feynman graphs. We obtain, for any n , that

$$\gamma_{j,t}^{(k)} = \mathcal{U}_0^{(k)}(t) \gamma_{j,0}^{(k)} + \sum_{m=1}^{n-1} \sum_{\Gamma \in \mathcal{F}_{m,k}} K_{\Gamma,t} \gamma_{j,0}^{(k+m)} - i \sum_{\Gamma \in \mathcal{F}_{n,k}} \int_0^t ds L_{\Gamma,t-s} \gamma_{j,s}^{(k+n)} \quad (3.33)$$

for $j = 1, 2$. Multiplying with the observable $J^{(k)}$ and taking the trace we obtain

$$\mathrm{Tr} J^{(k)} \gamma_{j,t}^{(k)} = \langle J^{(k)}, \mathcal{U}_0^{(k)}(t) \gamma_{j,0}^{(k)} \rangle + \sum_{m=1}^{n-1} \sum_{\Gamma \in \mathcal{F}_{m,k}} \langle J^{(k)}, K_{\Gamma,t} \gamma_{j,0}^{(m+k)} \rangle - i \sum_{\Gamma \in \mathcal{F}_{n,k}} \int_0^t ds \langle J^{(k)}, L_{\Gamma,t-s} \gamma_{j,s}^{(n+k)} \rangle \quad (3.34)$$

for $j = 1, 2$. From Theorem 3.3, it follows that the terms in the sum over m are bounded in absolute value by $C^m \|\gamma_{j,0}^{(m+k)}\|_{\mathcal{H}_{m+k}}$, in particular they are finite. Since $\gamma_{1,0}^{(k+m)} = \gamma_{2,0}^{(k+m)}$ for every $m \geq 1$, when we take the difference between $\mathrm{Tr} J^{(k)} \gamma_{1,t}^{(k)}$ and $\mathrm{Tr} J^{(k)} \gamma_{2,t}^{(k)}$, the free evolution terms $\langle J^{(k)}, \mathcal{U}_0^{(k)} \gamma_{j,0}^{(k)} \rangle$ and all the terms in the sum over m disappear and it only remains to bound the contributions from the last term in (3.34). From Theorem 3.3, and since $|\mathcal{F}_{n,k}| \leq C^{n+k}$, we obtain, under the assumption that $t \leq 1$ and $n \geq 10 + k/2$,

$$\left| \mathrm{Tr} J^{(k)} \left(\gamma_{1,t}^{(k)} - \gamma_{2,t}^{(k)} \right) \right| \leq C^n \int_0^t ds (t-s)^{\frac{n}{4}} \left(\|\gamma_{1,s}^{(n+k)}\|_{\mathcal{H}_{k+n}} + \|\gamma_{2,s}^{(n+k)}\|_{\mathcal{H}_{k+n}} \right) \leq C^{n+k} t^{\frac{n}{4}}, \quad (3.35)$$

where we used that, by assumption, $\sup_{s \in [0, T]} \|\gamma_{j,s}^{(n+k)}\|_{\mathcal{H}_{n+k}} \leq C^{n+k}$ for $j = 1, 2$. Hence, if we choose $t < \min(1, (1/2C)^4)$ we conclude that

$$\left| \mathrm{Tr} J^{(k)} \left(\gamma_{1,t}^{(k)} - \gamma_{2,t}^{(k)} \right) \right| \leq C^k 2^{-n}. \quad (3.36)$$

Since $n \geq 1$ is arbitrary, this clearly proves (3.32) for every $t \leq \min(1, (1/2C)^4)$. The proof can then be iterated to show that $\gamma_{1,t}^{(k)} = \gamma_{2,t}^{(k)}$ for all $t \in [0, T]$. \square

3.2.1 Proof of Theorem 3.3

The goal of this section is to present, mostly on a heuristic level, the main ideas used in [6] to prove Theorem 3.3. We discuss here the proof of (3.28), the proof of (3.29) is similar.

From (3.17) (after integrating out the frequencies associated with the trivial roots in $R_1(\Gamma)$) we obtain that

$$\begin{aligned} \langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle &= \int d\mathbf{q}_k d\mathbf{q}'_k d\mathbf{r}_{n+k} d\mathbf{r}'_{n+k} J^{(k)}(\mathbf{q}_k; \mathbf{q}'_k) \gamma^{(n+k)}(\mathbf{r}_{n+k}, \mathbf{r}'_{n+k}) \\ &\times \prod_{e \in R_1(\Gamma) = L_1(\Gamma)} (-i\tau_e) e^{-it\tau_e (q_{\pi_1}^{\#e})^2} \delta(q_{\pi_1}^{\#e} - r_{\pi_2}^{\#e}) \\ &\times \int \prod_{e \in E_2(\Gamma)} d\alpha_e dp_e \prod_{e \in R_2(\Gamma)} \delta(p_e - q_{\pi_1}^{\#e}) \prod_{e \in L_2(\Gamma)} \delta(p_e - r_{\pi_2}^{\#e}) e^{-it \sum_{e \in R_2(\Gamma)} \tau_e (\alpha_e + i\tau_e \eta_e)} \\ &\times \prod_{e \in E_2(\Gamma)} \frac{1}{\alpha_e - p_e^2 + i\tau_e \eta_e} \prod_{v \in V(\Gamma)} \delta\left(\sum_{e \in v} \pm \alpha_e\right) \delta\left(\sum_{e \in v} \pm p_e\right). \end{aligned} \quad (3.37)$$

Compared with (3.17), π_2 is now a fixed labeling of the leaves; this is a consequence of the fact that the density $\gamma^{(n+k)}$ is symmetric w.r.t. permutations, and thus the value of the r.h.s. of (3.37) is independent of π_2 (this removes the factor $1/(n+k)!$ and the summation over π_2 in (3.17)).

Since $K_{\Gamma,t}$ is independent of the choice of the family $\boldsymbol{\eta} = \{\eta_e\}_{e \in \Gamma}$, we can fix $\eta_e = 1$ for every $e \in L(\Gamma)$; it follows that $1 \leq \eta_e \leq 2n + 1$ for all $e \in E(\Gamma)$. With this choice, and using (3.27) to

bound the kernel of the observable $J^{(k)}$, we find that the absolute value of the l.h.s. of (3.37) can be estimated by

$$\begin{aligned} \left| \langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle \right| &\leq C e^{Cnt} \int \prod_{e \in E(\Gamma)} dp_e \prod_{e \in E_2(\Gamma)} d\alpha_e \prod_{e \in E_2(\Gamma)} \frac{1}{\langle \alpha_e - p_e^2 \rangle} \prod_{e \in R(\Gamma)} \frac{1}{\langle p_e \rangle^3} \\ &\times \prod_{v \in V(\Gamma)} \delta\left(\sum_{e \in v} \pm \alpha_e\right) \delta\left(\sum_{e \in v} \pm p_e\right) \left| \gamma^{(n+k)}(\{p_e\}_{e \in L(\Gamma)}) \right|, \end{aligned} \quad (3.38)$$

where we introduced the notation $\langle x \rangle = (1 + x^2)^{1/2}$. In (3.38), when we assign the momenta of the leaves to be the arguments of $\gamma^{(k+n)}$ we have to respect the pairing; the momenta of paired leaves have to be paired arguments in the kernel of $\gamma^{(k+n)}$ (the variable p_j and p'_j are paired in $\gamma^{(k+n)}(\mathbf{p}_{k+n}; \mathbf{p}'_{k+n})$). Note that, because of the choice $\eta_e = 1$ for all $e \in L(\Gamma)$, we lost all the dependence on t in the integrals. In particular, the r.h.s. of (3.38) does not converge to zero as $t \rightarrow 0$; this is fine, because for the bound (3.28) we are not interested in the time dependence. To prove (3.29), on the other hand, we have to choose $\eta_e = 1/t$ for all $e \in L(\Gamma)$, and then we have to keep track of the times more carefully.

Next, we have to bound all integrals over the three dimensional momentum variables p_e and over the one-dimensional variables α_e appearing in (3.38). Notice that, because of the singularity of the δ -potential in position space, we are faced here with a large momentum (“ultraviolet”) problem: we have to make sure that all integrals over p_e (and α_e) are convergent in the large p_e (respectively, large α_e) regime. Heuristically, this can be seen using a simple power counting argument. Fix $\kappa \gg 1$, and cutoff all momenta $|p_e| \geq \kappa$ and all frequencies $|\alpha_e| \geq \kappa^2$. Each p_e -integral scales then as κ^3 , and each α_e -integral scales as κ^2 . Since we have $2k + 3n$ edges in Γ , we have $2k + 3n$ momentum- and frequency integrations. However, because of the n delta functions (momentum and frequency conservation), we effectively only have to perform $2k + 2n$ momentum- and frequency-integrations. Therefore the whole integral in (3.38) carries a volume factor of the order $\kappa^{5(2k+2n)} = \kappa^{10k+10n}$. Now, since there are $2k + 2n$ leaves in the graph Γ , the estimate (3.3) guarantees a decay of the order $\kappa^{-5/2(2k+2n)} = \kappa^{-5k-5n}$. The $2k + 3n$ propagators, on the other hand, provide a decay of the order $\kappa^{-2(2k+3n)} = \kappa^{-4k-6n}$. Choosing the observable $J^{(k)}$ so that $\widehat{J}^{(k)}$ decays sufficiently fast at infinity, we can also gain an additional decay κ^{-6k} . Since

$$\kappa^{10k+10n} \cdot \kappa^{-5k-5n-4k-6n-6k} = \kappa^{-n-5k} \ll 1$$

for $\kappa \gg 1$, we can expect (3.38) to converge in the large momentum and large frequency regime. Remark the importance of the decay provided by the free evolution (through the propagators); without making use of it, we could not prove the convergence of the integrals.

To obtain a rigorous proof of the boundedness of the integral (3.38), we develop an integration scheme dictated by the structure of the Feynman graph Γ . We start by integrating over the variables p_e and α_e associated with the leaves of Γ . The momenta on the leaves are exactly the variables of the density $\gamma^{(n+k)}$. Because of the factor $\text{Tr}(1 - \Delta_1) \dots (1 - \Delta_{n+k}) \gamma^{(n+k)}$ on the r.h.s. of (3.28), we can assume that each leaf carries a decaying factor $|p_e|^{-(2+\lambda)}$ (for large p_e), for some $\lambda < 1/2$ (otherwise $\text{Tr}(1 - \Delta_1) \dots (1 - \Delta_{n+k}) \gamma^{(n+k)}$ would diverge). The idea then is that we integrate over all the p and α variables, starting from the leaves and moving towards the roots. At each step we propagate the momentum decay from the son-edges to the father edge of a certain vertex of Γ by integrating out the variables of the son-edges.

A typical step in the integration scheme is as follows: choose a vertex $v \in V(\Gamma)$ such that we already have demonstrated a decay $|p|^{-(2+\lambda)}$ in the momenta p_u, p_d, p_w of the three son edges of v (denoted by u, d and w , see Figure 6). This means that all the momentum- and α -variables of the

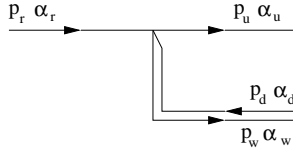


Figure 6: Integration scheme: a typical vertex

edges which are to the right of u, d and w in the graph have already been integrated out. Then we first perform the integration over the three α -variables of the son edges. We obtain, for arbitrary $\varepsilon > 0$,

$$\begin{aligned}
& \int d\alpha_u d\alpha_d d\alpha_w \delta(\alpha_r = \alpha_u + \alpha_d - \alpha_w) \frac{1}{\langle \alpha_u - p_u^2 \rangle \langle \alpha_d - p_d^2 \rangle \langle \alpha_w - p_w^2 \rangle} \\
&= \int d\alpha_u d\alpha_d \frac{1}{\langle \alpha_u - p_u^2 \rangle \langle \alpha_d - p_d^2 \rangle \langle \alpha_r - \alpha_u - \alpha_d + p_w^2 \rangle} \\
&\lesssim \frac{1}{\langle \alpha_r - p_u^2 - p_d^2 + p_w^2 \rangle^{1-\varepsilon}}.
\end{aligned} \tag{3.39}$$

On a heuristic level this follows by power counting (the exponent $1 - \varepsilon$ takes into account logarithmic factors produced in the integrations; for all practical purposes we can think of ε as being zero in this presentation). A rigorous proof of (3.39) can be obtained applying Lemma C.1 twice, once in the α_d and once in the α_w -integral (after estimating $\langle \alpha \rangle^{-1} \leq |\alpha|^{-1+\delta}$, for a sufficiently small $\delta > 0$).

Then we integrate over the momenta of the son-edges by using their decay factor. We find

$$\int \frac{dp_u dp_d dp_w}{|p_u|^{2+\lambda} |p_d|^{2+\lambda} |p_w|^{2+\lambda}} \frac{\delta(p_r = p_u + p_d - p_w)}{\langle \alpha_r - p_u^2 - p_d^2 + p_w^2 \rangle^{1-\varepsilon}} \leq \frac{\text{const}}{|p_r|^{2+\lambda}}. \tag{3.40}$$

Power counting (with $\varepsilon = 0$) requires that $3(2 + \lambda) + 2 - 6 > 2 + \lambda$ which holds for any $\lambda > 0$. A rigorous proof of the bound (3.40) (which requires more conditions on the exponents) is given in Proposition C.4.

From (3.40), we observe that the same decay in the large momentum regime propagates from the son-edges to the father edge. This procedure can then be iterated until we reach the roots of Γ . At this point we can complete the integration scheme by using the smoothness (momentum decay) of the observable $J^{(k)}$. Note that, in this formal computation, the dispersive nature of the free evolution is expressed via the decay in p and α of the resolvent $\langle \alpha - p^2 \rangle^{-1}$; as the above example shows, the use of this decay is crucial to complete the integration scheme.

