LECTURE NOTES III: ON A DERIVATION OF NLS FROM QUANTUM MANY BODY SYSTEMS

THOMAS CHEN, NATAŠA PAVLOVIĆ, AND NIKOLAOS TZIRAKIS

Abstract. The derivation of nonlinear dispersive PDE, such as the nonlinear Schrödinger (NLS) or nonlinear Hartree equations, from many body quantum dynamics is central topic in mathematical physics, which has been approached by many authors in a variety of ways. In particular, one way to derive NLS is via the Gross-Pitaevskii (GP) hierarchy, which is an infinite system of coupled linear non-homogeneous PDE. The most involved part in such a derivation of NLS consists in establishing uniqueness of solutions to the GP. That was achieved in seminal papers of Erdős-Schlein-Yau. Recently, in [8] a new, simpler proof of the unconditional uniqueness of solutions to the cubic Gross-Pitaevskii hierarchy in $\mathbb{R}^3$ was obtained, based on the quantum de Finetti theorem.

In the notes, we present a brief review of the derivation of NLS via the GP, and then describe main ideas of the new proof of uniqueness of solutions to the GP following [8].

Disclaimer. The notes are prepared as a study tool for participants of the MSRI summer school “Dispersive Partial Differential Equations”, June 16-27, 2014. Please keep in mind that the notes are in a raw format at the current stage.

In the notes we only give a short review of the derivation of the NLS from quantum many body systems via the GP hierarchy - we refer readers to excellent lecture notes by Schlein [54] for more details. The rest of the notes focuses on giving a global picture of the approach for proving uniqueness of the GP hierarchy, that the first two authors introduced in a collaboration with C. Hainzl and R. Seiringer in [8]. The approach is based on the use of the quantum de Finetti theorem, that in our context can be understood as a bridge between the NLS and the GP hierarchy.

The derivation of nonlinear dispersive PDE from many body quantum dynamics has experienced enormous progress recently: see [22, 23, 24, 25, 26, 43, 42, 53, 35, 36], and also [1, 2, 6, 27, 28, 29, 37, 34, 16, 38, 51, 52], as well as classical works [38, 31, 32, 56].

This problem is closely related to the phenomenon of Bose-Einstein condensation (BEC), in systems of interacting bosons, which was first experimentally verified in

---

The work of T.C. is supported in part by NSF grants DMS-1009448 and DMS-1151414 (CA-REER).

The work of N.P. is supported in part by NSF grant DMS-1101192.

The work of N.T. is supported in part by University of Illinois Research Board Grant RB-14054.

N.P. and N.T. are thankful to the MSRI staff for all help in organizing the workshop.
1. From Quantum many body systems to NLS

We start by giving a quick historical account of derivation of dispersive PDE from quantum many body systems. The derivation of the nonlinear Hartree equation (NLH) from an interacting Bose gas was first given by Hepp in [38] using the Fock space formalism and coherent states. The BBGKY hierarchy was prominently used in the works of Lanford for the study of classical mechanical systems in the infinite particle limit [44, 45]. Subsequently, the first derivation of the NLH via the BBGKY hierarchy was given by Spohn in [56]. More recently, this topic was revisited by Fröhlich, Tsai and Yau in [30], and in the last few years, Erdős, Schlein and Yau have further developed the BBGKY hierarchy approach to the derivation of the NLH and NLS in their seminal works [22, 23, 24, 25], which initiated much of the current widespread interest in this research topic. The proof strategy can be briefly summarized as follows:

**From N-body Schrödinger to BBGKY:** One considers $N$ bosons in $\mathbb{R}^d$ described by the wave function $\psi_N \in L^2_{\text{perm}}(\mathbb{R}^{dN})$, where $L^2_{\text{perm}}(\mathbb{R}^{dN})$ is the subspace of $L^2(\mathbb{R}^{dN})$ consisting of permutation symmetric functions. The wave function satisfies the Schrödinger equation

$$i\partial_t \psi_N = H_N \psi_N,$$

where the Hamiltonian $H_N$ is a self-adjoint operator acting on the Hilbert space $L^2_{\text{perm}}(\mathbb{R}^{dN})$,

$$H_N = \sum_{j=1}^N (-\Delta_{x_j}) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V_N(x_i - x_j).$$

The pair interaction potential has the form $V_N(x) = N^d \beta V(N^\beta x)$, with $V$ being spherically symmetric and in the Sobolev space $W^{r,s}(\mathbb{R}^d)$ for some suitable $r$, $s$. Here $\beta \in (0, 1]$.

When $\beta = 1$, the Hamiltonian (1.2) is called the Gross-Pitaevskii Hamiltonian. Thanks to the factor $\frac{1}{N}$ in front of the interaction potential, (1.2) can be formally interpreted as a mean field Hamiltonian. We note that physically (1.2) describes a very dilute gas, where interactions among particles are very rare and strong, while in a mean field Hamiltonian each particle usually reacts with all other particles via a very weak potential. However one can still apply to (1.2) similar mathematical methods as in the case of a mean field potential.
Since the Schrödinger equation \( (1.1) \) is linear and the Hamiltonian \( H_N \) is self-adjoint, global well-posedness of \( (1.1) \) is not an issue. But in terms of applications, one would like to have some information about qualitative and quantitative properties of the solution, which are hard to extract in physically relevant cases when number of particles \( N \) is very large (e.g. it varies from \( 10^3 \) for very dilute Bose-Einstein samples, to \( 10^{30} \) in stars). However physicists often care about macroscopic properties of the system, which can be obtained from averaging over a large number of particles. Further simplifications are related to obtaining a macroscopic behavior in the limit as \( N \to \infty \), with a hope that the limit will approximate properties observed in the experiments for a very large, but finite \( N \).

To study the limit as \( N \to \infty \), one introduces the \( N \)-particle density matrix

\[
\gamma_N(t; \underline{\underline{x}}_N; \underline{\underline{x}}_N') = \frac{\psi_N(t; \underline{\underline{x}}_N)\psi_N^*(t; \underline{\underline{x}}_N')}{\| \psi_N(t; \underline{\underline{x}}_N) \|^2}
\]

and its associated \( k \)-particle marginal density matrices

\[
\gamma^{(k)}_N(t; \underline{\underline{x}}_k; \underline{\underline{x}}_k') = \int \, dx_{N-k} \gamma_N(t; \underline{\underline{x}}_k; \underline{\underline{x}}_{N-k}; \underline{\underline{x}}_{N-k}),
\]

for \( k = 1, \ldots, N \), where \( \underline{\underline{x}}_k = (x_1, \ldots, x_k) \), \( \underline{\underline{x}}_{N-k} = (x_{k+1}, \ldots, x_N) \), that have an important role in the analysis of the system as \( N \to \infty \), because for every fixed \( k \), \( \gamma^{(k)}_N \) can have a well defined limit. Hence one studies the time evolution of \( k \)-particle marginals and observes that they satisfy the BBGKY hierarchy

\[
i\partial_t \gamma^{(k)}_N(t; \underline{\underline{x}}_k; \underline{\underline{x}}_k') = -\Delta \gamma^{(k)}_N(t; \underline{\underline{x}}_k; \underline{\underline{x}}_k') + \frac{1}{N} \sum_{1 \leq i < j \leq k} [V_N(x_i - x_j) - V_N(x_i' - x_j')] \gamma^{(k)}_N(t; \underline{\underline{x}}_k; \underline{\underline{x}}_k') + \frac{N - k}{N} \sum_{i=1}^{k} \int dx_{k+1} [V_N(x_i - x_{k+1}) - V_N(x_i' - x_{k+1})] \gamma^{(k+1)}_N(t; \underline{\underline{x}}_k, x_{k+1}; \underline{\underline{x}}'_k, x_{k+1})
\]

(1.6) where \( \Delta \underline{x}_k := \sum_{j=1}^{k} \Delta x_j \), and similarly for \( \Delta \underline{x}_k' \). We note that the size of the sum in (1.5) is \( \approx \frac{k^2}{N} \to 0 \) as \( N \to \infty \), and in (1.6) is \( \approx \frac{k(N-k)}{N} \to k \) as \( N \to \infty \). Indeed, it can be shown that, for a fixed \( k \), (1.5) disappears in the limit \( N \to \infty \) as described below, while (1.6) survives.