The complete proof of Theorem 3.3 is much more involved than the simple model calculations (3.39), (3.40). One complication comes from the local singularities. Notice that initially the leaves carry a decay $\langle p_e \rangle^{-2-\lambda}$ instead of $|p_e|^{-2-\lambda}$ but this locally regularized decay cannot be propagated; even if we replace $|p_j|^{-2-\lambda}$ by $\langle p_j \rangle^{-2-\lambda}$ (for $j = u, d, v$) on the l.h.s. of (3.40), on the r.h.s. the decay will not be regularized. This phenomenon stems from the singularity structure of the propagator (second factor on the l.h.s. of (3.40); for more details see the proof of Proposition C.4.

Another additional source of complications is the fact that, in order to use the decay in the momenta of the leaves, we need to apply a Schwarz inequality to (3.38). We define the sets

$$Q_1 := \{e \in L(\Gamma) : \tau_e = 1\}, \quad \text{and} \quad Q_2 = \{e \in L(\Gamma) : \tau_e = -1\}; \tag{3.41}$$

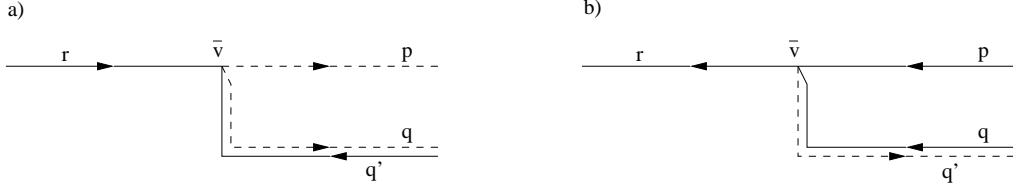


Figure 7: Vertices involving dead edges

that is Q_1 is the set of outward leaves and Q_2 is the set of inward leaves. Clearly $L(\Gamma) = Q_1 \cup Q_2$ and $|Q_1| = |Q_2| = n+k$. Assuming, without loss of generality that $\gamma^{(n+k)}(\mathbf{p}_{n+k}; \mathbf{p}'_{n+k}) = \psi(\mathbf{p}_{n+k})\bar{\psi}(\mathbf{p}'_{n+k})$ (in general the density $\gamma^{(n+k)}$ is a linear combination, with positive coefficients of terms like this one), and applying a weighted Schwarz inequality, we obtain (since $t \leq 1$ by assumption)

$$\begin{aligned}
& \left| \langle J^{(k)}, K_{\Gamma,t} \gamma^{(n+k)} \rangle \right| \\
& \leq C e^{Cn} \int \prod_{e \in E(\Gamma)} dp_e \prod_{e \in E_2(\Gamma)} \frac{d\alpha_e}{\langle \alpha_e - p_e^2 \rangle} \prod_{e \in R(\Gamma)} \frac{1}{\langle p_e \rangle^3} \prod_{v \in V(\Gamma)} \delta(\sum_{e \in v} \pm \alpha_e) \delta(\sum_{e \in v} \pm p_e) \\
& \quad \times \left(\frac{\prod_{e \in Q_1} p_e^2}{\prod_{e \in Q_2} p_e^2} |\psi(\{p_e\}_{e \in Q_1})|^2 + \frac{\prod_{e \in Q_2} p_e^2}{\prod_{e \in Q_1} p_e^2} |\psi(\{p_e\}_{e \in Q_2})|^2 \right) \\
& \leq C^n \int d\mathbf{p}_{n+k} p_1^2 \cdots p_{n+k}^2 |\psi(\mathbf{p}_{n+k})|^2 \\
& \quad \times \left(\sup_{\{p_e\}_{e \in Q_1}} \int \prod_{e \in E(\Gamma) \setminus Q_1} dp_e \prod_{e \in E_2(\Gamma)} \frac{d\alpha_e}{\langle \alpha_e - p_e^2 \rangle} \prod_{e \in R(\Gamma)} \frac{1}{\langle p_e \rangle^3} \prod_{e \in Q_2} \frac{1}{p_e^2} \prod_{v \in V(\Gamma)} \delta(\sum_{e \in v} \pm \alpha_e) \delta(\sum_{e \in v} \pm p_e) \right. \\
& \quad \left. + \sup_{\{p_e\}_{e \in Q_2}} \int \prod_{e \in E(\Gamma) \setminus Q_2} dp_e \prod_{e \in E_2(\Gamma)} \frac{d\alpha_e}{\langle \alpha_e - p_e^2 \rangle} \prod_{e \in R(\Gamma)} \frac{1}{\langle p_e \rangle^3} \prod_{e \in Q_1} \frac{1}{p_e^2} \prod_{v \in V(\Gamma)} \delta(\sum_{e \in v} \pm \alpha_e) \delta(\sum_{e \in v} \pm p_e) \right) \\
& =: A + B.
\end{aligned} \tag{3.42}$$

In the contribution A , resulting from the first term in the parenthesis, we take the supremum over all momenta p_e associated with the leaves in Q_1 . We say that these momenta are *frozen* and that the corresponding edges $e \in Q_1$ are *dead-edges* (the other edges, whose momenta are integrated out, are called *live-edges*). In the contribution B we froze all momenta of the leaves Q_2 .

We observe that, after performing the Schwarz inequality, the live leaves carry a decaying factor $|p_e|^{-2}$. This is still not enough to iterate the decay according to the scheme of (3.39), (3.40) (where we need a decay of the form $|p_e|^{-2-\lambda}$, for some $\lambda > 0$). We are saved by the presence of the dead leaves, which although their momentum is not integrated out, still allow us to gain an additional decay on the momenta associated with their father-edges. In fact there are two possible vertices involving dead-edges, drawn in Fig. 7 (dashed lines indicate dead-edges). Consider first the vertex b); in this case the son-edges are two live-leaves, carrying a decaying factor $|p_e|^{-2}$ (with $p_e = p$ and $p_e = q$), and one dead-leaf. To integrate out the vertex we need to perform three α -integration (effectively, only two α -integration, because of the delta-function) as in (3.39) but, due to the presence of the dead-edge, only two p -integration (effectively only one p -integration, because of the δ -function). It turns out that, as a result of these integrations, we obtain a decay $|r|^{-2-\lambda}$ for some $\lambda > 0$, in the momentum r of the father-edge, improving therefore on decay characterizing the son-

edges. The vertex a) in Fig. 7, however, is different: we have here two dead-leaves and only one live-leaf carrying the decay $|q'|^{-2}$. In this case we still have to perform the same α -integration as before, but this time, we effectively do not have to perform any p -integration. It turns out, in this case, that the decay in the momentum of the father edge cannot be boosted to $|p|^{-2-\lambda}$; instead, we gain an additional spherical decay coming from the propagator of the son-edges. In other words, in this case, we obtain a decay $|r|^{-2}\langle\alpha - (r - a)^2\rangle^{1-\varepsilon}$ in the momentum of the father-edge, for some a depending on the frozen momentum. This example makes clear that the process of *integrating out a vertex*, propagating the momentum-decay from the son- to the father-edges, until we reach the roots, is actually quite complicated, because there are several cases to consider, leading to different decays in the momenta of the father edges. Our algorithm involves altogether 7 types of vertices and 12 different transition steps. More details can be found in [6, Section 9.4 and 9.5].

4 A-Priori Estimates on Limit Points $\Gamma_{\infty,t}$

In this section we show how to prove the a-priori bounds (3.1), which are needed to apply Theorem 3.1 to the proof of Theorem 1.2.

Proposition 4.1. *Assume the conditions of Theorem 1.2 and the additional conditions A), B) stated at the end of Section 1 are verified. Suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1} \oplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ is a limit point of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ (the marginal densities associated with the solution $\psi_{N,t}$ of the N -particle Schrödinger equation). Then $\gamma_{\infty,t}^{(k)} \geq 0$ and there exists a constant C such that*

$$\text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{\infty,t}^{(k)} \leq C^k \quad (4.1)$$

for all $k \geq 1$ and $t \in [0, T]$.

The main difficulty in proving Proposition 4.1 is the fact that the estimate (4.1) does not hold true if we replace $\gamma_{\infty,t}^{(k)}$ by the marginal density $\gamma_{N,t}^{(k)}$. More precisely,

$$\text{Tr} (1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{N,t}^{(k)} \leq C^k \quad (4.2)$$

cannot hold true with a constant C independent of N . In fact, for finite N and $k > 1$, the k -particle density $\gamma_{N,t}^{(k)}$ still contains the short scale structure due to the correlations among the particles. For example, when particle one and particle two are very close to each other (at distances of order $1/N$), we can expect the two-particle density to be approximately given by

$$\gamma_{N,t}^{(2)}(\mathbf{x}_2, \mathbf{x}'_2) \simeq \text{const } f_N(x_1 - x_2) f_N(x'_1 - x'_2)$$

(the constant part takes into account factors which vary on a larger scale). It is then simple to check that

$$\text{Tr} (1 - \Delta_1)(1 - \Delta_2) \gamma_{N,t}^{(2)} \simeq N.$$

Only after taking the weak limit $N \rightarrow \infty$, the short scale correlation structure disappears (because it varies on a length scale of order $1/N$), and one can prove bounds like (4.1) (for a more detailed discussion on the short scale correlation structure developed by $\psi_{N,t}$ and by its marginal densities, we defer to Section 5; the resolution of this singularity is one of the main obstacles in proving the convergence to the infinite hierarchy).

To overcome this problem, we cutoff the wave function $\psi_{N,t}$ when two or more particles come at distances smaller than some intermediate length scale ℓ , with $N^{-1} \ll \ell \ll 1$ (more precisely, the

cutoff will be effective only when one or more particles come close to one of the variable x_j over which we want to take derivatives). For fixed $j = 1, \dots, N$, we define $\theta_j \in C^\infty(\mathbb{R}^{3N})$ such that

$$\theta_j(\mathbf{x}) \simeq \begin{cases} 1 & \text{if } |x_i - x_j| \gg \ell \text{ for all } i \neq j \\ 0 & \text{if there exists } i \neq j \text{ with } |x_i - x_j| \lesssim \ell \end{cases} .$$

It is important, for our analysis, that θ_j controls its derivatives (in the sense that, for example, $|\nabla_i \theta_j| \leq C\ell^{-1}\theta_j^{1/2}$); for this reason we cannot use standard compactly supported cutoffs, but instead we have to construct appropriate functions which decay exponentially when particles come close together (the prototype of such function is $\theta(x) = \exp(-\sqrt{(x/\ell)^2 + 1})$). Making use of the functions $\theta_j(\mathbf{x})$, we prove the following higher order energy estimates.

Proposition 4.2. *Choose $\ell \ll 1$ such that $N\ell^2 \gg 1$. Suppose that α is small enough. Then there exist constants C_1 and C_2 such that, for any $\psi \in L_s^2(\mathbb{R}^{3N})$,*

$$\langle \psi, (H_N + C_1 N)^k \psi \rangle \geq C_2 N^k \int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_{k-1}(\mathbf{x}) |\nabla_1 \dots \nabla_k \psi(\mathbf{x})|^2. \quad (4.3)$$

The meaning of the bound (4.3) is clear. The L^2 -norm of the k -th derivative $\nabla_1 \dots \nabla_k \psi$ can be controlled by the expectation of the k -th power of the energy per particle, if we restrict the integration domain to regions where the first $(k-1)$ particles are “isolated” (in the sense that there is no particle at distances smaller than ℓ from x_1, x_2, \dots, x_{k-1}).

Note that we can allow one “free derivative”; in (4.3) we take the derivative over x_k although there is no cutoff $\theta_k(\mathbf{x})$. The reason is that the correlation structure becomes singular, in the L^2 -sense, only when we derive it twice (if one uses the zero energy solution f_N introduced in (1.4) to describe the correlations, this can be seen by observing that $|\nabla f_N(x)| \leq 1/|x|$, which is locally square integrable). Remark that the condition $N\ell^2 \gg 1$ is a consequence of the fact that, if ℓ is too small, the error due to the localization of the kinetic energy on distances of order ℓ cannot be controlled. The proof of Proposition 4.2 is based on induction over k ; for details see Section 7 in [9].

From the estimates (4.3), using the preservation of the expectation of H_N^k along the time evolution and the additional condition (1.14), we obtain the following bounds for the solution $\psi_{N,t} = e^{-iH_N t} \psi_N$ of the Schrödinger equation (1.10).

$$\int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_{k-1}(\mathbf{x}) |\nabla_1 \dots \nabla_k \psi_{N,t}(\mathbf{x})|^2 \leq C^k \quad (4.4)$$

uniformly in N and t , and for all $k \geq 1$. Translating these bounds in the language of the density matrix $\gamma_{N,t}$, we obtain

$$\text{Tr} \theta_1 \dots \theta_{k-1} \nabla_1 \dots \nabla_k \gamma_{N,t} \nabla_1^* \dots \nabla_k^* \leq C^k. \quad (4.5)$$

The idea now is to use the freedom in the choice of the cutoff length ℓ . If we fix the position of all particles but x_j , it is clear that the cutoff θ_j is effective in a volume at most of the order $N\ell^3$. If we choose now ℓ such that $N\ell^3 \rightarrow 0$ as $N \rightarrow \infty$ (which is of course compatible with the condition that $N\ell^2 \gg 1$), then we can expect that, in the limit of large N , the cutoff becomes negligible. This approach yields in fact the desired results; starting from (4.5), and choosing ℓ such that $N\ell^3 \ll 1$, we can complete the proof of Proposition 4.1 (see Proposition 6.3 in [7] for more details).

5 Convergence to the Infinite Hierarchy

In this section we give some more details concerning Step 2 in the strategy outlined in Section 2. In [9, Theorem 8.1], we prove the following result.

Theorem 5.1. *Suppose that the assumptions of Theorem 1.2 are satisfied and fix $T > 0$. Suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ is a limit point of $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ (with respect to the product of the weak* topologies defined on \mathcal{L}_k^1). Then $\Gamma_{\infty,t}$ is a solution to the infinite hierarchy*

$$\gamma_{\infty,t}^{(k)} = \mathcal{U}^{(k)}(t)\gamma_{\infty,0}^{(k)} - 8\pi a_0 i \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_{\infty,s}^{(k+1)} \right] \quad (5.1)$$

with initial data $\gamma_{\infty,0}^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}$ (see (3.4) for the definition of $\mathcal{U}^{(k)}$).

To prove this theorem, we start with the BBGKY hierarchy (2.1), rewritten in integral form as

$$\begin{aligned} \gamma_{N,t}^{(k)} &= \mathcal{U}^{(k)}(t)\gamma_{N,0}^{(k)} - i \sum_{i < j}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \left[V_N(x_i - x_j), \gamma_{N,s}^{(k)} \right] \\ &\quad - i(N-k) \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[V_N(x_j - x_{k+1}), \gamma_{N,s}^{(k+1)} \right] \end{aligned} \quad (5.2)$$

Assuming (by passing to an appropriate subsequence) that $\Gamma_{N,t} \rightarrow \Gamma_{\infty,t}$ as $N \rightarrow \infty$ with respect to the product of the weak* topologies (uniformly in $t \in [0, T]$) it is simple to prove that the l.h.s. and the first term on the r.h.s. of (5.2) converge, as $N \rightarrow \infty$, to the l.h.s. and, respectively, to the first term on the r.h.s. of (5.1). The second term on the r.h.s. of (5.2), on the other hand, can be proven to vanish in the limit $N \rightarrow \infty$. In fact, compared with the third term on the r.h.s. of (5.2), the second term is, at least formally, smaller by a factor N (the limit $N \rightarrow \infty$ has to be taken with fixed $k \geq 1$). The fact that the second term on the r.h.s. of (5.2) is negligible in the limit $N \rightarrow \infty$ (compared with the third term) corresponds to the physical intuition that the interactions among the first k particles affect their time-evolution less than their interaction with the other $(N - k)$ particles.

To conclude the proof of Theorem 5.1, we only need to show that the third term on the r.h.s. of (5.2) converges, as $N \rightarrow \infty$, to the last term on the r.h.s. of (5.1). As already remarked in (2.3) and (2.4), this convergence relies critically on the correlation structure characterizing the $(k + 1)$ -particle density $\gamma_{N,t}^{(k+1)}$. A naive approach, based on the observation that $(N - k)V_N(x_j - x_{k+1}) \simeq N^3 V(N(x_j - x_{k+1})) \simeq b_0 \delta(x_j - x_{k+1})$ for large N , fails to explain the coupling constant in front of the last term on the r.h.s. of (5.1). The emergence of the scattering length can only be understood taking into account the correlation structure of $\gamma_{N,t}^{(k+1)}$. Assuming for a moment that the correlations can be described, in good approximation, by the solution f_N to the zero-energy scattering equation (1.6), then we can expect that, for large N ,

$$\gamma_{N,t}^{(k+1)}(\mathbf{x}_{k+1}; \mathbf{x}'_{k+1}) \simeq f_N(x_j - x_{k+1}) \gamma_{\infty,t}^{(k+1)}(\mathbf{x}_{k+1}; \mathbf{x}'_{k+1}) \quad (5.3)$$

in the region where $x_j - x_{k+1}$ is of the order $1/N$ (and all other particles are at larger distances). Assuming some regularity of the limit point $\gamma_{\infty,t}^{(k+1)}$, and using (1.5), the approximation (5.3) imme-

diately leads to

$$\begin{aligned}
& \left(\text{Tr}_{k+1}(N-k)V_N(x_j - x_{k+1})\gamma_{N,t}^{(k+1)} \right) (\mathbf{x}_k; \mathbf{x}'_k) \\
& \simeq \int dx_{k+1} N^3 V(N(x_j - x_{k+1})) f(N(x_j - x_{k+1})) \gamma_{\infty,t}^{(k+1)} (\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1}) \\
& = \int dy V(y) f(y) \gamma_{\infty,t}^{(k+1)} \left(\mathbf{x}_k, x_j + \frac{y}{N}; \mathbf{x}'_k, x_j + \frac{y}{N} \right) \\
& \simeq \left(\int dy V(y) f(y) \right) \gamma_{\infty,t}^{(k+1)} (\mathbf{x}_k, x_j; \mathbf{x}'_k, x_j) \\
& = 8\pi a_0 \int dx_{k+1} \delta(x_j - x_{k+1}) \gamma_{\infty,t}^{(k+1)} (\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1})
\end{aligned} \tag{5.4}$$

and thus explains the emergence of the scattering length on the r.h.s. of (5.1) (note that the third term on r.h.s. of (5.2) is a commutator and thus produces two summands; in (5.4) we only consider one of these terms, the other can be handled analogously). This heuristic argument shows that in order to prove Theorem 5.1 we need to identify the short scale structure of the marginal densities and prove that it can be described by the function f_N as in (5.3). To this end we are going to use energy estimates. In [7] and [9], we developed two different approaches to this problem. The first approach is simpler, but it only works for sufficiently small interaction potentials. The second approach is a little bit more involved, but it can be used for all potentials satisfying the assumptions of Theorem 1.2. In the following we will concentrate on the first, simpler, approach; in the next section, we present then some of the main ideas of the second approach.

To measure the strength of the interaction potential V , we define the dimensionless constant

$$\rho = \sup_{x \in \mathbb{R}^3} |x|^2 V(x) + \int \frac{dx}{|x|} V(x) \tag{5.5}$$

Proposition 5.2. *Assume that the potential V satisfies the conditions of Theorem 1.2, and suppose that ρ is sufficiently small. Then there exists $C > 0$ such that*

$$\langle \psi, H_N^2 \psi \rangle \geq CN^2 \int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \tag{5.6}$$

for all $i \neq j$ and for all $\psi \in L_s^2(\mathbb{R}^{3N}, d\mathbf{x})$.

Making use of this energy estimate it is possible to deduce strong a-priori bounds on the solution $\psi_{N,t}$ of the Schrödinger equation (1.10).

Corollary 5.3. *Under the assumptions of Theorem 1.2 (and the additional condition (B), for $k = 2$), for ρ small enough we have*

$$\int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \leq C \tag{5.7}$$

for all $i \neq j$, uniformly in $N \in \mathbb{N}$ and $t \in \mathbb{R}$. Therefore, if $\gamma_{N,t}^{(k)}$ denote the k -particle marginal associated with $\psi_{N,t}$, we have, for every $1 \leq i, j \leq k$ with $i \neq j$,

$$\text{Tr} (1 - \Delta_i)(1 - \Delta_j) \frac{1}{f_N(x_i - x_j)} \gamma_{N,t}^{(k)} \frac{1}{f_N(x_i - x_j)} \leq C$$

uniformly in $N \in \mathbb{N}$ and in $t \in \mathbb{R}$.

Proof. Using (5.6), the conservation of the energy along the time evolution, and the assumption (B) on the initial wave function ψ_N , we find

$$\int d\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \leq CN^{-2} \langle \psi_{N,t}, H_N^2 \psi_{N,t} \rangle = CN^{-2} \langle \psi_N, H_N^2 \psi_N \rangle \leq C. \quad (5.8)$$

□

Remark that the a-priori bounds (5.7) cannot hold true if we do not divide the solution $\psi_{N,t}$ of the Schrödinger equation by $f_N(x_i - x_j)$. In fact, using that $f_N(x) \simeq 1 - a_0/(N|x| + 1)$, it is simple to check that

$$\int dx |\nabla^2 f_N(x)|^2 \simeq N.$$

This implies that, if we replace $\psi_{N,t}(\mathbf{x})/f_N(x_i - x_j)$ by $\psi_N(\mathbf{x})$ the integral in (5.7) would be of order N . Only after removing the singular factor $f_N(x_i - x_j)$ from $\psi_{N,t}(\mathbf{x})$ we can obtain useful bounds on the regular part of the wave function. These a-priori bounds allow us to identify the correlation structure of the wave function $\psi_{N,t}$ and to show that, when x_i and x_j are close to each other, $\psi_{N,t}(\mathbf{x})$ can be approximated by the time independent correlation factor $f_N(x_i - x_j)$, which varies on the length scale $1/N$, multiplied with a regular part which only varies on scales of order one. In other words, the bounds (5.7) establish a strong separation of scales for the solution $\psi_{N,t}$ of the N -particle Schrödinger equation, and for its marginal densities; on length scales of order $1/N$, $\psi_{N,t}$ is characterized by a singular, time independent, short scale correlation structure described by the the solution f_N to the zero-energy scattering equation. On scales of order one, on the other hand, $\psi_{N,t}$ is regular, and, as it follows from Theorem 1.2, it can be approximated, in an appropriate sense, by products of the solution to the time-dependent Gross-Pitaevskii equation. Remark that although the short-scale correlation structure is time independent, it still affects, in a non-trivial way, the time-evolution on length scales of order one (because it produces the scattering length in the Gross-Pitaevskii equation).

Since it is quite short and it shows why the solution $f_N(x_i - x_j)$ to the zero energy scattering equation (1.4) can be used to describe the two-particle correlations, we reproduce next the proof Proposition 5.2.

Proof of Proposition 5.2. We decompose the Hamiltonian (1.9) as

$$H_N = \sum_{j=1}^N h_j \quad \text{with} \quad h_j = -\Delta_j + \frac{1}{2} \sum_{i \neq j} V_N(x_i - x_j).$$

For an arbitrary permutation symmetric wave function ψ and for any fixed $i \neq j$, we have

$$\langle \psi, H_N^2 \psi \rangle = N \langle \psi, h_i^2 \psi \rangle + N(N-1) \langle \psi, h_i h_j \psi \rangle \geq N(N-1) \langle \psi, h_i h_j \psi \rangle.$$

Using the positivity of the potential, we find

$$\langle \psi, H_N^2 \psi \rangle \geq N(N-1) \left\langle \psi, \left(-\Delta_i + \frac{1}{2} V_N(x_i - x_j) \right) \left(-\Delta_j + \frac{1}{2} V_N(x_i - x_j) \right) \psi \right\rangle. \quad (5.9)$$

Next, we define $\phi(\mathbf{x})$ by $\psi(\mathbf{x}) = f_N(x_i - x_j) \phi(\mathbf{x})$ (ϕ is well defined because $f_N(x) > 0$ for all $x \in \mathbb{R}^3$); note that the definition of the function ϕ depends on the choice of i, j . Then

$$\frac{1}{f_N(x_i - x_j)} \Delta_i (f_N(x_i - x_j) \phi(\mathbf{x})) = \Delta_i \phi(\mathbf{x}) + \frac{(\Delta f_N)(x_i - x_j)}{f_N(x_i - x_j)} \phi(\mathbf{x}) + \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \nabla_i \phi(\mathbf{x}).$$

From (1.4) it follows that

$$\frac{1}{f_N(x_i - x_j)} \left(-\Delta_i + \frac{1}{2} V_N(x_i - x_j) \right) f_N(x_i - x_j) \phi(\mathbf{x}) = L_i \phi(\mathbf{x})$$

and analogously

$$\frac{1}{f_N(x_i - x_j)} \left(-\Delta_j + \frac{1}{2} V_N(x_i - x_j) \right) f_N(x_i - x_j) \phi(\mathbf{x}) = L_j \phi(\mathbf{x})$$

where we defined

$$L_\ell = -\Delta_\ell + 2 \frac{\nabla_\ell f_N(x_i - x_j)}{f_N(x_i - x_j)} \nabla_\ell, \quad \text{for } \ell = i, j.$$

Remark that, for $\ell = i, j$, the operator L_ℓ satisfies

$$\int d\mathbf{x} f_N^2(x_i - x_j) L_\ell \bar{\phi}(\mathbf{x}) \psi(\mathbf{x}) = \int d\mathbf{x} f_N^2(x_i - x_j) \bar{\phi}(\mathbf{x}) L_\ell \psi(\mathbf{x}) = \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_\ell \bar{\phi}(\mathbf{x}) \nabla_\ell \psi(\mathbf{x}).$$

Therefore, from (5.9), we obtain

$$\begin{aligned} \langle \psi, H_N^2 \psi \rangle &\geq N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) L_i \bar{\phi}(\mathbf{x}) L_j \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_i L_j \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) L_j \nabla_i \phi(\mathbf{x}) \\ &\quad + N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \nabla_i \bar{\phi}(\mathbf{x}) [\nabla_i, L_j] \phi(\mathbf{x}) \\ &= N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) |\nabla_j \nabla_i \phi(\mathbf{x})|^2 \\ &\quad + N(N-1) \int d\mathbf{x} f_N^2(x_i - x_j) \left(\nabla_i \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \right) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_j \phi(\mathbf{x}). \end{aligned} \tag{5.10}$$