**From BBGKY to GP:** In the case when one starts with factorized initial wave function \( \psi_N(\underline{\underline{x}}_N) = \prod_{j=1}^{N} \phi(x_j) \), it is proven in \([22, 23, 26]\) that, for a suitable topology on the space of marginal density matrices, and as \( N \to \infty \), one can extract convergent subsequences \( \gamma^{(k)}_N \to \gamma^{(k)} \) for \( k \in \mathbb{N} \), which satisfy the Gross-Pitaevskii (GP) hierarchy:

\[
i\partial_t \gamma^{(k)} = \sum_{j=1}^{k} [-\Delta x_j, \gamma^{(k)}] + \lambda B_{k+1} \gamma^{(k+1)}, \quad k \in \mathbb{N},
\]

(1.7) for suitable initial data \( (\gamma^{(k)}(0))_{k \in \mathbb{N}} \), where \( \gamma^{(k)}(t; \underline{\underline{x}}_k; \underline{\underline{x}}'_k) \) is fully symmetric under permutations separately of the components of \( \underline{\underline{x}}_k := (x_1, \ldots, x_k) \), and of the components of \( \underline{\underline{x}}'_k := (x'_1, \ldots, x'_k) \). The interaction term for the \( k \)-particle marginal is defined by

\[
B_{k+1} \gamma^{(k+1)} = B_{k+1}^+ \gamma^{(k+1)} - B_{k+1}^- \gamma^{(k+1)},
\]

(1.8)
where
\[ B_{k+1}^+ \gamma^{(k+1)} = \sum_{j=1}^{k} B_{j,k+1}^+ \gamma^{(k+1)} \] (1.9)
and
\[ B_{k+1}^- \gamma^{(k+1)} = \sum_{j=1}^{k} B_{j,k+1}^- \gamma^{(k+1)}, \] (1.10)
with
\[ \left( B_{j,k+1}^+ \gamma^{(k+1)} \right) (t, x_1, \ldots, x_k; x'_1, \ldots, x'_k) = \int dx_{k+1} dx'_{k+1} \delta(x_j - x_{k+1}) \delta(x_j - x'_{k+1}) \gamma^{(k+1)} (t, x_1, \ldots, x_{k+1}; x'_1, \ldots, x'_{k+1}) = \gamma^{(k+1)} (t, x_1, \ldots, x_j, x_k; x'_1, \ldots, x'_j, x'_k), \] (1.11)
and
\[ \left( B_{j,k+1}^- \gamma^{(k+1)} \right) (t, x_1, \ldots, x_k; x'_1, \ldots, x'_k) = \int dx_{k+1} dx'_{k+1} \delta(x'_j - x_{k+1}) \delta(x'_j - x'_{k+1}) \gamma^{(k+1)} (t, x_1, \ldots, x_{k+1}; x'_1, \ldots, x'_{k+1}) = \gamma^{(k+1)} (t, x_1, \ldots, x_k; x'_1, \ldots, x'_j, x'_k; x'_j). \] (1.12)

We say that \( B_{j,k+1}^+ \) contracts the triple of variables \( x_j, x_{k+1}, x'_{k+1} \), and that \( B_{j,k+1}^- \) contracts the triple of variables \( x'_j, x_{k+1}, x'_{k+1} \). The GP hierarchy is said to be defocusing if \( \lambda = 1 \), and focusing if \( \lambda = -1 \) (we are assuming the normalization condition \( |\lambda| = 1 \) for simplicity).

**NLS and factorized solutions of GP:** The link between the original bosonic \( N \)-body system and solutions of the NLS is established via noticing that the factorized \( k \)-particle marginals
\[ \gamma^{(k)} (t, x_k; x'_k) = |\phi(t, x_j) \rangle \langle \phi(t, x'_j)| \otimes^k := \prod_{j=1}^{k} \phi(t, x_j) \overline{\phi(t, x'_j)} \]
are a solution of the GP hierarchy (1.7) if \( \phi(t, x) \) solves the defocusing\(^1\) cubic NLS
\[ i \partial_t \phi = -\Delta x \phi + |\phi|^2 \phi. \] (1.13)

**Uniqueness of solutions to the GP:** While the existence of factorized solutions can be easily obtained, as outlined above, the proof of uniqueness of solutions of the GP hierarchy (which encompass non-factorized solutions) is the most difficult part in this analysis. It was originally obtained by Erdős-Schlein-Yau [22, 23, 24, 25] in the space \( \{ \gamma^{(k)} | \| \gamma^{(k)} \|_{h^1} < \infty \} \), where
\[ \| \gamma^{(k)} \|_{h^1} := \text{Tr}(|S^{(k,\alpha)} \gamma^{(k)}|), \] (1.14)
\(^1\)The first derivation of the focusing NLS was obtained recently in [19].
ON A DERIVATION OF NLS

with \( S^{(k,\alpha)} := \prod_{j=1}^{k} (\nabla_{x_j})^{\alpha}(\nabla'_{x_j})^{\alpha} \). This is a crucial, and very involved part of Erdős-Schlein-Yau’s method for deriving the cubic defocusing NLS. Roughly speaking, the method employed in [22, 23, 24, 25] consists of:

(1) Proving compactness of the sequence \( \{\gamma^{(k)}_{N}(t)\}_{k=1}^{N} \) with respect to an appropriate weak topology.

(2) Proving that every limit point of \( \{\gamma^{(k)}_{N}(t)\}_{k=1}^{N} \) as \( N \to \infty \) solves the GP hierarchy.

(3) Proving that the solution to the GP hierarchy is unique, which implies that for factorized initial data, the solutions of the GP hierarchy are determined by a cubic NLS. In particular, the uniqueness proof of Erdős-Schlein-Yau uses a sophisticated and extensive construction involving Feynman graph expansions, and high dimensional singular integral estimates. A key ingredient in their proof is a powerful combinatorial method that resolves the problem of the factorial growth of number of terms in iterated Duhamel expansions.

Subsequently, Klainerman-Machedon [43] gave a much shorter proof of the uniqueness of solutions to the GP hierarchy in the space of density matrices for which the Hilbert-Schmidt type Sobolev norms are finite \( \{\gamma^{(k)} || \| \gamma^{(k)} \|_{\dot{H}^{1}} < \infty \} \), where

\[
\|\gamma^{(k)}\|_{\dot{H}^{\alpha}} := \|\mathcal{R}^{(k,\alpha)}\gamma^{(k)}\|_{L^{2}}
\]

with \( \mathcal{R}^{(k,\alpha)} := \prod_{j=1}^{k} |\nabla_{x_j}|^{\alpha}|\nabla'_{x_j}|^{\alpha} \). However the result is conditional on the assumption that

\[
\|B_{j,k+1}\gamma^{(k+1)}\|_{L^{2}_{t}\dot{H}^{1}} < C_{k}
\]

holds for some finite constant \( C \) independent of \( k \). Their approach uses techniques from the analysis of dispersive nonlinear PDE, together with the combinatorial method of [22, 23, 24, 25], which Klainerman-Machedon presented as the “boardgame argument”. Starting with the work [42] for the cubic GP hierarchy on \( \mathbb{R}^{2} \) and \( \mathbb{T}^{2} \), the approach of Klainerman-Machedon was used by various authors for the derivation of the NLS from interacting Bose gases [9, 13, 17, 18, 42, 15, 60].

2. From NLS to quantum many body systems via the GP

The GP is a system of linear coupled PDE that describes the dynamics of a gas of infinitely many interacting bosons, while at the same time retains some of the features of a dispersive PDE. Based on these dispersive features, one can investigate solutions to the GP hierarchy and illustrate that, in some instances, the GP can be studied using generalizations of methods of dispersive PDE. We review what has been done in that direction:

The \( p \)-GP hierarchy: Let \( p \in \{2,4\} \). To unify the notation for cubic and quintic GP hierarchies, the \( p \)-GP hierarchy can be introduced as follows (see [10] for details):

\[
i\partial_{t}\gamma^{(k)} = - (\Delta_{x_k} - \Delta_{x'_{k}})\gamma^{(k)} + \mu B_{k+\frac{p}{2}} \gamma^{(k+\frac{2}{p})}
\]

where the operator \( B_{k+\frac{p}{2}} \gamma^{(k+\frac{2}{p})} \) accounts for \( \frac{p}{2} \) + 1-body interactions between the Bose particles and is given via:

\[
B_{k+\frac{p}{2}} \gamma^{(k+\frac{2}{p})} = B_{k+\frac{p}{2}}^{+} \gamma^{(k+\frac{2}{p})} - B_{k+\frac{p}{2}}^{-} \gamma^{(k+\frac{2}{p})},
\]
where
\[ B_{k+\frac{p}{2}}^+ \gamma^{(k+\frac{p}{2})} = \sum_{j=1}^k B_{j;k+1,...,k+\frac{p}{2}}^+ \gamma^{(k+\frac{p}{2})}, \quad B_{-k-\frac{p}{2}}^- \gamma^{(k+\frac{p}{2})} = \sum_{j=1}^k B_{j;k+1,...,k+\frac{p}{2}}^- \gamma^{(k+\frac{p}{2})} \]

with
\[ \left( B_{j;k+1,...,k+\frac{p}{2}}^+ \gamma^{(k+\frac{p}{2})} \right)(t, x_1, \ldots, x_k; x_1', \ldots, x_k') = \int dx_{k+1} \cdots dx_{k+\frac{p}{2}} dx_{k+1}' \cdots dx_{k+\frac{p}{2}} \]
\[ \prod_{\ell=k+1}^{k+\frac{p}{2}} \delta(x_j - x_{\ell}) \delta(x_j' - x_{\ell}') \gamma^{(k+\frac{p}{2})}(t, x_1, \ldots, x_k; x_1', \ldots, x_k') \]
and
\[ \left( B_{j;k+1,...,k+\frac{p}{2}}^- \gamma^{(k+\frac{p}{2})} \right)(t, x_1, \ldots, x_k; x_1', \ldots, x_k') = \int dx_{k+1} \cdots dx_{k+\frac{p}{2}} dx_{k+1}' \cdots dx_{k+\frac{p}{2}} \]
\[ \prod_{\ell=k+1}^{k+\frac{p}{2}} \delta(x_j' - x_{\ell}) \delta(x_j - x_{\ell}') \gamma^{(k+\frac{p}{2})}(t, x_1, \ldots, x_k; x_1', \ldots, x_k') \].

We refer to (2.1) as the cubic GP hierarchy if \( p = 2 \), and as the quintic GP hierarchy if \( p = 4 \). Moreover, for \( \mu = 1 \) or \( \mu = -1 \) we refer to the GP hierarchies as being defocusing or focusing, respectively.

We note that for factorized solutions of (2.1) the corresponding 1-particle wave function satisfies the \( p \)-NLS: \( i\partial_t \phi = -\Delta \phi + \mu |\phi|^p \phi \).

For a derivation of the quintic NLS see [9]. A general power type NLS was recently derived from the corresponding quantum many body system by Xie in [60].

**The spaces:** In [10] the following space was introduced:
\[ \mathcal{S} := \bigoplus_{k=1}^{\infty} L^2(\mathbb{R}^d \times \mathbb{R}^d) \]
of sequences of density matrices
\[ \Gamma := (\gamma^{(k)})_{k \in \mathbb{N}} \]
where \( \gamma^{(k)} \geq 0 \), \( \text{Tr} \gamma^{(k)} = 1 \), and where every \( \gamma^{(k)}(x_k, x_k') \) is symmetric in all components of \( x_k \), and in all components of \( x_k' \), respectively.

Given \( \xi > 0 \), we define the Sobolev space \( \mathcal{H}_\xi^\alpha = \{ \Gamma \in \mathcal{S} \mid \| \Gamma \|_{\mathcal{H}_\xi^\alpha} < \infty \} \) where
\[ \| \Gamma \|_{\mathcal{H}_\xi^\alpha} := \sum_{k \in \mathbb{N}} \xi^k \| \gamma^{(k)} \|_{H^\alpha}, \quad (2.3) \]
and where \( \| \gamma^{(k)} \|_{H^\alpha} := \| S^{(k,\alpha)} \gamma^{(k)} \|_{L^2} \) is the non-homogenous version of the norm in [43]. The parameter \( \alpha \) determines the regularity of the solution. If \( \Gamma \in \mathcal{H}_\xi^\alpha \), then \( \xi^{-1} \) an upper bound on the typical \( H^\alpha \)-energy per particle.

**Results motivated by techniques from nonlinear dispersive PDE:** Having introduced a topology on the space of sequences of density matrices, so that a fixed point argument can be used, in [10], the local well-posedness was obtained for energy subcritical focusing and defocusing cubic and quintic GP hierarchies.
in a subspace of $\mathcal{H}_\xi^2$ defined by a condition related to the Klainerman-Machedon condition (1.16). Subsequently, in [14] we identify a conserved energy functional and prove virial identities for solutions of GP hierarchies, and use those to prove a finite-time blow up for $L^2$-critical and supercritical focusing GP hierarchies, whenever energy is negative and the variance is finite. In [11], an infinite family of multiplicative energy functionals is identified and used to prove global well-posedness for $H^1$ subcritical defocusing GP hierarchies, and for $L^2$ subcritical focusing GP hierarchies.

In [12], Chen-Pavlović prove the existence of solutions to the GP hierarchy, without the assumption of the Klainerman-Machedon condition. This is achieved via showing that the limit of solutions to a truncated GP hierarchy exists as the truncation parameter goes to infinity, and that this limit is a solution to the GP. Such a “truncation-based” proof of existence of solutions to the GP motivated us to try to implement a similar approach at the level of the BBGKY hierarchy, which is what has been done in [13]. In such a way, it was shown that there are solutions to the cubic GP hierarchy, constructed from solutions to the BBGKY hierarchy, that satisfy the Klainerman-Machedon condition in dimension $d = 3$ (for $d \leq 2$, it is known to be the case, [9, 42]). The work [13] illustrates that techniques from the NLS (such as Strichartz estimates and well-posedness theory) can actually be introduced at the level of the quantum many body systems. This line of work was continued by X. Chen [17], X. Chen-Holmer [18] and T. Chen-K.Taliaferro [15].

3. Uniqueness of solutions to the GP via quantum de Finetti theorems

Until recently the only available proof of unconditional uniqueness of solutions in $L_{t \in [0, T]}^\infty \mathcal{H}_1$ to the cubic GP hierarchy in $\mathbb{R}^3$ was the one given in the works of Erdős-Schlein-Yau, [22]-[25], using an involved construction based on Feynman graph expansions and high-dimensional singular integral estimates. Here for $\alpha \geq 0$, $\mathcal{S}_\alpha$ denotes the trace class Sobolev space defined for the entire sequence $(\gamma^{(k)})_{k \in \mathbb{N}}$ via:

$$\mathcal{S}_\alpha := \left\{ (\gamma^{(k)})_{k \in \mathbb{N}} \mid \text{Tr}(S^{(k,\alpha)}(\gamma^{(k)})) < M^{2k} \text{ for some constant } M < \infty \right\}. \quad (3.1)$$

Recently, a new, simpler proof of uniqueness of solutions in $L_{t \in [0, T]}^\infty \mathcal{H}_1$ to the cubic GP hierarchy in $\mathbb{R}^3$ was obtained in [8], which is based on the use of quantum de Finetti theorems. Subsequently the new approach for proving uniqueness for the GP based on quantum de Finetti theorems has been applied to obtain uniqueness of solutions to the cubic GP in $\mathbb{R}^3$ in low regularity spaces $L_{t \in [0, T]}^\infty \mathcal{S}_s$, for certain values of $s$ in [40], and very recently in the context of the GP hierarchy on $\mathbb{T}^3$ in [55], as well as in the context of the infinite hierarchy that appears in a connection to the Chern-Simons-Schrödinger system in [20].

In the rest of the notes we give a brief overview of this new approach for proving uniqueness of solutions to the GP. We start by giving a precise statement of the result proved in [8]. The result concerns a mild solution to the GP hierarchy, which is introduced as follows.
A mild solution in the space \( L^\infty_{t \in [0, T)} \mathcal{F}^1 \), to the GP hierarchy with initial data 
\((\gamma^{(k)}(0))_{k \in \mathbb{N}} \in \mathcal{F}^1 \), is a solution of the integral equation

\[
\gamma^{(k)}(t) = U^{(k)}(t)\gamma^{(k)}(0) + i\lambda \int_0^t U^{(k)}(t-s)B_{k+1}\gamma^{(k+1)}(s)ds , \quad k \in \mathbb{N},
\]

(3.2)
satisfying

\[
\sup_{t \in [0, T)} \text{Tr}(|S^{(k,1)} \gamma^{(k)}(t)|) < M^{2k}
\]

(3.3)
for a finite constant \( M \) independent of \( k \). Here,

\[
U^{(k)}(t) := \prod_{\ell=1}^k e^{it(\Delta_{x^\ell} - \Delta_{x^\ell'})}
\]

(3.4)
denotes the free \( k \)-particle propagator.

**Theorem 3.1.** Let \((\gamma^{(k)}(t))_{k \in \mathbb{N}} \) be a mild solution in \( L^\infty_{t \in [0, T)} \mathcal{F}^1 \) to the (de)focusing cubic GP hierarchy in \( \mathbb{R}^3 \) with initial data \((\gamma^{(k)}(0))_{k \in \mathbb{N}} \in \mathcal{F}^1 \), which is either admissible, or obtained at each \( t \) from a weak-* limit.

Then, \((\gamma^{(k)}(k))_{k \in \mathbb{N}} \) is the unique solution for the given initial data.