To control the second term on the right hand side of the last equation we use bounds on the function f_N , which can be derived from the zero energy scattering equation (1.4):

$$1 - C\rho \leq f_N(x) \leq 1, \quad |\nabla f_N(x)| \leq C \frac{\rho}{|x|}, \quad |\nabla^2 f_N(x)| \leq C \frac{\rho}{|x|^2} \tag{5.11}$$

for constants C independent of N and of the potential V (recall the definition of the dimensionless constant ρ from (5.5)). Therefore, for $\rho < 1$,

$$\begin{aligned} &\left| \int d\mathbf{x} f_N^2(x_i - x_j) \left(\nabla_i \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \right) \nabla_i \bar{\phi}(\mathbf{x}) \nabla_j \phi(\mathbf{x}) \right| \\ &\leq C\rho \int d\mathbf{x} \frac{1}{|x_i - x_j|^2} |\nabla_i \phi(\mathbf{x})| |\nabla_j \phi(\mathbf{x})| \\ &\leq C\rho \int d\mathbf{x} \frac{1}{|x_i - x_j|^2} (|\nabla_i \phi(\mathbf{x})|^2 + |\nabla_j \phi(\mathbf{x})|^2) \\ &\leq C\rho \int d\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2 \end{aligned} \tag{5.12}$$

where we used Hardy inequality. Thus, from (5.10), and using again the first bound in (5.11), we obtain

$$\langle \psi, H_N^2 \psi \rangle \geq N(N-1)(1 - C\rho) \int d\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2$$

which implies (5.6). \square

Equipped with the a-priori bounds of Corollary 5.3, we can now come back to the problem of proving the convergence of the last term on the r.h.s. of (5.2) to the last term on the r.h.s. of (5.1). For simplicity, we consider the case $k = 1$, and we only discuss the term with the interaction potential sitting on the left of the density (the commutator also has a term with the interaction being on the right of the density, which can be handled analogously). After multiplying with a smooth one-particle observable $J^{(1)}$ (a compact operator on $L^2(\mathbb{R}^3)$, with sufficiently smooth kernel), we need to prove that

$$\mathrm{Tr} \left(\mathcal{U}^{(1)}(s-t)J^{(1)} \right) \left(N^3V(N(x_1-x_2))\gamma_{N,t}^{(2)} - 8\pi a_0\delta(x_1-x_2)\gamma_{\infty,t}^{(2)} \right) \rightarrow 0 \quad (5.13)$$

as $N \rightarrow \infty$. To this end we decompose the difference in several terms. We use the notation $J_t^{(1)} = \mathcal{U}^{(1)}(t)J^{(1)}$, and, for a bounded function $h(x) \geq 0$ with $\int dx h(x) = 1$, we define $h_\alpha(x) = \alpha^{-3}h(\alpha^{-1}x)$ for all $\alpha > 0$. Then we have

$$\begin{aligned} & \mathrm{Tr} \left(\mathcal{U}^{(1)}(s-t)J^{(1)} \right) \left(N^3V(N(x_1-x_2))\gamma_{N,t}^{(2)} - 8\pi a_0\delta(x_1-x_2)\gamma_{\infty,t}^{(2)} \right) \\ &= \mathrm{Tr} J_{s-t}^{(1)} N^3V(N(x_1-x_2))f(N(x_1-x_2)) \frac{1}{f(N(x_1-x_2))} \gamma_{N,t}^{(2)} \frac{1}{f(N(x_1-x_2))} (f(N(x_1-x_2)) - 1) \\ & \quad + \mathrm{Tr} J_{s-t}^{(1)} (N^3V(N(x_1-x_2))f(N(x_1-x_2)) - 8\pi a_0\delta(x_1-x_2)) \frac{1}{f(N(x_1-x_2))} \gamma_{N,t}^{(2)} \frac{1}{f(N(x_1-x_2))} \\ & \quad + 8\pi a_0 \mathrm{Tr} J_{s-t}^{(1)} (\delta(x_1-x_2) - h_\alpha(x_1-x_2)) \frac{1}{f(N(x_1-x_2))} \gamma_{N,t}^{(2)} \frac{1}{f(N(x_1-x_2))} \\ & \quad + 8\pi a_0 \mathrm{Tr} J_{s-t}^{(1)} h_\alpha(x_1-x_2) \left(\frac{1}{f(N(x_1-x_2))} \gamma_{N,t}^{(2)} \frac{1}{f(N(x_1-x_2))} - \gamma_{N,t}^{(2)} \right) \\ & \quad + 8\pi a_0 \mathrm{Tr} J_{s-t}^{(1)} h_\alpha(x_1-x_2) \left(\gamma_{N,t}^{(2)} - \gamma_{\infty,t}^{(2)} \right) \\ & \quad + 8\pi a_0 \mathrm{Tr} J_{s-t}^{(1)} (h_\alpha(x_1-x_2) - \delta(x_1-x_2)) \gamma_{\infty,t}^{(2)}. \end{aligned} \quad (5.14)$$

The idea here is that in order to compare the N -dependent potential $N^3V(N(x_1-x_2))$ with the limiting δ -potential, we have to test it against a regular density (using an appropriate Poincaré inequality). For this reason, we first regularize the density $\gamma_{N,t}^{(2)}$ in the variable (x_1-x_2) dividing it by the correlation function $f_N(x_1-x_2)$ on the left and the right (first term on the r.h.s. of the last equation). Using the regularity of $f_N^{-1}(x_1-x_2)\gamma_{N,t}^{(2)}f_N^{-1}(x_1-x_2)$ from Corollary 5.3, we can then compare, in the regime of large N , the interaction potential with the delta-function (second term on the r.h.s.). At this point we are still not done, because, in order to remove the regularizing factors $f_N^{-1}(x_1-x_2)$ (fourth term on the r.h.s. of (5.14)) and in order to replace the density $\gamma_{N,t}^{(2)}$ by its limit point $\gamma_{\infty,t}^{(2)}$ (fifth term on the r.h.s. of (5.14)), we need to test the density against a compact observable. For this reason, in the third term on the r.h.s. of (5.14), we replace the δ -function (which is of course not bounded) by the function h_α which approximate the delta-function on the length-scale α ; it is important here that α is now decoupled from N . In the last term, after having removed all N dependence, we go back to the δ -potential using the regularity of the limiting density $\gamma_{\infty,t}^{(2)}$.

To control the first and fourth term on the r.h.s. of (5.14), we use the fact that $1 - f_N(x_1-x_2) \simeq 1/(N|x_1-x_2| + 1)$ varies on a length scale of order $1/N$. It follows that the first term converges to zero as $N \rightarrow \infty$, as well as the fourth term, for every fixed $\alpha > 0$. To estimate the second, the third and the last term, we make use of appropriate Poincaré inequalities, combined with the result of Corollary 5.3 and, for the last term, of Proposition 4.1 (we present an example of a Poincaré

inequality, which can be used to estimate these terms in Appendix D). It follows that the second term converges to zero as $N \rightarrow \infty$, and that the third and the fifth terms converge to zero as $\alpha \rightarrow 0$, uniformly in N . Finally, the fifth term on the r.h.s. of (5.14) converges to zero as $N \rightarrow \infty$, for every fixed α ; this follows from the assumption that $\gamma_{N,t}^{(2)} \rightarrow \gamma_{\infty,t}^{(2)}$ as $N \rightarrow \infty$ with respect to the weak* topology (some additional work has to be done here, because the operator $J_{s-t}^{(1)} h_\alpha(x_1 - x_2)$ is not compact). Therefore, if we first fix $\alpha > 0$ and let $N \rightarrow \infty$ and then we let $\alpha \rightarrow 0$ all terms on the r.h.s. of (5.14) converge to zero; this concludes the proof of Theorem 5.1.

6 Convergence for Large Interaction Potentials

As pointed out in Section 5, the energy estimate, Proposition 5.2, which was the basis for the proof of Theorem 5.1, only holds for sufficiently small potentials (for sufficiently small values of the parameter ρ defined in (5.5)). For large potentials, we need a different approach. The new technique, developed in [9], is based on the use of the wave operator associated with the one-particle Hamiltonian $\mathfrak{h}_N = -\Delta + (1/2)V_N$, defined through the strong limit

$$W_N = s - \lim_{t \rightarrow \infty} e^{i\mathfrak{h}_N t} e^{i\Delta t}. \quad (6.1)$$

Under the assumptions of Theorem 1.2 on the potential V , it is simple to show that the limit (6.1) exists, that the wave operator W_N is complete, in the sense that

$$W_N^{-1} = W_N^* = s - \lim_{t \rightarrow \infty} e^{-i\Delta t} e^{-i\mathfrak{h}_N t}, \quad (6.2)$$

and that it satisfies the intertwining relation

$$W_N^* \mathfrak{h} W_N = -\Delta. \quad (6.3)$$

It is also important to observe that the wave operator W_N is related by simple scaling to the wave operator W associated with the one-particle Hamiltonian $\mathfrak{h} = -\Delta + (1/2)V$ (and defined analogously to (6.1)). In fact, if $W_N(x; x')$ and $W(x; x')$ denote the kernels of W_N and, respectively, of W , we have

$$W_N(x; x') = N^3 W(Nx; Nx') \quad \text{and} \quad W_N^*(x; x') = N^3 W^*(Nx; Nx').$$

In particular this implies that the norm of W_N , as an operator from $L^p(\mathbb{R}^3)$ to $L^p(\mathbb{R}^3)$, for arbitrary $1 \leq p \leq \infty$, is independent of N . From the work of Yajima, see [15, 16], we know that, under the conditions on V assumed in Theorem 1.2, the wave operator and its inverse, are bounded on any L^p -space. Therefore

$$\|W_N\|_{L^p \rightarrow L^p} = \|W\|_{L^p \rightarrow L^p} < \infty \quad \text{for all } 1 \leq p \leq \infty.$$

In the following we will denote by $W_{N,(i,j)}$ the wave operator W_N acting only on the relative variable $x_j - x_i$. In other words, the action of $W_{N,(i,j)}$ on a N -particle wave function $\psi_N \in L^2(\mathbb{R}^{3N})$ is given by

$$(W_{N,(i,j)} \psi_N)(\mathbf{x}) = \int dv W_N(x_j - x_i; v) \psi_N \left(x_1, \dots, \frac{x_i + x_j}{2} + \frac{v}{2}, \dots, \frac{x_i + x_j}{2} - \frac{v}{2}, \dots, x_N \right) \quad (6.4)$$

if $j < i$ (the formula for $i > j$ is similar). Similarly, we define $W_{N,(i,j)}^*$.

Using the wave operator we have the following energy estimate, which replaces Proposition 5.2, and whose proof can be found in [9, Proposition 5.2].

Proposition 6.1. *Suppose $V \geq 0$, $V \in L^1(\mathbb{R}^3)$ and $V(x) = V(-x)$ for all $x \in \mathbb{R}^3$. Then we have, for every $i \neq j$,*

$$\langle \psi_N, H_N^2 \psi_N \rangle \geq CN^2 \int dx \left| (\nabla_i \cdot \nabla_j) W_{N,(i,j)}^* \psi_N \right|^2. \quad (6.5)$$

From Proposition 6.1, we obtain immediately an a-priori bound on $\psi_{N,t}$ and on its marginal densities without the smallness condition on ρ .

Corollary 6.2. *Under the assumptions of Theorem 1.2 (and the additional condition (B), for $k = 2$), we have, for all $i \neq j$,*

$$\int dx \left| (\nabla_i \cdot \nabla_j) W_{N,(i,j)}^* \psi_{N,t}(\mathbf{x}) \right|^2 \leq C \quad (6.6)$$

uniformly in $N \in \mathbb{N}$ and $t \in \mathbb{R}$. Therefore, if $\gamma_{N,t}^{(k)}$ denote the k -particle marginal associated with $\psi_{N,t}$, we have, for every $1 \leq i, j \leq k$ with $i \neq j$,

$$\text{Tr} \left((\nabla_i \cdot \nabla_j)^2 - \Delta_i - \Delta_j + 1 \right) W_{N,(i,j)}^* \gamma_{N,t}^{(k)} W_{N,(i,j)} \leq C$$

uniformly in $N \in \mathbb{N}$ and in $t \in \mathbb{R}$.

The philosophy of the bounds (6.6) and (5.7) is the same; first we have to regularize the wave function $\psi_{N,t}$, and then we can prove useful bounds on its derivatives. There are however important differences. In (5.7) we regularized $\psi_{N,t}$ in position space, by factoring out the short scale correlation structure $f_N(x_i - x_j)$. In (6.6), instead, we regularize $\psi_{N,t}$ applying the wave operator $W_{N,(i,j)}^*$. Another important difference is that (6.6) is weaker than (5.7); in fact, (6.6) only gives a control on the particular combination $\sum_{\alpha=1}^3 \partial_{x_{i,\alpha}} \partial_{x_{j,\alpha}}$ of second derivatives, while (5.7) controls $\partial_{x_{i,\alpha}} \partial_{x_{j,\beta}}$ for all $1 \leq \alpha, \beta \leq 3$. The weakness of the bound (6.6) makes the proof of the convergence more difficult. In particular we have to establish new Poincaré inequalities, which only require control of the inner product $\nabla_i \cdot \nabla_j$. It turns out that the weaker control provided by (6.6) is still enough to conclude the proof of convergence to the infinite hierarchy (Theorem 5.1). For more details, see [9, Section 8].

A Uniqueness for Bounded Interactions and for a Coulomb Potential

The main difficulty in proving the uniqueness of the infinite hierarchy (3.2) is the singularity of the δ -function. For more regular potential, the proof of the uniqueness of the infinite hierarchy does not require an expansion in Feynman graphs. In this section we show the uniqueness of the infinite hierarchy for bounded interaction, and then, in a different space, for a Coulomb potential. The proof in the case of bounded potential is due to Spohn, see [14]. For Coulomb potential, the proof was obtained by Erdős and Yau in [10].