Moreover, assume that the initial data \((\gamma^{(k)}(0))_{k \in \mathbb{N}} \in \mathcal{F}^1 \) satisfy

\[
\gamma^{(k)}(0) = \int d\mu(\phi)(|\phi\rangle\langle\phi|)^\otimes k , \quad \forall k \in \mathbb{N},
\]

(3.5)
where \( \mu \) is a Borel probability measure supported either on the unit sphere or on the unit ball in \( L^2(\mathbb{R}^3) \), and invariant under multiplication of \( \phi \in \mathcal{H} \) by complex numbers of modulus one. Then,

\[
\gamma^{(k)}(t) = \int d\mu(\phi)(|S_t(\phi)\rangle\langle S_t(\phi)|)^\otimes k , \quad \forall k \in \mathbb{N},
\]

(3.6)
where \( S_t : \phi \mapsto \phi_t \) is the flow map of the cubic (de)focusing NLS, for \( t \in [0, T) \). That is, \( \phi_t \) satisfies (1.13) with initial data \( \phi \).

### 3.1. Preliminaries

The proof in [8] uses the following two ingredients:

1. The boardgame combinatorial organization as presented by Klainerman and Machedon [43]
2. The quantum de Finetti theorem, which is a quantum analogue of the Hewitt-Savage theorem in probability theory, [39].

We start by presenting a brief description of each of those two techniques.

#### 3.1.1. The boardgame combinatorial organization as presented by Klainerman and Machedon

To prove uniqueness, we will show that the trace norm of \( \gamma^{(k)} \) is zero if the initial data is zero. We will use the combinatorial method of Erdős, Schlein and Yau [22, 23, 24, 25], which was presented in an elegant and accessible form by Klainerman and Machedon in [43] as a ”boardgame argument”.
To begin with, we consider the \( r \)-fold iterate of the Duhamel formula (3.2) for \( \gamma^{(k)} \), with initial data \( \gamma_0^{(k)} = 0 \), for some arbitrary \( r \in \mathbb{N} \),

\[
\gamma^{(k)}(t) = (i\lambda)^r \int_{t_1 \geq t_2 \geq \cdots \geq t_r} dt_1 \cdots dt_r U^{(k)}(t - t_1) B_{k+1} U^{(k+1)}(t_1 - t_2) \cdots \cdots U^{(k+r-1)}(t_{r-1} - t_r) B_{k+r} \gamma^{(k+r)}(t_r)
\]

\[=: \int_{t_1 \geq t_2 \geq \cdots \geq t_r} dt_1 \cdots dt_r J^k(t_r), \quad t_r := (t_1, \ldots, t_r). \tag{3.7}\]

We will prove that the trace norm of the right hand side converges to zero as \( r \to \infty \), for \( t \in [0, T) \) and \( T > 0 \) sufficiently small (where the smallness condition on \( T \) is uniform in \( k \)).

A key difficulty in this approach stems from the fact that the interaction operator \( B_{\ell+1} \) is the sum of \( O(\ell) \) terms, therefore (3.7) contains \( O(\frac{(k+r-1)!}{(k-1)!}) = O(r!) \) terms. The boardgame argument allows one to control this rapid increase of the number of terms as \( r \to \infty \). We give a short summary of the method.

Recalling that \( B_{\ell+1} = \sum_{j=1}^{\ell} B_{j; \ell+1} \), we write

\[
J^k(t_r) = \sum_{\rho \in \mathcal{M}_{k,r}} J^k(\rho; t_r), \tag{3.8}
\]

where

\[
J^k(\rho; t_r) := (i\lambda)^r U^{(k)}(t - t_1) B_{\rho(k+1), k+1} U^{(k+1)}(t_1 - t_2) \cdots \cdots U^{(k+\ell-1)}(t_{\ell-1} - t_\ell) B_{\rho(k+\ell), k+\ell} \cdots U^{(k+r-1)}(t_{r-1} - t_r) B_{\rho(k+r), k+r} \gamma^{(k+r)}(t_r),
\]

and \( \rho \) is a map

\[
\rho : \{k+1, r+2, \ldots, k+r\} \to \{1, 2, \ldots, k+r-1\}, \quad \rho(2) = 1, \quad \rho(j) < j \quad \forall j. \tag{3.10}
\]

Here \( \mathcal{M}_{k,r} \) denotes the set of all such mappings \( \rho \).

We observe that each map \( \rho \) can be represented by highlighting one nonzero entry \( B_{\rho(k+\ell), k+\ell} \) in each column of an \((k+r-1) \times r\) matrix \([A_{i,\ell}]\) with entries \( A_{i,\ell} = B_{i, k+\ell} \) for \( i < k + \ell \), and \( A_{i,\ell} = 0 \) for \( i \geq k + \ell \). As an example, consider

\[
\begin{bmatrix}
B_{1, k+1} & B_{1, k+2} & \cdots & \cdots & \cdots & B_{1, k+r} \\
\vdots & B_{2, k+2} & \cdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \ddots & \cdots & \cdots & \vdots \\
B_{k, k+1} & B_{k, k+2} & \cdots & B_{\rho(k+\ell), k+\ell} & \cdots & \vdots \\
0 & B_{k+1, k+2} & \cdots & \cdots & \cdots & \vdots \\
\vdots & 0 & \cdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \cdots & \cdots & \cdots & \vdots \\
\vdots & \vdots & \cdots & 0 & \cdots & \vdots \\
0 & 0 & \cdots & 0 & \cdots & B_{k+r-1, k+r}
\end{bmatrix}. \tag{3.11}
\]

Then,

\[
\gamma^{(k)}(t) = \sum_{\rho \in \mathcal{M}_{k,r}} \int_{t_1 \geq t_2 \geq \cdots \geq t_r} J^k(\rho; t_r) \ dt_{1} \cdots dt_r, \tag{3.12}
\]
where the time domains are given by the same simplex \( \{ t > t_1 > \cdots > t_r \} \subset [0, t]^r \) for all integrals in the sum over \( \rho \).

We next consider the integrals with permuted time integration orders

\[
I(\rho, \pi) = \int_{\{ t > t_1 > \cdots > t_r \}} J^k(\rho; \underline{t}) \, dt_1 \cdots dt_r,
\]

where \( \pi \) is a permutation of \( \{1, 2, \ldots, r\} \). This corresponds to replacing the simplex \( \{ t > t_1 > \cdots > t_r \} \subset [0, t]^r \) by an isometric image in \( [0, t]^r \). One can associate to \( I(\rho, \pi) \) the matrix

\[
\begin{bmatrix}
  t_{\pi^{-1}(1)} & t_{\pi^{-1}(2)} & \cdots & t_{\pi^{-1}(r)} \\
  B_{1,k+1} & B_{1,k+2} & \cdots & B_{1,k+r} \\
  \vdots & \vdots & \ddots & \vdots \\
  0 & \cdots & \cdots & 0 \\
  0 & 0 & \cdots & B_{k+r-1,k+r}
\end{bmatrix}
\]

whose columns are labeled 1 through \( r \) and whose rows are labeled 0, 1, \ldots, \( k+r-1 \), and where the highlighted entries correspond to \( B_{\rho(k+\ell),k+\ell} \).

Using the combinatorial method in [22, 23, 24, 25] in the form presented in [43], a board game is introduced on the set of such matrices. A acceptable move is characterized as follows: If \( \rho(k+\ell) < \rho(k+\ell-1) \), the player is allowed to do the following three changes at the same time:

- exchange the highlights in columns \( \ell \) and \( \ell+1 \),
- exchange the highlights in rows \( k+\ell-1 \) and \( k+\ell \),
- exchange \( t_{\pi^{-1}(\ell)} \) and \( t_{\pi^{-1}(\ell+1)} \).

We note that the rows \( k+\ell \) and \( k+\ell+1 \) do not necessarily contain highlights.

A main property of the integrals \( I(\rho, \pi) \) is invariance under acceptable moves, [22, 23, 24, 25, 43]:

**Lemma 3.2.** If \((\rho, \pi)\) is transformed into \((\rho', \pi')\) by an acceptable move, then \( I(\rho, \pi) = I(\rho', \pi') \).