Theorem A.1 (Bounded potential, [14]). *Suppose that $V \in L^\infty(\mathbb{R}^3)$. Fix $T > 0$ and $\Gamma = \{\gamma^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} \mathcal{L}_k^1$. Then there exists at most one solution $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ to the infinite hierarchy*

$$\gamma_t^{(k)} = \mathcal{U}^{(k)}(t) \gamma_0^{(k)} - i \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[V(x_j - x_{k+1}), \gamma_s^{(k+1)} \right] \quad (\text{A.1})$$

with $\text{Tr} |\gamma_t^{(k)}| \leq 1$ for all $k \geq 1$ and $t \in [0, T]$ and with $\Gamma_{t=0} = \Gamma$. In (A.1), Tr_{k+1} denotes the partial trace over the degrees of freedom of the $(k+1)$ -th particle and $\mathcal{U}^{(k)}(t)$ is defined in (3.4).

Proof. We define $B^{(k)}$ as a map from \mathcal{L}_{k+1}^1 into \mathcal{L}_k^1 by

$$B^{(k)}\gamma^{(k+1)} = \sum_{j=1}^k \text{Tr}_{k+1} \left[V(x_j - x_{k+1}), \gamma^{(k+1)} \right]$$

Using that

$$\text{Tr}^{(k)} |\text{Tr}_{k+1} A| \leq \text{Tr}^{(k+1)} |A|$$

for every $A \in \mathcal{L}_{k+1}^1$ (here we use the notation $\text{Tr}^{(k)}$ to indicate the trace of a k -particle operator; in the following we will skip the superscript, and the meaning of the symbol Tr will be clear from the context), and the bound $\text{Tr}|AB| \leq \|A\|\text{Tr}|B|$, we obtain that

$$\begin{aligned} \text{Tr} \left| B^{(k)}\gamma^{(k+1)} \right| &\leq \sum_{j=1}^k \left(\text{Tr} \left| V(x_j - x_{k+1})\gamma^{(k+1)} \right| + \text{Tr} \left| \gamma^{(k+1)}V(x_j - x_{k+1}) \right| \right) \\ &\leq 2k\|V\|\text{Tr} \left| \gamma^{(k+1)} \right|, \end{aligned} \quad (\text{A.2})$$

where $\|V\|$ indicates the operator norm of the multiplication operator V , which is the same as the L^∞ -norm of the function $V(x)$. Iterating the integral equation (A.1), we obtain that

$$\begin{aligned} \gamma_t^{(k)} &= \mathcal{U}^{(k)}(t)\gamma_0^{(k)} \\ &+ \sum_{m=1}^{n-1} (-i)^m \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) \dots \\ &\quad \times B^{(k+m-1)} \mathcal{U}^{(k+m)}(s_m) \gamma_0^{(k+m)} \\ &+ (-i)^n \int_0^t ds_1 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) \dots B^{(k+n-1)} \gamma_{s_n}^{(k+n)}. \end{aligned} \quad (\text{A.3})$$

Suppose now that $\Gamma_{1,t} = \{\gamma_{1,t}^{(k)}\}_{k \geq 1}$ and $\Gamma_{2,t} = \{\gamma_{2,t}^{(k)}\}_{k \geq 1}$ are two solutions of (A.1), with the same initial data. Then we can expand both of them in the Duhamel series (A.3) of order $n \geq 1$. Taking the difference between the two expansions, we find

$$\begin{aligned} \gamma_{t,1}^{(k)} - \gamma_{t,2}^{(k)} &= (-i)^n \int_0^t ds_1 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1) B^{(k)} \mathcal{U}^{(k+1)}(s_1-s_2) \dots \\ &\quad \times B^{(k+n-1)} \left(\gamma_{1,s_n}^{(k+n)} - \gamma_{2,s_n}^{(k+n)} \right). \end{aligned} \quad (\text{A.4})$$

Taking the trace norm, using (A.2) and the fact that

$$\text{Tr} \left| \mathcal{U}^{(k)}(t)\gamma^{(k)} \right| = \text{Tr} \left| \gamma^{(k)} \right|$$

we obtain that

$$\begin{aligned} \text{Tr} \left| \gamma_{t,1}^{(k)} - \gamma_{t,2}^{(k)} \right| &\leq k(k+1) \dots (k+n) 2^n \|V\|^n \int_0^t ds_1 \dots \int_0^{s_{n-1}} ds_n \text{Tr} \left| \gamma_{1,s_n}^{(k+n)} - \gamma_{2,s_n}^{(k+n)} \right| \\ &\leq 2(2\|V\|t)^n \frac{(k+n)!}{k!n!} \\ &\leq 2^{k+1} (4\|V\|t)^n. \end{aligned} \quad (\text{A.5})$$

Since the l.h.s. is independent of n , it follows that it must vanish, for every fixed k and for all $t \leq 1/(8\|V\|)$. This proves the uniqueness for short times; the argument can then be iterated to prove uniqueness for all times. \square

The Coulomb potential $V(x) = \pm 1/|x|$ is not bounded, and therefore the previous proof does not apply. It turns out, however, that the Coulomb potential is bounded by the kinetic energy. In fact, as an operator inequality, we have, in three dimensions,

$$\frac{1}{|x|} \leq \frac{\pi}{2} |\nabla| \leq \frac{\pi}{2} (1 - \Delta).$$

This bound suggests to consider the uniqueness problem in the space of densities with bounded H^1 -norm. Actually the $H^{1/2}$ -norm would be enough, but then the proof is more involved (see [5], where the pseudo-relativistic Hartree equation is derived; in this case, the kinetic energy is essentially only $|\nabla|$ instead of $-\Delta$); we present here only the easier case. Note that, in three dimensions, the δ -function interaction cannot be bounded by the kinetic energy (in fact $\delta(x) \leq C(1 - \Delta)^\alpha$, only if $\alpha > 3/2$); this explains why the proof of the uniqueness in the case of a δ -interaction is more involved.

Theorem A.2 (Coulomb potential, [10]). *Let $S_j = (1 - \Delta_j)^{1/2}$ and fix $T > 0$. Then, for every $\Gamma = \{\gamma^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} \mathcal{L}_k^1$, there exists at most one solution $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \bigoplus_{k \geq 1} C([0, T], \mathcal{L}_k^1)$ to the infinite hierarchy*

$$\gamma_t^{(k)} = \mathcal{U}^{(k)}(t) \gamma_0^{(k)} - i \sum_{j=1}^k \int_0^t ds \mathcal{U}^{(k)}(t-s) \text{Tr}_{k+1} \left[\frac{1}{|x_j - x_{k+1}|}, \gamma_s^{(k+1)} \right] \quad (\text{A.6})$$

with $\Gamma_{t=0} = \Gamma$ and such that there exists a constant $D > 0$ with

$$\|\gamma_t^{(k)}\|_{\mathcal{H}_k} = \text{Tr} |S_1 \dots S_k \gamma_t^{(k)} S_k \dots S_1| \leq D^k \quad (\text{A.7})$$

for all $k \geq 1$ and all $t \in [0, T]$.

Proof. Using again the notation

$$B^{(k)} \gamma^{(k+1)} = \sum_{j=1}^k \text{Tr}_{k+1} \left[\frac{1}{|x_j - x_{k+1}|}, \gamma^{(k+1)} \right]$$

we observe that there exists a constant $C > 0$, with

$$\|B^{(k)} \gamma^{(k+1)}\|_{\mathcal{H}_k} \leq Ck \|\gamma^{(k+1)}\|_{\mathcal{H}_{k+1}}. \quad (\text{A.8})$$

To prove (A.8), we write

$$\begin{aligned} \|B^{(k)} \gamma^{(k+1)}\|_{\mathcal{H}_k} &\leq \sum_{j=1}^k \text{Tr}^{(k)} \left| S_1 \dots S_k \left(\text{Tr}_{k+1} \frac{1}{|x_j - x_{k+1}|} \gamma^{(k+1)} \right) S_k \dots S_1 \right| \\ &\quad + \sum_{j=1}^k \text{Tr}^{(k)} \left| S_1 \dots S_k \left(\text{Tr}_{k+1} \gamma^{(k+1)} \frac{1}{|x_j - x_{k+1}|} \right) S_k \dots S_1 \right|. \end{aligned} \quad (\text{A.9})$$

All terms can be handled similarly. We show how to bound the summand with $j = 1$ on the first

line.

$$\begin{aligned}
& \text{Tr}^{(k)} \left| S_1 \dots S_k \left(\text{Tr}_{k+1} \frac{1}{|x_1 - x_{k+1}|} \gamma^{(k+1)} \right) S_k \dots S_1 \right| \\
&= \text{Tr}^{(k)} \left| S_1 \dots S_k \left(\text{Tr}_{k+1} S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_{k+1} \gamma^{(k+1)} S_{k+1} \right) S_k \dots S_1 \right| \\
&\leq \text{Tr}^{(k+1)} \left| S_1 S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1^{-1} S_1 \dots S_k S_{k+1} \gamma^{(k+1)} S_{k+1} S_k \dots S_1 \right| \quad (\text{A.10}) \\
&\leq \|S_1 S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1^{-1}\| \|\gamma^{(k+1)}\|_{\mathcal{H}_{k+1}} \\
&\leq C \|\gamma^{(k+1)}\|_{\mathcal{H}_{k+1}}
\end{aligned}$$

where in the second line we used the cyclicity of the partial trace, and, in the last line, we used the bound (without restriction of generality, we can assume that $k = 1$)

$$\|S_1 S_2^{-1} \frac{1}{|x_1 - x_2|} S_2^{-1} S_1^{-1}\| < \infty. \quad (\text{A.11})$$

To prove (A.11), we write

$$S_1 S_2^{-1} \frac{1}{|x_1 - x_2|} S_2^{-1} S_1^{-1} = S_2^{-1} \frac{1}{|x_1 - x_2|} S_2^{-1} + S_2^{-1} \left[S_1, \frac{1}{|x_1 - x_2|} \right] S_2^{-1}. \quad (\text{A.12})$$

The norm of the first term is finite, because of the operator inequality

$$\frac{1}{|x_1 - x_2|} \leq \frac{\pi}{2} |\nabla_2| \leq \frac{\pi}{2} (1 - \Delta_2) = \frac{\pi}{2} S_2^2.$$

The second term on the r.h.s. of (A.12) is also bounded. In fact, expanding the commutator, we find

$$\begin{aligned}
S_2^{-1} \left[S_1, \frac{1}{|x_1 - x_2|} \right] S_2^{-1} &= \frac{2}{\pi} \int_0^\infty ds s^{1/2} S_2^{-1} \frac{1}{s+1-\Delta_1} \left(\nabla_1 \frac{1}{|x_1 - x_2|} \right) \frac{1}{s+1-\Delta_1} S_2^{-1} \\
&= \frac{2}{\pi} \int_0^\infty ds s^{1/2} \frac{1}{s+1-\Delta_1} S_2^{-1} \frac{(x_1 - x_2)}{|x_1 - x_2|^3} S_2^{-1} \frac{1}{s+1-\Delta_1}. \quad (\text{A.13})
\end{aligned}$$

Taking the norm, and using that, by Hardy's inequality

$$\pm \frac{(x_1 - x_2)}{|x_1 - x_2|^3} \leq 4S_2^2,$$

we obtain

$$\left\| S_2^{-1} \left[S_1, \frac{1}{|x_1 - x_2|} \right] S_2^{-1} \right\| \leq C \int_0^\infty ds s^{1/2} \left\| \frac{1}{s+1-\Delta_1} \right\|^2 \leq C \int_0^\infty ds s^{1/2} \frac{1}{(s+1)^2} \leq C. \quad (\text{A.14})$$

As in the proof of Theorem A.1, we are led to the expansion (A.4) for the difference $\gamma_{1,t}^{(k)} - \gamma_{2,t}^{(k)}$ of two hypothetical solutions. The \mathcal{H}_k -norm of this difference can then be estimated, using (A.8) and the fact that $\|\mathcal{U}^{(k)} \gamma^{(k)}\|_{\mathcal{H}_k} = \|\gamma^{(k)}\|_{\mathcal{H}_k}$, by

$$\begin{aligned}
\left\| \gamma_{1,t}^{(k)} - \gamma_{2,t}^{(k)} \right\|_{\mathcal{H}_k} &\leq (2C)^n \frac{(k+n)!}{k!} \int_0^t ds_1 \dots \int_0^{s_{n-1}} ds_n \|\gamma_{1,s_n}^{(k+n)} - \gamma_{2,s_n}^{(k+n)}\|_{\mathcal{H}_{k+n}} \\
&\leq 2(2Ct)^n \frac{(k+n)!}{k!n!} D^{k+n} \\
&\leq 2^{k+1} D^k (4CDt)^n
\end{aligned} \quad (\text{A.15})$$

for any n . Here we used the a-priori bounds (A.7). For $t \leq 1/(8CD)$, the l.h.s. must vanish. This shows uniqueness for short time, and thus, by iteration, for all times. \square