We say that a matrix of the type (3.11) is in upper echelon form if each highlighted entry in a row is to the left of each highlighted entry in a lower row. For example, the following matrix is in upper echelon form (with \( k = 1 \) and \( r = 4 \)):

\[
\begin{bmatrix}
  B_{1,2} & B_{1,3} & B_{1,4} & B_{1,5} \\
  0 & B_{2,3} & B_{2,4} & B_{2,5} \\
  0 & 0 & B_{3,4} & B_{3,5} \\
  0 & 0 & 0 & B_{4,5}
\end{bmatrix}
\]

Then, the following normal form property holds, [22, 23, 24, 25, 43]:
**Lemma 3.3.** For each matrix in $\mathcal{M}_{k,r}$, there is a finite number of acceptable moves that transforms the matrix into upper echelon form. Moreover, let $C_{k,r}$ denote the number of upper echelon matrices of size $(k + r - 1) \times r$. Then,

$$C_{k,r} \leq 2^{k+r}.$$  \hspace{1cm} (3.14)

Let $\mathcal{N}_{k,r}$ denote the subset of matrices in $\mathcal{M}_{k,r}$ which are in upper echelon form. Let $\sigma$ account for a matrix in $\mathcal{N}_{k,r}$. We write $\rho \sim \sigma$ if the matrix corresponding to $\rho$ can be transformed into that corresponding to $\sigma$ in finitely many acceptable moves. We note that $\sigma$ satisfies the same properties (3.10) as $\rho$, but in addition,

$$\sigma(j) \leq \sigma(j') \quad \forall j < j'.$$  \hspace{1cm} (3.15)

Then, the following key theorem holds, [22, 23, 24, 25, 43]:

**Theorem 3.4.** Suppose $\sigma \in \mathcal{N}_{k,r}$. Then, there exists a subset of $[0, t]^r$, denoted by $D(\sigma, t)$, such that

$$\sum_{\rho \sim \sigma} \int_{t_1 \geq \cdots \geq t_r} J^k(\rho; t_r) \ dt_1 \cdots dt_r = \int_{D(\sigma, t)} J^k(\sigma; t_r) \ dt_1 \cdots dt_r.$$  \hspace{1cm} (3.16)

Let $\mathcal{D}(\sigma, t)$ be the union of all simplices $\{t > t_{\pi(1)} > \cdots > t_{\pi(r)}\} \subset [0, t]^r$ obtained under acceptable moves for the fixed upper echelon form $\sigma$; notably, the interiors of these simplices are all pairwise disjoint. We emphasize that the main point of Theorem 3.4 is the reduction of a sum of $O(r!)$ terms to a sum of $O(C^r)$ terms. This concludes our summary of the Erdős-Schlein-Yau combinatorial method [22, 23, 24, 25], formulated in boardgame form following Klainerman-Machedon [43].

### 3.1.2. On quantum de Finetti theorems

The strong version of the quantum de Finetti theorem is due to Hudson-Moody, and Stormer, [41, 58], and applies to sequences of density matrices that are admissible, i.e., $\gamma^{(k)} = \text{Tr}_{k+1}(\gamma^{(k+1)})$, $\forall k \in \mathbb{N}$. We quote it in the formulation presented by Lewin-Nam-Rougerie in [46] ([41, 58] state it in the $C^*$-algebraic context).

**Theorem 3.5.** (Strong Quantum de Finetti) Let $\mathcal{H}$ be any separable Hilbert space and let $\mathcal{H}^k = \bigotimes_{\text{sym}}^k \mathcal{H}$ denote the corresponding bosonic $k$-particle space. Let $\Gamma$ denote a collection of admissible bosonic density matrices on $\mathcal{H}$, i.e., $\Gamma = (\gamma^{(1)}, \gamma^{(2)}, \ldots)$ with $\gamma^{(k)}$ a non-negative trace class operator on $\mathcal{H}^k$, and $\gamma^{(k)} = \text{Tr}_{k+1}(\gamma^{(k+1)})$, where $\text{Tr}_{k+1}$ denotes the partial trace over the $(k + 1)$-th factor. Then, there exists a unique Borel probability measure $\mu$, supported on the unit sphere $S \subset \mathcal{H}$, and invariant under multiplication of complex numbers of modulus one, such that

$$\gamma^{(k)} = \int d\mu(\phi) (|\phi\rangle \langle \phi|)^{\otimes k}, \quad \forall k \in \mathbb{N}.$$  \hspace{1cm} (3.17)

The limiting hierarchies obtained via weak-* limits from the BBGKY hierarchy of bosonic $N$-body Schrödinger systems as in [22]-[25] do not necessarily satisfy admissibility. A weak version of the quantum de Finetti theorem then still applies; in [8] we use the version that was recently proven by Lewin-Nam-Rougerie [46]. Previously, Ammari-Nier proved an equivalent result in [4, 5].

In our case, we consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$. 
3.2. Setup of the proof of Theorem 3.1. Now we give a precise formulation of the framework in which we prove Theorem 3.1. Let us assume that we have two positive semidefinite solutions \((\gamma_j^{(k)}(t))_{k \in \mathbb{N}} \in L^\infty_{t \in [0,T]} S^1\) satisfying the same initial data, \((\gamma_1^{(k)}(0))_{k \in \mathbb{N}} = (\gamma_2^{(k)}(0))_{k \in \mathbb{N}} \in S^1\). Then,

\[
\gamma^{(k)}(t) := \gamma_1^{(k)}(t) - \gamma_2^{(k)}(t), \quad k \in \mathbb{N},
\]

is a solution to the GP hierarchy with initial data \(\gamma^{(k)}(0) = 0 \forall k \in \mathbb{N}\), and it suffices to prove that \(\gamma^{(k)}(t) = 0 \forall k \in \mathbb{N}\), and for all \(t \in [0,T]\). This is due to the linearity of the GP hierarchy.

We note that \(\gamma^{(k)}\), as a difference of positive semidefinite marginal density matrices, is not in general positive semidefinite.

From the assumptions of Theorem 3.1, we have that

\[
\sup_{t \in [0,T]} \text{Tr}(\mathcal{S}_i^{(k,1)\gamma_i^{(k)}(t)}(t)) < M^2k, \quad k \in \mathbb{N}, \quad i = 1, 2,
\]

for some finite constant \(M\) independent of \(k\) and \(t\).

To ensure the applicability of the quantum de Finetti theorem (by which we henceforth refer to either the strong or the weak version), we note that if

\[
\gamma_j^{(k)} = \text{Tr}_{k+1}(\gamma_j^{(k+1)}), \quad \forall k \in \mathbb{N}, \quad j = 1, 2,
\]

are admissible, it follows immediately that \((\gamma^{(k)})_{k \in \mathbb{N}}\) is admissible. Moreover if both \((\gamma_1^{(k)})\) and \((\gamma_2^{(k)})\) are obtained from a weak-* limit, then so is \((\gamma^{(k)})\).

Thus, from the quantum de Finetti theorem, we have that

\[
\gamma_j^{(k)}(t) = \int d\mu_t^{(j)}(\phi)(|\phi\rangle \langle \phi|)^{\otimes k}, \quad j = 1, 2,
\]

\[
\gamma^{(k)}(t) = \int d\overline{\mu}_t(\phi)(|\phi\rangle \langle \phi|)^{\otimes k},
\]

where \(\overline{\mu}_t := \mu_t^{(1)} - \mu_t^{(2)}\) is the difference of two probability measures on the unit ball in \(L^2(\mathbb{R}^3)\). We remark that (3.19) is equivalent to

\[
\int d\mu_t^{(j)}(\phi)\|\phi\|_{H^1}^{2k} < M^2k, \quad j = 1, 2,
\]

for all \(k \in \mathbb{N}\), where \(H^1 = \{ f \in L^2(\mathbb{R}^3) \mid \|\nabla_x f\|_{L^2} < \infty\}\), and \(\langle \nabla \rangle := \sqrt{1 - \Delta}\).

From here on, we will consider the representation of the expansion (3.7) for \(\gamma^{(k)}(t)\) in upper echelon normal form, given by the right hand side of (3.16). Then,

\[
\begin{align*}
\gamma^{(k)}(t) &= \sum_{\sigma \in \mathcal{N}_{k}, r} \int_{D(\sigma,t)} dt_1 \cdots dt_r U^{(k)}(t - t_1)B_{\sigma(k+1), k+1} U^{(k+1)}(t_1 - t_2) \cdots \\
&\quad \cdots U^{(k+r-1)}(t_{r-1} - t_r)B_{\sigma(k+r), k+r} \gamma^{(k+r)}(t_r).
\end{align*}
\]

The sum with respect to \(\sigma\) extends over all inequivalent upper echelon forms.
Using the quantum de Finetti theorem, we obtain

$$\gamma^{(k)}(t) = \sum_{\sigma \in \mathbb{N}_{k,\sigma}} \int_{D(\sigma, t)} dt_1, \ldots, dt_r \int d\mu_{t_r}(\phi) J^k(\sigma; t, t_1, \ldots, t_r),$$  \hspace{1cm} (3.24)$$

where

$$J^k(\sigma; t, t_1, \ldots, t_r; \mathcal{E}_k; \mathcal{E}_k^*) = \left( U^{(k)}(t - t_1)B_{\sigma(k+1),k+1}U^{(k+1)}(t_1 - t_2) \right)$$

$$\cdot \cdots U^{(k+\ell)}(t_{\ell} - t_{\ell+1})B_{\sigma(k+\ell+1),k+\ell+1}U^{(k+\ell+1)}(t_{\ell+1} - t_{\ell+2}) \cdots$$

$$\cdot U^{(k+r-1)}(t_{r-1} - t_r)B_{\sigma(k+r),k+r}(|\phi\rangle\langle\phi|)^{(k+r)}(\mathcal{E}_k; \mathcal{E}_k^*).$$ \hspace{1cm} (3.25)$$