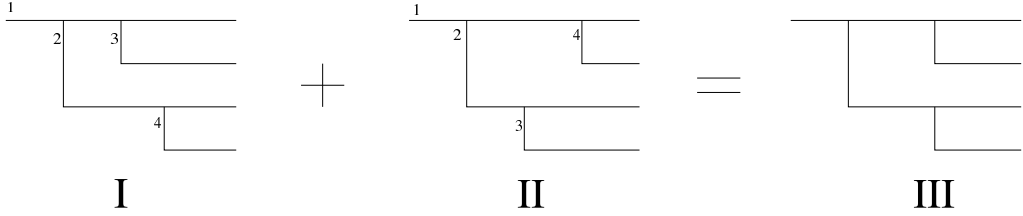


Figure 8: Removing the order

B Removing the Time Ordering

In this section we show, through a simple example, how the total time-ordering characterizing the Duhamel expansion (3.11) disappears when we switch to the representation (3.20) or (3.22) in terms of Feynman graphs. We start with the two contributions to the Duhamel expansion which can be naturally associated with the ordered graphs I and II in Fig. 8; the graphs here just describe the collision histories of the terms we are interested in (since this effect can be understood on the level of classical graphs, we work with the graphs drawn in Fig. 8 and we always write the interaction on the left of the density). The contributions associated with the graphs I and II are given, respectively, by

$$\begin{aligned}
\text{I} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \mathcal{U}^{(1)}(t-s_1) \\
&\quad \times \text{Tr}_{2,3,4} \delta(x_1-x_2) \mathcal{U}^{(2)}(s_1-s_2) \delta(x_2-x_3) \mathcal{U}^{(3)}(s_2-s_3) \delta(x_1-x_4) \mathcal{U}^{(4)}(s_3) \gamma^{(4)} \\
&= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_1} ds_3 \chi(s_2 \geq s_3) \mathcal{U}^{(1)}(t-s_1) \\
&\quad \times \text{Tr}_{2,3,4} \delta(x_1-x_2) \mathcal{U}^{(2)}(s_1-s_2) \delta(x_2-x_3) \mathcal{U}^{(3)}(s_2-s_3) \delta(x_1-x_4) \mathcal{U}^{(4)}(s_3) \gamma^{(4)}
\end{aligned} \tag{B.1}$$

and by

$$\begin{aligned}
\text{II} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \mathcal{U}^{(1)}(t-s_1) \\
&\quad \times \text{Tr}_{2,3,4} \delta(x_1-x_2) \mathcal{U}^{(2)}(s_1-s_2) \delta(x_1-x_3) \mathcal{U}^{(3)}(s_2-s_3) \delta(x_2-x_4) \mathcal{U}^{(4)}(s_3) \gamma^{(4)}.
\end{aligned} \tag{B.2}$$

Here $\text{Tr}_{2,3,4}$ denotes the partial trace over x_2, x_3, x_4 , and the operator $\mathcal{U}^{(k)}(t)$ is defined in (3.4). The contribution (B.2) looks, at first sight, quite different from (B.1). We want to show that they are actually quite similar. To this end, we start by observing that, since x_3 and x_4 are just integration variables (because we take the partial trace over x_2, x_3, x_4), we can interchange them. We obtain (assuming that the density $\gamma^{(4)}$ is invariant w.r.t. permutations and using the notation $p_j = -i\nabla_j$)

$$\begin{aligned}
\text{II} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \mathcal{U}^{(1)}(t-s_1) \text{Tr}_{2,3,4} \delta(x_1-x_2) \\
&\quad \times \left(e^{i(p_1^2+p_2^2)(s_1-s_2)} \delta(x_1-x_4) e^{i(p_1^2+p_2^2+p_4^2)(s_2-s_3)} \delta(x_2-x_3) e^{i(p_1^2+p_2^2+p_3^2+p_4^2)s_3} \gamma^{(4)} \right. \\
&\quad \left. \times e^{-i(p_1^2+p_2^2+p_3^2+p_4^2)s_3} e^{-i(p_1^2+p_2^2+p_4^2)(s_2-s_3)} e^{-i(p_1^2+p_2^2)(s_1-s_2)} \right).
\end{aligned} \tag{B.3}$$

(Note that since we exchanged x_3 and x_4 , we also had to interchange the momenta p_3 and p_4). Next, we observe that the operator in the parenthesis, on the left of the density $\gamma^{(4)}$, can be reorganized as

$$\begin{aligned}
&e^{i(p_1^2+p_2^2)(s_1-s_2)} e^{ip_2^2(s_2-s_3)} \delta(x_1-x_4) \delta(x_2-x_3) e^{i(p_1^2+p_4^2)(s_2-s_3)} e^{i(p_1^2+p_2^2+p_3^2+p_4^2)s_3} \\
&= e^{i(p_1^2+p_2^2)(s_1-s_3)} \delta(x_2-x_3) e^{i(p_1^2+p_2^2+p_3^2)(s_3-s_2)} \delta(x_1-x_4) e^{i(p_1^2+p_2^2+p_3^2+p_4^2)s_2}.
\end{aligned} \tag{B.4}$$

Here we used the fact that p_j commutes with x_i , if $i \neq j$. Also the operator on the right of the density $\gamma^{(4)}$ in (B.3) can be clearly rearranged as

$$\begin{aligned} & e^{-i(p_1^2+p_2^2+p_3^2+p_4^2)s_3} e^{-i(p_1^2+p_2^2+p_4^2)(s_2-s_3)} e^{-i(p_1^2+p_2^2)(s_1-s_2)} \\ &= e^{-i(p_1^2+p_2^2+p_3^2+p_4^2)s_2} e^{-i(p_1^2+p_2^2+p_3^2)(s_3-s_2)} e^{-i(p_1^2+p_2^2)(s_1-s_3)}. \end{aligned} \quad (\text{B.5})$$

Inserting the last two equations on the r.h.s. of (B.3), we find that

$$\begin{aligned} \text{II} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_2} ds_3 \mathcal{U}^{(1)}(t-s_1) \\ &\quad \times \text{Tr}_{2,3,4} \delta(x_1-x_2) \mathcal{U}^{(2)}(s_1-s_3) \delta(x_2-x_3) \mathcal{U}^{(3)}(s_3-s_2) \delta(x_1-x_4) \mathcal{U}^{(4)}(s_2) \gamma^{(4)}. \end{aligned} \quad (\text{B.6})$$

Exchanging the two times s_2 and s_3 we obtain

$$\begin{aligned} \text{II} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_1} ds_3 \chi(s_2 \leq s_3) \mathcal{U}^{(1)}(t-s_1) \\ &\quad \times \text{Tr}_{2,3,4} \delta(x_1-x_2) \mathcal{U}^{(2)}(s_1-s_2) \delta(x_2-x_3) \mathcal{U}^{(3)}(s_2-s_3) \delta(x_1-x_4) \mathcal{U}^{(4)}(s_3) \gamma^{(4)}. \end{aligned} \quad (\text{B.7})$$

Comparing with (B.1), we conclude that the two ordered graphs I and II in Fig. 8 have the same value, with the only difference that the order of the times s_2 and s_3 is inverted. Therefore, we can define a single Feynman graph (graph III in Figure 8) with no ordering between the vertices associated with the times s_2 and s_3 , whose value is given by sum of I and II.

$$\begin{aligned} \text{III} = \text{I} + \text{II} &= \int_0^t ds_1 \int_0^{s_1} ds_2 \int_0^{s_1} ds_3 \mathcal{U}^{(1)}(t-s_1) \text{Tr}_{2,3,4} \delta(x_1-x_2) \\ &\quad \times \mathcal{U}^{(2)}(s_1-s_2) \delta(x_2-x_3) \mathcal{U}^{(3)}(s_2-s_3) \delta(x_1-x_4) \mathcal{U}^{(4)}(s_3) \gamma^{(4)}. \end{aligned} \quad (\text{B.8})$$

C Integral Estimates

In this section we collect some of the estimates for integrals over frequency- and momentum-variables needed to bound the contributions associated with Feynman graphs.

The first lemma is used to integrate out frequency variables (for example, to prove (3.39)).

Lemma C.1. *For every $\varepsilon, \lambda, \eta$ with $0 \leq \varepsilon < \lambda < 1$ and $0 < \eta < \lambda - \varepsilon$ there exists a constant $C_{\lambda, \varepsilon, \eta}$ such that*

$$\int_{-\infty}^{\infty} \frac{d\beta}{\langle \alpha - \beta \rangle^{1-\varepsilon} |\beta|^\lambda} \leq \frac{C_{\lambda, \varepsilon, \eta}}{\langle \alpha \rangle^{\lambda-\varepsilon-\eta}} \quad (\text{C.1})$$

for all $\alpha \in \mathbb{R}$.

Proof. If $|\alpha| \leq 1$, then $\langle \alpha \rangle \sim 1$, $\langle \alpha - \beta \rangle \sim \langle \beta \rangle$ and (C.1) is trivial. For $|\alpha| \geq 1$ we split the integral into two parts. For $|\beta| \leq |\alpha|/2$, we use

$$\frac{1}{\langle \alpha - \beta \rangle^{1-\varepsilon}} \lesssim \frac{1}{\langle \alpha - \beta \rangle^{1-\lambda+\eta} \langle \alpha \rangle^{\lambda-\varepsilon-\eta}}$$

and we obtain

$$\begin{aligned} \int_{|\beta| \leq |\alpha|/2} \frac{d\beta}{\langle \alpha - \beta \rangle^{1-\varepsilon} |\beta|^\lambda} &\leq \frac{C}{\langle \alpha \rangle^{\lambda-\varepsilon-\eta}} \int_{|\beta| \leq |\alpha|/2} \frac{d\beta}{\langle \alpha - \beta \rangle^{1-\lambda+\eta} |\beta|^\lambda} \\ &\leq \frac{C}{\langle \alpha \rangle^{\lambda-\varepsilon-\eta}} \left(\int_{|\beta| \leq 1/2} \frac{d\beta}{|\beta|^\lambda} + \int d\beta \left(\frac{1}{\langle \beta \rangle^{1+\eta}} + \frac{1}{\langle \alpha - \beta \rangle^{1+\eta}} \right) \right) \\ &\leq \frac{C}{\langle \alpha \rangle^{\lambda-\varepsilon-\eta}} \end{aligned} \quad (\text{C.2})$$

where we used the Schwarz inequality and the fact that, if $|\beta| \geq 1/2$, $|\beta| \sim \langle \beta \rangle$. For $|\beta| \geq |\alpha|/2$, on the other hand, we use

$$\frac{1}{|\beta|^\lambda} \lesssim \frac{1}{|\alpha|^{\lambda-\varepsilon-\eta} |\beta|^{\varepsilon+\eta}} \lesssim \frac{1}{\langle \alpha \rangle^{\lambda-\varepsilon-\eta} |\beta|^{\varepsilon+\eta}}$$

and conclude similarly. \square

The next two lemmas, on the other hand, are used to integrate out momenta. The first one, in particular, is used when we have to face lack of decay on planes (propagators of the form $\langle \alpha - p \cdot a \rangle^{-1}$ do not decay as $|p| \rightarrow \infty$ with $p \cdot a = \alpha$). The second one on the other hand deals with spherical denominators of the form $\langle \alpha - (p-a)^2 \rangle^{-1}$. Note the plane-singularities result from spherical denominators like $\langle \alpha - p^2 + (q-p)^2 \rangle^{-1} = \langle \alpha + q^2 - 2q \cdot p \rangle^{-1}$ (integrating over p for fixed q); such terms are encountered, for example, in Proposition C.4 below.

Lemma C.2. *For any $\varepsilon, \delta, \eta$ with $0 \leq \varepsilon < 2\delta < 1$, and $0 < \eta < 2\delta - \varepsilon$, there exists a constant $C_{\delta, \eta, \varepsilon}$ such that*

$$I = \int \frac{dp}{|p|^{2+2\delta} \langle \alpha - p \cdot a \rangle^{1-\varepsilon}} \leq \frac{C_{\delta, \eta, \varepsilon}}{\langle \alpha \rangle^{2\delta-\varepsilon-\eta} |a|^{1-2\delta}} \quad (\text{C.3})$$

for every $a \in \mathbb{R}^3$, $\alpha \in \mathbb{R}$.

Proof. By rotational symmetry, we can assume $a = (|a|, 0, 0)$. Introducing the variable $\varrho = p_2^2 + p_3^2$, we find

$$I \lesssim \int_{\mathbb{R}} \frac{dp_1}{\langle \alpha - p_1 |a| \rangle^{1-\varepsilon}} \int_0^\infty \frac{d\varrho}{|p_1^2 + \varrho|^{1+\delta}} \lesssim \int_{\mathbb{R}} \frac{dp_1}{\langle \alpha - p_1 |a| \rangle^{1-\varepsilon} |p_1|^{2\delta}} = \frac{1}{|a|^{1-2\delta}} \int_{\mathbb{R}} \frac{dy}{\langle \alpha - y \rangle^{1-\varepsilon} |y|^{2\delta}}$$

and we conclude by (C.1). \square

Lemma C.3. *For every $\varepsilon, \delta, \gamma$ with $0 \leq \varepsilon < 1$, $\delta < (1/2) - \varepsilon$, $\delta > -1/2$, and $0 \leq \gamma < \min(1 - \varepsilon; 1 + 2\delta; 1 - 2\delta - 2\varepsilon)$, and for every $\eta > 0$ sufficiently small (depending on $\varepsilon, \delta, \gamma$), there exists a constant $C = C_{\delta, \varepsilon, \gamma, \eta}$ with*

$$I = \int \frac{dp}{|p|^{2-2\delta} \langle \alpha - (p-a)^2 \rangle^{1-\varepsilon}} \leq \frac{C}{\langle a \rangle^\gamma \langle \alpha - a^2 \rangle^{\frac{1}{2} - \frac{\gamma}{2} - \delta - \varepsilon - \eta}} \quad (\text{C.4})$$

for all $\alpha \in \mathbb{R}$ and $a \in \mathbb{R}^3$.

Proof. We consider first the case $|a| < 1$. Then $\langle \alpha - a^2 \rangle \sim \langle \alpha \rangle$ and $\langle a \rangle \sim 1$, so it is sufficient to prove the estimate (C.4) when a^2 and $\langle a \rangle$ are removed from the r.h.s. of (C.4). We now distinguish two cases, depending on the size of $|\alpha|$.

If $|\alpha| \leq 10$, then the integral I is comparable with

$$I \lesssim \int \frac{dp}{|p|^{2-2\delta} \langle p-a \rangle^{2-2\varepsilon}} \lesssim \int_{|p| \leq 1} \frac{dp}{|p|^{2-2\delta}} + \int dp \left(\frac{1}{\langle p \rangle^{4-2\delta-2\varepsilon}} + \frac{1}{\langle p-a \rangle^{4-2\delta-2\varepsilon}} \right)$$

which is uniformly bounded in α and a . Here we applied a Schwarz inequality, and we used that, by assumption, $\delta > -1/2$ and $\delta + \varepsilon < 1/2$. Since in this case $\langle \alpha \rangle \simeq 1$, this proves (C.4).

If $|\alpha| \geq 10$, then we split the dp -integration into three different regimes. In the regime $p^2 \leq |\alpha|/2$ we have $\langle \alpha - (p-a)^2 \rangle \sim \langle \alpha \rangle$ and, putting $y = p^2$,

$$\int_{|p|^2 \leq |\alpha|/2} \frac{dp}{|p|^{2-2\delta} \langle \alpha - (p-a)^2 \rangle^{1-\varepsilon}} \lesssim \frac{1}{\langle \alpha \rangle^{1-\varepsilon}} \int_0^{|\alpha|/2} dy \frac{1}{|y|^{\frac{1}{2}-\delta}} \lesssim \frac{1}{\langle \alpha \rangle^{\frac{1}{2}-\varepsilon-\delta}} \quad (\text{C.5})$$

because $\delta > -1/2$. In the regime $|\alpha|/2 \leq p^2 \leq 2|\alpha|$ we have

$$\begin{aligned} \int_{|\alpha|/2 \leq p^2 \leq 2|\alpha|} \frac{dp}{|p|^{2-2\delta} \langle \alpha - (p-a)^2 \rangle^{1-\varepsilon}} &\lesssim \frac{1}{\langle \alpha \rangle^{1-\delta}} \int_{|\alpha|/2 \leq p^2 \leq 2|\alpha|} \frac{dp}{\langle \alpha - (p-a)^2 \rangle^{1-\varepsilon}} \\ &\leq \frac{1}{\langle \alpha \rangle^{1-\delta}} \int_{|\alpha|/2 \leq (q+a)^2 \leq 2|\alpha|} \frac{dq}{\langle \alpha - q^2 \rangle^{1-\varepsilon}} \leq \frac{1}{\langle \alpha \rangle^{1-\delta}} \int_{|\alpha|/3 \leq q^2 \leq 3|\alpha|} \frac{dq}{\langle \alpha - q^2 \rangle^{1-\varepsilon}} \\ &\lesssim \frac{1}{\langle \alpha \rangle^{1-\delta}} \int_{|\alpha|/3}^{3|\alpha|} \frac{dy \sqrt{y}}{\langle \alpha - y \rangle^{1-\varepsilon}} \lesssim \frac{1}{\langle \alpha \rangle^{\frac{1}{2}-\delta}} \int_{|\alpha|/3}^{3|\alpha|} \frac{dy}{|\alpha - y|^{1-\varepsilon}} \lesssim \frac{1}{\langle \alpha \rangle^{\frac{1}{2}-\varepsilon-\delta}}. \end{aligned} \quad (\text{C.6})$$

Finally, for $p^2 \geq 2|\alpha|$, we have $\langle \alpha - (p-a)^2 \rangle \sim p^2$ and hence

$$\int_{p^2 \geq 2|\alpha|} \frac{dp}{|p|^{2-2\delta} \langle \alpha - (p-a)^2 \rangle^{1-\varepsilon}} \lesssim \int_{p^2 \geq 2|\alpha|} \frac{dp}{|p|^{4-2\delta-2\varepsilon}} \lesssim \frac{1}{\langle \alpha \rangle^{\frac{1}{2}-\varepsilon-\delta}}. \quad (\text{C.7})$$

Combining (C.5), (C.6), and (C.7), we obtain (C.4) for arbitrary $\gamma \geq 0$ and $\eta > 0$.

Now we turn to the case $|a| \geq 1$. By rotational symmetry, we can assume that $a = (|a|, 0, 0)$. After a change of variables and introducing $\varrho := p_2^2 + p_3^2$ we find

$$I \lesssim \int_{\mathbb{R}} dp_1 \int_0^\infty \frac{d\varrho}{|\varrho + p_1^2|^{1-\delta} \langle \alpha - a^2 - \varrho - p_1^2 + 2|a|p_1 \rangle^{1-\varepsilon}}.$$

We define the new variables:

$$u := \varrho + p_1^2, \quad v := \alpha - a^2 - u + 2|a|p_1.$$

The map $D \ni (u, v) \rightarrow (p_1, \varrho) \in \mathbb{R} \times [0, \infty)$ is one-to-one if we choose

$$D = \left\{ (u, v) \in \mathbb{R}^2 : u \geq \left(\frac{\alpha - a^2 - u - v}{2|a|} \right)^2 \right\}.$$

Computing the Jacobian of this transformation, we obtain

$$I \lesssim \frac{1}{|a|} \int_D \frac{dudv}{|u|^{1-\delta} \langle v \rangle^{1-\varepsilon}}.$$

Using the definition of the domain D , we get, for $0 \leq \gamma \leq 1$,

$$I \lesssim \frac{1}{|a|} \int_D \frac{dudv}{|u|^{\frac{1}{2}+\frac{\gamma}{2}-\delta} \langle v \rangle^{1-\varepsilon} \left| \frac{\alpha - a^2 - u - v}{2|a|} \right|^{1-\gamma}} \lesssim \frac{1}{|a|^\gamma} \int_{\mathbb{R}^2} \frac{dudv}{|u|^{\frac{1}{2}+\frac{\gamma}{2}-\delta} |\alpha - a^2 - u - v|^{1-\gamma} \langle v \rangle^{1-\varepsilon}}. \quad (\text{C.8})$$

Applying the bound (C.1) twice, to integrate first over v and then over u , and using the assumptions that $0 \leq \gamma < \min(1 - \varepsilon; 1 + 2\delta; 1 - 2\delta - 2\varepsilon)$ and that η is small enough, we find

$$I \lesssim \frac{1}{|a|^\gamma} \int_{\mathbb{R}} \frac{du}{|u|^{\frac{1}{2}+\frac{\gamma}{2}-\delta} \langle \alpha - a^2 - u \rangle^{1-\gamma-\varepsilon-\frac{\eta}{2}}} \lesssim \frac{C_{\delta, \varepsilon, \gamma, \varepsilon}}{\langle a \rangle^\gamma \langle \alpha - a^2 \rangle^{\frac{1}{2}-\frac{\gamma}{2}-\delta-\varepsilon-\eta}}. \quad (\text{C.9})$$

Here we used that $|a| \geq 1$, to replace $|a|$ by $\langle a \rangle$. \square

Using the last two lemmas, we can now show how the bound (3.40), needed to integrate out the momenta of three son-edges and obtain decay in the momentum of the father edge, can be established rigorously.

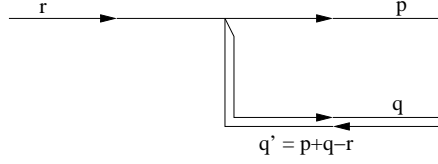


Figure 9: The vertex of Prop. C.4

Proposition C.4. *Suppose $\kappa_1, \kappa_2, \kappa_3 \geq 0$ with $0 < \kappa_1 + \kappa_2 + \kappa_3 < 1$. Let $0 \leq \kappa < \kappa_1 + \kappa_2 + \kappa_3$, and $\varepsilon < (\kappa_1 + \kappa_2 + \kappa_3 - \kappa)/2$. Then there is a constant $C = C(\kappa_1, \kappa_2, \kappa_3, \kappa, \varepsilon)$ such that*

$$\sup_{\alpha} \int \frac{dp dq}{|p|^{2+\kappa_1} |q|^{2+\kappa_2} |r-p-q|^{2+\kappa_3}} \frac{1}{\langle \alpha - p^2 - q^2 + (r-p-q)^2 \rangle^{1-\varepsilon}} \leq \frac{1}{|r|^{2+\kappa}} \quad (\text{C.10})$$

Proof. Using

$$\frac{1}{|p|^{\kappa_1} |q|^{\kappa_2} |r-p-q|^{\kappa_3}} \leq \left(\frac{1}{|p|^{\theta}} + \frac{1}{|q|^{\theta}} + \frac{1}{|r-p-q|^{\theta}} \right)$$

with $\theta = \kappa_1 + \kappa_2 + \kappa_3$, and the symmetry of the integrand w.r.t. the exchange $p \leftrightarrow q$, the l.h.s. of (C.10) is bounded by

$$\begin{aligned} & 2 \sup_{\alpha} \int \frac{dp dq}{|p|^{2+\theta} |q|^2 |r-p-q|^2} \frac{1}{\langle \alpha - p^2 - q^2 + (r-p-q)^2 \rangle^{1-\varepsilon}} \\ & + \sup_{\alpha} \int \frac{dp dq}{|p|^2 |q|^{2+\theta} |r-p-q|^{2+\theta}} \frac{1}{\langle \alpha - p^2 - q^2 + (r-p-q)^2 \rangle^{1-\varepsilon}} \\ & \lesssim \sup_{\alpha} \int \frac{dq}{|q|^2 |r-q|^2} \int dp \left(\frac{1}{|p|^{2+\theta}} + \frac{1}{|r-q-p|^{2+\theta}} \right) \frac{1}{\langle \alpha - p^2 - q^2 + (r-p-q)^2 \rangle^{1-\varepsilon}} \quad (\text{C.11}) \\ & \lesssim \sup_{\alpha_1} \int \frac{dq}{|q|^2 |r-q|^2} \int \frac{dp}{|p|^{2+\theta}} \frac{1}{\langle \alpha_1 - 2r \cdot q - 2p \cdot (r-q) \rangle^{1-\varepsilon}} \\ & + \sup_{\alpha_2} \int \frac{dq}{|q|^2 |r-q|^2} \int \frac{dp}{|p|^{2+\theta}} \frac{1}{\langle \alpha_2 - 2(q - \frac{r}{2})^2 + 2p \cdot (r-q) \rangle^{1-\varepsilon}} \end{aligned}$$

where we applied the inequality

$$\frac{1}{|a|^{\alpha} |b-a|^{\beta}} \leq \frac{C}{|b|^{\gamma}} \left(\frac{1}{|a|^{\alpha+\beta-\gamma}} + \frac{1}{|b-a|^{\alpha+\beta-\gamma}} \right) \quad (\text{C.12})$$

valid for all $\alpha, \beta > 0$ with $0 \leq \gamma \leq \min(\alpha, \beta)$, and, to obtain the last term, we shifted the variable $q \rightarrow (r-p-q)$. Applying Lemma C.2 we conclude that the l.h.s. of (C.10) can be estimated by

$$\begin{aligned} & \sup_{\alpha} \int \frac{dp dq}{|p|^{2+\kappa_1} |q|^{2+\kappa_2} |r-p-q|^{2+\kappa_3}} \frac{1}{\langle \alpha - p^2 - q^2 + (r-p-q)^2 \rangle^{1-\varepsilon}} \\ & \lesssim \sup_{\alpha_1} \int \frac{dq}{|q|^2 |r-q|^{3-\theta}} \frac{1}{\langle \alpha_1 - 2r \cdot q \rangle^{\theta-\varepsilon-\eta}} \quad (\text{C.13}) \\ & + \sup_{\alpha_2} \int \frac{dq}{|q|^2 |r-q|^{3-\theta}} \frac{1}{\langle \alpha_2 - 2(q - \frac{r}{2})^2 \rangle^{\theta-\varepsilon-\eta}}, \end{aligned}$$

for any sufficiently small $\eta > 0$. To bound the first term we use again (C.12) and Lemma C.2:

$$\begin{aligned}
& \sup_{\alpha_1} \int \frac{dq}{|q|^2|r-q|^{3-\theta}} \frac{1}{\langle \alpha_1 - 2r \cdot q \rangle^{\theta-\varepsilon-\eta}} \\
& \lesssim \frac{1}{|r|^{2-\frac{\theta-\kappa}{2}}} \sup_{\alpha_1} \int dq \left(\frac{1}{|q|^{3-\frac{\theta+\kappa}{2}}} + \frac{1}{|r-q|^{3-\frac{\theta+\kappa}{2}}} \right) \frac{1}{\langle \alpha_1 - 2r \cdot q \rangle^{\theta-\varepsilon-\eta}} \\
& \lesssim \frac{1}{|r|^{2+\kappa}} \sup_{\alpha_1} \frac{1}{\langle \alpha_1 \rangle^{\frac{\theta-\kappa}{2}-\varepsilon-2\eta}} \lesssim \frac{1}{|r|^{2+\kappa}},
\end{aligned} \tag{C.14}$$

because $\kappa < \theta$, $0 \leq 2\varepsilon < \theta - \kappa$ and $\eta > 0$ is arbitrarily small. Using (C.12) and Lemma C.3 (with $\gamma = \kappa$), the second term on the r.h.s. of (C.13) can be controlled by:

$$\begin{aligned}
& \sup_{\alpha_2} \int \frac{dq}{|q|^2|r-q|^{3-\theta}} \frac{1}{\langle \alpha_2 - 2(q - \frac{r}{2})^2 \rangle^{\theta-\varepsilon-\eta}} \\
& \lesssim \frac{1}{|r|^2} \sup_{\alpha_2} \int dp \left(\frac{1}{|q|^{3-\theta}} + \frac{1}{|r-q|^{3-\theta}} \right) \frac{1}{\langle \alpha_2 - 2(q - \frac{r}{2})^2 \rangle^{\theta-\varepsilon-\eta}} \\
& \lesssim \frac{1}{|r|^{2+\kappa}} \sup_{\alpha_3} \frac{1}{\langle \alpha_3 \rangle^{\frac{\theta-\kappa}{2}-\varepsilon-2\eta}} \lesssim \frac{1}{|r|^{2+\kappa}},
\end{aligned} \tag{C.15}$$

because $\theta > \kappa$ and $2\varepsilon < \theta - \kappa$, and η is arbitrarily small. This completes the proof of (C.10). \square

D Non-Standard Sobolev- and Poincaré Inequalities

In this section, we collect some non-standard Sobolev- and Poincaré-type inequalities which are very useful when dealing with singular potentials.