Here, we may think of the time variable $t_\ell$ as being attached to the interaction operator $B_{\sigma(k+\ell),k+\ell}$. For fixed $\phi$, we note that since

$$\left(|\phi\rangle\langle\phi|\right)^{(k+r)}(\mathcal{E}_k; \mathcal{E}_k^*) = \prod_{i=1}^{k+r}(|\langle\phi|\langle\phi|)(x_i; x_i')$$ \hspace{1cm} (3.26)$$

is given by a product of 1-particle kernels, it follows that

$$J^k(\sigma; t, t_1, \ldots, t_r; \mathcal{E}_k; \mathcal{E}_k^*) = \prod_{j=1}^{k} J^j_{\sigma}(\sigma_j; t, t_{\ell_{j,1}}, \ldots, t_{\ell_{j,m_j}}; x_j; x_j')$$ \hspace{1cm} (3.27)$$

likewise has product form, for each fixed $\sigma$. This is because in (3.25), the operators $B_{\sigma(k+\ell),k+\ell}$ and $U^{(k+\ell)}(t_\ell - t_{\ell+1})$ each map products of 1-particle kernels to products of 1-particle kernels (but the operators $B_{\sigma(k+\ell),k+\ell}$ do in general not preserve positive semidefiniteness). Each 1-particle kernel $J^j_{\sigma}$ can be written as a Duhamel expansion in itself, with interaction operators inherited from those appearing in $J^j$. We label the interaction operators in $J^j_{\sigma}$ “internally” with $\sigma_j$, $j = 1, \ldots, k$, (which are automatically in upper echelon form relative to $J^j_{\sigma}$).

For a fixed $k$, the number of inequivalent echelon forms is bounded by $C^r$, using Lemma 3.3. Hence,

$$\text{Tr}(|\gamma^{(k)}|) \leq C^r \sup_{i=1,2} \int_{[0,t]} dt_1 \cdots dt_r \int d\mu_{t_r}(\phi) \prod_{j=1}^{k} \text{Tr}\left(J^j_{\sigma}(\sigma_j; t, t_{\ell_{j,1}}, \ldots, t_{\ell_{j,m_j}}; x_j; x_j')\right).$$ \hspace{1cm} (3.28)$$

The time variable $t_{\ell_{j,\alpha}}$ corresponds to the one attached to the $\alpha$-th interaction operator (counting from the left) appearing in the factor $J^j_{\sigma}$ (every $t_{\ell_{j,\alpha}}$ corresponds uniquely to one of the time variables $t_\ell$ in (3.25)). We will prove that the right hand side tends to zero as $r \to \infty$, for $t \in [0, T)$, and sufficiently small $T > 0$. Since $r$ is arbitrary, this implies that the left hand side equals zero, thus establishing uniqueness. By iterating this argument on the union of intervals $[0, T) \cup [T, 2T) \cup \ldots$, uniqueness extends to the entire time of existence for a given solution. We also note that in (3.28), the distinction between focusing and defocusing GP hierarchy has disappeared, since $|\lambda| = 1$ in both cases.

### 3.3. Definition of binary trees

We now introduce binary tree graphs as a bookkeeping device to keep track of the complicated contraction structures imposed by the interaction operators inside the iterated Duhamel formula (3.25).
To this end, we associate (3.25) to the union of $k$ disjoint binary tree graphs, $(\tau_j)_{j=1}^k$. We note that these appear as "skeleton graphs" for the more complicated graphs in [22, 23, 24, 25]. We assign:

- An **internal vertex** $v_\ell$, $\ell = 1, \ldots, r$, to each operator $B_{\sigma(k+\ell), k+\ell}$. Accordingly, the time variable $t_\ell$ in (3.25) is thought of as being attached to the vertex $v_\ell$.
- A **root vertex** $w_j$, $j = 1, \ldots, k$ to each factor $J_j^j \cdots (x_j^j; x_j')$ in (3.27).
- A **leaf vertex** $u_i$, $i = 1, \ldots, k + r$, to the factor $\langle \phi \rangle \langle \phi \rangle (x_i; x_i')$ in (3.26).

For the sake of concreteness, we draw graphs as follows: We consider the strip in $[0, 1]$. We draw all root vertices $(w_j)_{j=1}^k$, ordered vertically, on the line $x = 0$, all internal vertices $(v_\ell)_{\ell=1}^r$ in the region $x \in (0, 1)$, where $v_\ell$ is on the right of $v_\ell'$ if $\ell' > \ell$. Finally, we draw all leaf vertices $(u_i)_{i=1}^{k+r}$, ordered vertically, on the line $x = 1$.

Next, we introduce the equivalence relation "~" of connectivity between vertices. Between any pair of connected vertices, we draw a connecting line, which we refer to as an **edge**:

- Let $v_\ell$ be the internal vertex with smallest value of $\ell$ such that $\sigma(\ell) = j$; then, we say that $v_\ell$ is connected to the root vertex $w_j$, that is, $w_j \sim v_\ell$.
- If there is no internal vertex connected to $w_j$, we draw an edge connecting $w_j$ to the leaf vertex $u_j$, and say that they are connected, $w_j \sim u_j$.
- Given $k < \ell \leq k + r$, if there exists $\ell' > \ell$ such that $\ell = \sigma(\ell')$ or $\ell = \sigma(\ell')$, we say that $v_\ell \sim v_{\ell'}$ are connected.
  
  $v_\ell$ is then called a **parent vertex** of $v_{\ell'}$, and $v_{\ell'}$ is called a **child vertex** of $v_\ell$. We denote the two child vertices of $v_\ell$ by $v_{\kappa_-(\ell)}$ and $v_{\kappa_+(\ell)}$, using the condition $\kappa_-(\ell) < \kappa_+(\ell)$.

  If there exists no internal vertex $v_{\ell'}$ with $\ell' > \ell$ such that $\ell = \sigma(\ell')$, we say that $v_\ell$ is connected to the leaf vertex $u_\ell$, $v_\ell \sim u_\ell$; if there exists no internal vertex $v_{\ell'}$ with $\ell' > \ell$ such that $\sigma(\ell) = \sigma(\ell')$, we say that $v_\ell$ is connected to the leaf vertex $u_{\sigma(\ell)}$, $v_\ell \sim u_{\sigma(\ell)}$. In these cases, $v_\ell$ is the **parent vertex** of $u_\ell$ (or $u_{\sigma(\ell)}$), and $u_\ell$ (or $u_{\sigma(\ell)}$) is a **child vertex** of $v_\ell$.

This implies that every internal vertex has precisely two child vertices, which can either be internal or leaf vertices (they do not need to be of the same type). Every root vertex has precisely one child vertex, which could be of internal or of leaf type. Every internal or leaf vertex has exactly one parent vertex.

We conclude that the graph thus obtained is the disjoint union of $k$ binary trees, which we denote by $(\tau_j)_{j=1}^k$, where the root of $\tau_j$ is the root vertex $w_j$ (if $w_j \sim u_j$ without internal vertices inbetween, then the binary tree consists trivially only of a single edge connecting one root and one leaf vertex).

We say that the tree $\tau_j$ is **distinguished** if $v_r \in \tau_j$, and **regular** if $v_r \not\in \tau_j$. We call the two leaf vertices connected to $v_r$ **distinguished leaf vertices**, and all others **regular leaf vertices**. Clearly, there are $k - 1$ regular trees, and one distinguished tree in this construction.
Figure 1. The disjoint union of three tree graphs $\tau_j$, $j = 1, 2, 3$, corresponding to the case $k = 3$, $r = 4$, and

$$J^3(\sigma; t, t_1, \ldots, t_4) = U^{(3)}_{0,1}B_2u^{(4)}_{1,2}B_2B_5u^{(5)}_{2,3}B_6u^{(6)}_{3,4}B_{5,7}(|\phi\rangle\langle\phi|)^{\otimes 7},$$

where $U^{(j)}_{i,i'}$ denotes $U^{(j)}(t_i - t_{i'})$ with the convention that $t_0 = t$. The root vertex $w_j$ belongs to the tree $\tau_j$, $j = 1, 2, 3$. The internal vertices correspond to $v_1 \sim B_2, v_2 \sim B_2, v_3 \sim B_3, v_4 \sim B_5$. The leaf vertices $u_5$ and $u_7$, and the internal vertex $v_4 \sim B_5$ are distinguished. The distinguished tree $\tau_2$ is drawn with thick edges.

3.4. An illustrative example. A roadmap of the proof consists of the following two steps:

1. recognize that a certain product structure gets preserved from right to left (via recursively introducing kernels that account for contractions performed by B operators)

2. get an estimate on integrals in upper echelon form via recursively performing Strichartz estimates (at the level of the Schrödinger equation) from left to right

In particular, to illustrate the strategy of the proof we considering an example of a distinguished tree, which we obtain from setting $k = 1, r = 3$ in (3.24) (if $k = 1$, there is only one tree, and it is necessarily distinguished). From (3.24) and (3.25), we have

$$\gamma^{(1)}(t) = (i\lambda)^3 \sum_{\sigma \in N_{1,3}} \int_{D(\sigma,t)} dt_1 dt_2 dt_3 \int d\tilde{\mu}_{t_3}(\phi)U^{(1)}(t)(t_2-t_1)B_{1,2}U^{(2)}(t_1-t_2)$$

$$B_{\sigma(3),3}U^{(3)}(t_2-t_3)B_{\sigma(4),4}(|\phi\rangle\langle\phi|)^{\otimes 4},$$

(3.30)
where $D(\sigma, t) \subseteq [0, t]^3$. For a fixed $\sigma$ (with, say, $\sigma(3) = 2$ and $\sigma(4) = 3$), we consider, as an example, the contribution to the bound (3.28) of the form

$$
\int_{[0,T]^3} dt_1 dt_2 dt_3 \int d\mu_{t_3}(i) \text{Tr} \left( \left| \left( U^{(1)}(t-t_1) B_{1,2} U^{(2)}(t-t_2) B_{2,3} U^{(3)}(t_2-t_3) B_{3,4}(|\phi\rangle \langle \phi|)^{\otimes 4} \right) \right| \right),
$$

(3.31)

where $t \in [0, T)$, and noting that $|i\lambda| = 1$.

3.4.1. Recursive determination of contraction structure. Clearly, $(|\phi\rangle \langle \phi|)^{\otimes 4}$ is a product of 1-particle density matrices. We observe that the interaction operators $B_{i,j}$ preserve the product structure (while changing the explicit expressions for each factor), and contract two factors at a time (the $i$-th and the $j$-th). On all other factors, $B_{i,j}$ acts as the identity. We introduce kernels $\Theta_\alpha$, $\alpha = 1, \ldots, 3$ that account for the contractions performed by $B_{\sigma(\alpha+1),\alpha+1}$, which we write in the normal form

$$
\Theta_\alpha(x, x') = \sum_{\beta_\alpha} c^\alpha_{\beta_\alpha} \chi^\alpha_{\beta_\alpha}(x) \overline{\psi^\alpha_{\beta_\alpha}}(x')
$$

(3.32)

where $\chi^\alpha_{\beta_\alpha}, \psi^\alpha_{\beta_\alpha}$ are certain functions that will be recursively determined, and $c^\alpha_{\beta_\alpha}$ are coefficients with values in $\{1, -1\}$.

- The kernel $\Theta_3$: We start at the last interaction operator $B_{3,4}$ in (3.31). It acts nontrivially only on the 3-rd and 4-th factor in $(|\phi\rangle \langle \phi|)^{\otimes 4}$,

$$
B_{3,4}(|\phi\rangle \langle \phi|)^{\otimes 4} = (|\phi\rangle \langle \phi|)^{\otimes 2} \otimes \Theta_3.
$$

(3.33)

The kernel $\Theta_3$ is obtained from contracting a two particle density matrix to a one particle density matrix via the interaction operator $B_{1,2}$ (which acts on a two-particle kernel $f(x, y; x', y')$ by $(B_{1,2}f)(x, x') = f(x, x'; x) - f(x, x'; x')$).

$$
\Theta_3(x, x') := B_{1,2} \left( (|\phi\rangle \langle \phi|)^{\otimes 2} \right)(x, x') = \overline{\psi(x)} \overline{\phi(x')} - \overline{\phi(x)} \overline{\psi(x')}
$$

$$
=: \sum_{\beta_3=1}^2 c^3_{\beta_3} \chi^3_{\beta_3}(x) \overline{\psi^3_{\beta_3}}(x')
$$

(3.34)

where

$$
\overline{\psi} := |\phi|^2 \phi.
$$

(3.35)

Here, we have $c^3_1 = 1$, $c^3_2 = -1$, $\chi^3_1 = \overline{\psi}$, $\chi^3_2 = \phi$, $\psi^3_1 = \phi$, $\psi^3_2 = \overline{\psi}$.

Main difficulty: The main difficulty in estimating (3.31) stems from the fact that the term $\overline{\psi} = |\phi|^2 \phi$ can only be controlled in $L^2$, where by Sobolev embedding, $\|\psi\|_{L^2} \leq C\|\phi\|_{H^1}$, which can then be controlled by (3.22), see (4.9) below. Our objective thus is to apply the triangle inequality to the trace norm inside (3.31), and to recursively “propagate” the resulting $L^2$ norm through all intermediate terms until we reach $\overline{\psi}$, see (3.40) below. We remark that if $\|\psi\|_{H^1}$ could be controlled by $\|\phi\|_{H^1}$ (which is not the case), a straightforward application of the method of [43] would suffice to carry out our analysis.

We now re-interpret $\overline{\psi}$ in (3.34) as a function that is independent of $\phi$, $\overline{\phi}$. Only at the end of our analysis, we will substitute $\overline{\psi} := |\phi|^2 \phi$. We call a factor $\chi^\alpha_{\beta_\alpha}$,
3.4.2. Recursive bounds. We may now return to (3.31), and perform the following recursive bounds with respect to time integration.

- The kernel $\Theta_2$: Next, we consider the terms contracted by $B_{2,3}$ in (3.31),

$$B_{2,3}U^{(3)}(t_2 - t_3)\left(\langle \phi | \phi \rangle \otimes \Theta_3\right) = \left(U^{(1)}(t_2 - t_3)\langle \phi | \phi \rangle \otimes \Theta_2\right),$$

using (3.33), which defines the kernel

$$\Theta_2(x, x') = B_{1,2}\left(\left(U^{(1)}(t_2 - t_3)\langle \phi | \phi \rangle \otimes (U^{(1)}(t_2 - t_3)\Theta_3)\right)(x, x')\right)$$

$$= (U_{2,3}\phi)(x)(U_{2,3}\phi)(x') \sum_{\beta_3 = 1}^2 c_{\beta_3}^3 \left[(U_{2,3}\chi_{\beta_3}^3)(x)(U_{2,3}\psi_{\beta_3}^3)(x)\right.$$

$$\left.\quad - (U_{2,3}\chi_{\beta_3}^3)(x')(U_{2,3}\psi_{\beta_3}^3)(x')\right]$$

$$=: \sum_{\beta_2 = 1}^4 c_{\beta_2}^3 \chi_{\beta_2}^3(x)\overline{\psi_{\beta_2}^3}(x'),$$

(3.37)

where

$$U_{i,j} := e^{i(t_i - t_j)\Delta}.$$  

(3.38)

Since for every $\beta_3$, only one out of the two factors $\chi_{\beta_3}^3, \psi_{\beta_3}^3$ is distinguished, it follows from (3.37) that for every $\beta_2 \in \{1, \ldots, 4\}$, only one out of the two factors $\chi_{\beta_2}^2, \psi_{\beta_2}^2$ is distinguished. The coefficients $c_{\beta_2}^2$ again have values in $\{1, -1\}$.

- The kernel $\Theta_1$: Finally, we consider the terms contracted by $B_{1,2}$ in (3.31), corresponding to

$$\Theta_1(x, x') = B_{1,2}\left(\left(U^{(1)}(t_1 - t_2)U^{(1)}(t_2 - t_3)\langle \phi | \phi \rangle \otimes (U^{(1)}(t_1 - t_2)\Theta_2)\right)(x, x')\right)$$

$$= (U_{1,3}\phi)(x)(U_{1,3}\phi)(x') \sum_{\beta_2 = 1}^4 c_{\beta_2}^2 \left[(U_{1,2}\chi_{\beta_2}^2)(x)(U_{1,2}\psi_{\beta_2}^2)(x)\right.$$

$$\left.\quad - (U_{1,2}\chi_{\beta_2}^2)(x')(U_{1,2}\psi_{\beta_2}^2)(x')\right]$$

$$=: \sum_{\beta_1 = 1}^8 c_{\beta_1}^1 \chi_{\beta_1}^1(x)\overline{\psi_{\beta_1}^1}(x').$$

(3.39)