Lemma D.1 (Sobolev-type inequalities). *Let $\psi \in L^2(\mathbb{R}^6, dx_1 dx_2)$. If $V \in L^{3/2}(\mathbb{R}^3)$, we have*

$$\langle \psi, V(x_1 - x_2)\psi \rangle \leq C \|V\|_{3/2} \langle \psi, (1 - \Delta_1)\psi \rangle. \tag{D.1}$$

If $V \in L^1(\mathbb{R}^3)$, then

$$\langle \psi, V(x_1 - x_2)\psi \rangle \leq C \|V\|_1 \langle \psi, (1 - \Delta_1)(1 - \Delta_2)\psi \rangle \tag{D.2}$$

The first bound follows from a Hölder inequality followed by a standard Sobolev inequality (in the variable x_1 , with fixed x_2). The proof of (D.2) can be obtained by following the same arguments as in the proof of the next Poincaré-type inequality (with $\kappa = 0$),

Lemma D.2 (Poincaré-type inequality). *Suppose that $h \in L^1(\mathbb{R}^3)$ is a probability density with $\int dx |x|^{1/2} h(x) < \infty$. For $\alpha > 0$, let $h_\alpha(x) = \alpha^{-3} h(x/\alpha)$. Then we have, for every $0 \leq \kappa < 1/2$,*

$$|\langle \varphi, (h_\alpha(x_1 - x_2) - \delta(x_1 - x_2))\psi \rangle| \leq C \alpha^\kappa \langle \varphi, (1 - \Delta_1)(1 - \Delta_2)\varphi \rangle^{1/2} \langle \psi, (1 - \Delta_1)(1 - \Delta_2)\psi \rangle^{1/2}.$$

Proof. We rewrite the inner product in Fourier space.

$$\begin{aligned}
& \langle \varphi, \left(h_\alpha(x_1 - x_2) - \delta(x_1 - x_2) \right) \psi \rangle \\
& = \int dp_1 dp_2 dq_1 dq_2 dx \delta(p_1 + p_2 - q_1 - q_2) \widehat{\varphi}(p_1, p_2) \widehat{\psi}(q_1, q_2) h(x) \left(e^{i\alpha(p_1 - q_1) \cdot x} - 1 \right).
\end{aligned} \tag{D.3}$$

Using that $|e^{i\alpha(p_1 - q_1) \cdot x} - 1| \leq \alpha^\kappa |x|^\kappa |p_1 - q_1|^\kappa$, we obtain

$$\begin{aligned} & \left| \langle \varphi, (h_\alpha(x_1 - x_2) - \delta(x_1 - x_2)) \psi \rangle \right| \\ & \leq \alpha^\kappa \left(\int dx h(x) |x|^\kappa \right) \\ & \quad \times \int dp_1 dp_2 dq_1 dq_2 \delta(p_1 + p_2 - q_1 - q_2) (|p_1|^\kappa + |q_1|^\kappa) |\widehat{\varphi}(p_1, p_2)| |\widehat{\psi}(q_1, q_2)|. \end{aligned}$$

We show how to control the term proportional to $|p_1|^\kappa$; the other term can be handled similarly.

$$\begin{aligned} & \left| \langle \varphi, (h_\alpha(x_1 - x_2) - \delta(x_1 - x_2)) \psi \rangle \right| \\ & \leq C \alpha^\kappa \int dp_1 dp_2 dq_1 dq_2 \delta(p_1 + p_2 - q_1 - q_2) \frac{|p_1|^\kappa (1 + p_1^2)^{(1-\kappa)/2} (1 + p_2^2)^{1/2}}{(1 + q_1^2)^{1/2} (1 + q_2^2)^{1/2}} |\widehat{\varphi}(p_1, p_2)| \\ & \quad \times \frac{(1 + q_1^2)^{1/2} (1 + q_2^2)^{1/2}}{(1 + p_1^2)^{(1-\kappa)/2} (1 + p_2^2)^{1/2}} |\widehat{\psi}(q_1, q_2)| \\ & \leq C \alpha^\kappa \left(\int dp_1 dp_2 dq_1 dq_2 \delta(p_1 + p_2 - q_1 - q_2) \frac{(1 + p_1^2)(1 + p_2^2)}{(1 + q_1^2)(1 + q_2^2)} |\widehat{\varphi}(p_1, p_2)|^2 \right)^{1/2} \\ & \quad \times \left(\int dp_1 dp_2 dq_1 dq_2 \delta(p_1 + p_2 - q_1 - q_2) \frac{(1 + q_1^2)(1 + q_2^2)}{(1 + p_1^2)^{1-\kappa} (1 + p_2^2)} |\widehat{\psi}(q_1, q_2)|^2 \right)^{1/2} \\ & \leq C \alpha^{1/2} \langle \varphi, (1 - \Delta_1)(1 - \Delta_2) \varphi \rangle^{1/2} \langle \psi, (1 - \Delta_1)(1 - \Delta_2) \psi \rangle^{1/2} \\ & \quad \times \left(\sup_p \int dq \frac{1}{(1 + q^2)(1 + (p - q)^2)} \right)^{1/2} \left(\sup_q \int dp \frac{1}{(1 + p^2)(1 + (q - p)^2)^{1-\kappa}} \right)^{1/2} \end{aligned}$$

The claim follows because

$$\sup_{q \in \mathbb{R}^3} \int dp \frac{1}{(1 + p^2)(1 + (q - p)^2)^{1-\kappa}} \leq C \quad (\text{D.4})$$

for all $\kappa < 1/2$. To prove (D.4) we consider the three regions $|p| > 2|q|$, $|q|/2 \leq |p| \leq 2|q|$ and $|p| < |q|/2$ separately. Since $|p - q| > |p|/2$ for $|p| > 2|q|$, it follows that

$$\int_{|p| > 2|q|} \frac{dp}{(1 + p^2)(1 + (q - p)^2)^{1-\kappa}} \leq \int_{|p| > 2|q|} \frac{dp}{\left(1 + \frac{p^2}{4}\right)^{2-\kappa}} < C \int \frac{dp}{(1 + p^2)^{2-\kappa}} < \infty$$

for $\kappa < 1/2$, uniformly in q . For $|p| < |q|/2$, we use the fact that $|q - p| > |q|/2$, and we obtain

$$\int_{|p| < |q|/2} \frac{dp}{(1 + p^2)(1 + (q - p)^2)^{1-\kappa}} \leq \frac{C}{(1 + q^2)^{1-\kappa}} \int_{|p| < |q|/2} \frac{dp}{1 + p^2} \leq \frac{C|q|}{(1 + q^2)^{1-\kappa}}$$

which is bounded uniformly in q . Finally, in the region $|q|/2 \leq |p| \leq 2|q|$, we use that

$$\int_{|q|/2 < |p| < 2|q|} \frac{dp}{(1 + p^2)(1 + (q - p)^2)^{1-\kappa}} \leq \frac{C}{(1 + q^2)} \int_{|p| < 3|q|} \frac{dp}{(1 + p^2)^{1-\kappa}} \leq C \frac{|q|^{2\kappa+1}}{1 + q^2} < \infty \quad (\text{D.5})$$

uniformly in $q \in \mathbb{R}^3$, for all $\kappa < 1/2$. □

In the approach developed in [9] for the case of large interaction potential we can only prove weaker estimates on the solution $\psi_{N,t}$ of the Schrödinger equation. As discussed in Section 6, we can only prove that

$$\langle W_{N,(i,j)}^* \psi_{N,t}, ((\nabla_i \cdot \nabla_j)^2 - \Delta_i - \Delta_j + 1) W_{N,(i,j)}^* \psi_{N,t} \rangle \leq C$$

uniformly in N and t . For this reason, we need estimates which only require the boundedness of the expectation of this particular combination of derivatives. The next lemma gives a Sobolev inequality of this type.

Lemma D.3. *Suppose $V \in L^1(\mathbb{R}^3)$. Then*

$$|\langle \varphi, V(x_1 - x_2) \psi \rangle| \leq C \|V\|_1 \langle \psi, ((\nabla_1 \cdot \nabla_2)^2 - \Delta_1 - \Delta_2 + 1) \psi \rangle^{1/2} \times \langle \varphi, ((\nabla_1 \cdot \nabla_2)^2 - \Delta_1 - \Delta_2 + 1) \varphi \rangle^{1/2} \quad (\text{D.6})$$

for every $\psi, \varphi \in L^2(\mathbb{R}^6, dx_1 dx_2)$.

Proof. Switching to Fourier space, we find

$$\langle \varphi, V(x_1 - x_2) \psi \rangle = \int dp_1 dp_2 dq_1 dq_2 \overline{\widehat{\varphi}(p_1, p_2)} \widehat{\psi}(q_1, q_2) \widehat{V}(q_1 - p_1) \delta(p_1 + p_2 - q_1 - q_2). \quad (\text{D.7})$$

Therefore, by a weighted Schwarz inequality,

$$\begin{aligned} & \left| \langle \varphi, V(x_1 - x_2) \psi \rangle \right| \\ & \leq \|\widehat{V}\|_\infty \left(\int dp_1 dp_2 dq_1 dq_2 \frac{(p_1 \cdot p_2)^2 + p_1^2 + p_2^2 + 1}{(q_1 \cdot q_2)^2 + q_1^2 + q_2^2 + 1} |\widehat{\varphi}(p_1, p_2)|^2 \delta(p_1 + p_2 - q_1 - q_2) \right)^{1/2} \\ & \quad \times \left(\int dp_1 dp_2 dq_1 dq_2 \frac{(q_1 \cdot q_2)^2 + q_1^2 + q_2^2 + 1}{(p_1 \cdot p_2)^2 + p_1^2 + p_2^2 + 1} |\widehat{\psi}(q_1, q_2)|^2 \delta(p_1 + p_2 - q_1 - q_2) \right)^{1/2} \quad (\text{D.8}) \\ & \leq \|V\|_1 \left(\sup_p \int dq \frac{1}{(q \cdot (p - q))^2 + q^2 + (p - q)^2 + 1} \right) \\ & \quad \times \langle \psi, ((\nabla_1 \cdot \nabla_2)^2 - \Delta_1 - \Delta_2 + 1) \psi \rangle^{1/2} \langle \varphi, ((\nabla_1 \cdot \nabla_2)^2 - \Delta_1 - \Delta_2 + 1) \varphi \rangle^{1/2}. \end{aligned}$$

The lemma will then follow from

$$\sup_{p \in \mathbb{R}^3} \int dq \frac{1}{(q \cdot (p - q))^2 + q^2 + (p - q)^2 + 1} < \infty. \quad (\text{D.9})$$

To prove (D.9), we proceed as follows.

$$\begin{aligned} \int dq \frac{1}{(q \cdot (p - q))^2 + q^2 + (p - q)^2 + 1} &= \int_{|q - \frac{p}{2}| > |p|} dq \frac{1}{\left(\left(q - \frac{p}{2} \right)^2 - \frac{p^2}{4} \right)^2 + q^2 + (p - q)^2 + 1} \\ & \quad + \int_{|q - \frac{p}{2}| < |p|} dq \frac{1}{\left(\left(q - \frac{p}{2} \right)^2 - \frac{p^2}{4} \right)^2 + q^2 + (p - q)^2 + 1}. \end{aligned} \quad (\text{D.10})$$

The first term on the r.h.s. of the last equation is bounded by

$$\begin{aligned} \int_{|q - \frac{p}{2}| > |p|} dq \frac{1}{\left(\left(q - \frac{p}{2} \right)^2 - \frac{p^2}{4} \right)^2 + q^2 + (p - q)^2 + 1} &\leq \int_{|q - \frac{p}{2}| > |p|} dq \frac{1}{\frac{9}{16} \left| q - \frac{p}{2} \right|^4 + 1} \\ &\leq \frac{16}{9} \int_{\mathbb{R}^3} dq \frac{1}{|q|^4 + 1} < \infty, \end{aligned} \quad (\text{D.11})$$

uniformly in $p \in \mathbb{R}^3$. As for the second term on the r.h.s. of (D.10), we observe that

$$\begin{aligned}
& \int_{|q-\frac{p}{2}|<|p|} dq \frac{1}{\left((q-\frac{p}{2})^2 - \frac{p^2}{4}\right)^2 + q^2 + (p-q)^2 + 1} \\
&= \int_{|x|<|p|} dx \frac{1}{\left(x^2 - \frac{p^2}{4}\right)^2 + \left(x + \frac{p}{2}\right)^2 + \left(x - \frac{p}{2}\right)^2 + 1} \\
&= 4\pi \int_0^{|p|} dr \frac{r^2}{\left(r^2 - \frac{|p|^2}{4}\right)^2 + 2r^2 + \frac{|p|^2}{2} + 1} \\
&\leq C|p|^2 \int_{-|p|/2}^{|p|/2} dr \frac{1}{r^2 (r + |p|)^2 + \left(r + \frac{|p|}{2}\right)^2 + \frac{|p|^2}{4} + 1} \\
&\leq C \int_{-|p|/2}^{|p|/2} dr \frac{1}{r^2 + 1} \leq C \int_{\mathbb{R}} dr \frac{1}{r^2 + 1} < \infty,
\end{aligned} \tag{D.12}$$

uniformly in p . □

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