Again, since for every $\beta_2$, only one out of the two functions $\chi_{\beta_2}^2, \psi_{\beta_2}^2$ is distinguished, it follows that for every $\beta_1 \in \{1, \ldots, 8\}$, only one out of the two functions $\chi_{\beta_1}^1, \psi_{\beta_1}^1$ is distinguished. The coefficients $c_{\beta_1}^1$ again have values in $\{1, -1\}$.
• **Integral in** $t_1$. Applying Cauchy-Schwarz with respect to the integral in $t_1$ and the triangle inequality for the trace norm, we obtain that

\[
(3.31) = \int_{[0,T]^3} dt_1 dt_2 dt_3 \int d\mu_{i3}^{(i)}(\phi) \text{Tr} \left( \left| U^{(1)}(t-t_1)\Theta_1 \right| \right)
\]

\[
\leq \sum_{\beta_1=1}^{8} T^{3/2} \int_{[0,T]^2} dt_2 dt_3 \int d\mu_{i3}^{(i)}(\phi) \left\| \chi_{\beta_1}^1 \right\|_{L^2} \left\| \psi_{\beta_1}^1 \right\|_{L^2} \left\| \psi_{\beta_2}^2 \right\|_{L^2_{t_1 \in [0,T]}},
\]

using that $|e_{\beta_1}^1| = 1$. From (3.39), we see that given $\beta_1 \in \{1, \ldots, 8\}$, there exists $\beta_2$ such that

\[
\chi_{\beta_1}^1(x) = (U_{1,3}\phi)(x)
\]

\[
\psi_{\beta_1}^1(x) = (U_{1,3}\phi)(x)(U_{1,2}\chi_{\beta_2}^2)(x)(U_{1,2}\psi_{\beta_2}^2)(x)
\]

(3.41)

(or with a cubic expressions for $\chi_{\beta_1}^1$ and a linear expression for $\psi_{\beta_1}^1$). Therefore,

\[
\left\| \chi_{\beta_1}^1 \right\|_{L^2} \left\| \psi_{\beta_1}^1 \right\|_{L^2} \left\| \psi_{\beta_2}^2 \right\|_{L^2_{t_1 \in [0,T]}},
\]

\[
= \left\| \phi \right\|_{L^2} \left| (U_{1,3}\phi)(x)(U_{1,2}\chi_{\beta_2}^2)(x)(U_{1,2}\psi_{\beta_2}^2)(x) \right| \left\| \psi_{\beta_2}^2 \right\|_{L^2_{t_1 \in [0,T]}},
\]

using that $U_{1,3}$ is unitary, and that $\phi$ does not depend on $t_1$.

Next, we observe that

\[
\left\| (e^{it\Delta} f_1)(x)(e^{it\Delta} f_2)(x)(e^{it\Delta} f_3)(x) \right\|_{L^2_t L^6_x(\mathbb{R}^3)}
\]

\[
\leq \left\| e^{it\Delta} f_1 \right\|_{L^\infty_t L^6_x} \left\| e^{it\Delta} f_2 \right\|_{L^\infty_t L^6_x} \left\| e^{it\Delta} f_3 \right\|_{L^2_t L^6_x}
\]

\[
\leq C \left\| f_1 \right\|_{H^1_t} \left\| f_2 \right\|_{H^1_t} \left\| f_3 \right\|_{H^1_t},
\]

(3.43)

using the Hölder inequality, the Sobolev inequality, and the Strichartz estimate $\left\| e^{it\Delta} f \right\|_{L^2_t L^6_x} \leq C \left\| f \right\|_{L^2}$ for the free Schrödinger evolution. We make the important observation that in (3.43), we can place the $L^2_t$-norm on any of the three functions $f_j$, $j = 1, 2, 3$, and not only on $f_3$. Similarly, if a derivative is included,

\[
\left\| \nabla_x (e^{it\Delta} f_1)(x)(e^{it\Delta} f_2)(x)(e^{it\Delta} f_3)(x) \right\|_{L^2_t L^2_x(\mathbb{R}^3)}
\]

\[
\leq \sum_{j=1}^{3} \left\| e^{it\Delta} \nabla_x f_j \right\|_{L^2_t L^6_x} \prod_{1 \leq i \neq j \leq 3} \left\| e^{it\Delta} f_i \right\|_{L^\infty_t L^6_x}
\]

\[
\leq C \left\| f_1 \right\|_{H^1_t} \left\| f_2 \right\|_{H^1_t} \left\| f_3 \right\|_{H^1_t},
\]

(3.44)

which, together with (3.43), implies that

\[
\left\| (e^{it\Delta} f_1)(x)(e^{it\Delta} f_2)(x)(e^{it\Delta} f_3)(x) \right\|_{L^2_t H^1_x(\mathbb{R}^3)} \leq C \prod_{j=1}^{3} \left\| f_j \right\|_{H^1_t}.
\]

(3.45)

Only one of the factors $\chi_{\beta_2}^2$, $\psi_{\beta_2}^2$ is distinguished, say for instance $\psi_{\beta_2}^2$. We then use (3.43) in such a way that the $L^2_t$-norm is applied to this term. All terms in
(3.40) can be treated in the same manner, thus obtaining

\[
(3.31) \leq C T^{1/2} \sum_{\beta_1 = 1}^{8} \int_{[0,T)^2} dt_2 dt_3 \int d\mu_{t_3}^{(i)}(\phi) \|\phi\|_{H^1}^2 \|\chi_{\beta_2}^2 \|_{H^1} \|\psi_{\beta_2}^2 \|_{L^2},
\]

where the indices \(\beta_2\) depend on \(\beta_1\). Next, we use the defining relation (3.37) for the functions \(\chi_{\beta_2}^2, \psi_{\beta_2}^3\), and consider the integral in \(t_2\).

- **Integral in \(t_2\).** By assumption, the factor \(\psi_{\beta_2}^2\) is distinguished, while \(\chi_{\beta_2}^2\) is not. Moreover, one of the functions \(\chi_{\beta_2}^2, \psi_{\beta_2}^3\) is linear, while the other one is a cubic expression in the functions after the second equality sign in (3.37) (the distinguished factor could be either). Our goal is to bound the distinguished factor in \(L^2\). From comparing terms in (3.37), one possible combination is

\[
\chi_{\beta_2}^2(x) = (U_{2,3}\phi)(x), \quad \psi_{\beta_2}^3(x) = (U_{2,3}\phi)(x)(U_{2,3}\chi_{\beta_1})^2(x)(U_{2,3}\psi_{\beta_3}^3)(x),
\]

that is, the distinguished factor \(\psi_{\beta_2}^3\) is a cubic expression. We apply Cauchy-Schwarz in the \(L^2\)-integral in such a way that the \(L^2\) norm falls on the cubic term. (If, on the other hand, \(\chi_{\beta_2}^2\) is the cubic term, we use Cauchy-Schwarz in \(t_2\) to get \(\|\psi_{\beta_2}^3\|_{L^2} \leq \chi_{\beta_2}^3 \|L^2\) and \(\|\chi_{\beta_2}^2\|_{L^2} \leq C \|\phi\|_{H^1}\) from (3.45).) We then get

\[
(3.46) \leq C T \sum_{\beta_1 = 1}^{8} \int_{[0,T)} dt_3 \int d\mu_{t_3}^{(i)}(\phi) \|\phi\|_{H^1}^2 \|\chi_{\beta_2}^2 \|_{L^2} \|\psi_{\beta_2}^3 \|_{L^2} \|U_{2,3}\phi(x)(U_{2,3}\chi_{\beta_1})^2(x)(U_{2,3}\psi_{\beta_3}^3)(x)\|_{L^2} \leq C \|\phi\|_{H^1},
\]

where only one of the three factors inside the norm on the last line is distinguished. We may assume it is \(\psi_{\beta_3}^3\). By comparing terms in (3.34), we then find that \(\psi_{\beta_3}^3 = \tilde{\psi}\), and \(\chi_{\beta_3}^3 = \phi\). We then apply (3.43) again, and use the \(L^2\)-bound for \(\psi_{\beta_3}^3 = \tilde{\psi}\). At this point, we substitute \(\tilde{\psi} = |\phi|^2 \phi\).

- **Using de Finetti for the last step.** Subsequently, we obtain

\[
(3.31) \leq C T \sum_{\beta_1 = 1}^{8} \int_{[0,T)} dt_3 \int d\mu_{t_3}^{(i)}(\phi) \|\phi\|_{H^1}^5 \|\tilde{\psi}\|_{L^2} \leq 8CT^2 \sup_{t_3 \in [0,T]} \int d\mu_{t_3}^{(i)}(\phi) \|\phi\|_{H^1}^8 \leq 8CT^2 M^4,
\]

where we used \(\|\tilde{\psi}\|_{L^2} \leq C \|\phi\|_{H^1}\) from Sobolev embedding, and the bound (3.22) related to the de Finetti theorem, which is uniform in \(t_3\). This is the desired estimate in our example calculation.

The strategy presented in this example can be applied in the general case and details are in [8].
References


ON A DERIVATION OF NLS


[60] Z. Xie, Uniqueness of Gross Pitaevskii (GP) solution on 1D and 2D nonlinear Schrödinger equation, Preprint, arXiv:1305.7240

T. Chen, Department of Mathematics, University of Texas at Austin.

E-mail address: tc@math.utexas.edu

N. Pavlović, Department of Mathematics, University of Texas at Austin.

E-mail address: natasa@math.utexas.edu

N. Tzirakis, University of Illinois at Urbana-Champaign.

E-mail address: tzirakis@math.uiuc.edu