

Dynamics of Bose-Einstein Condensates

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INTERACTING MANY-BODY QUANTUM SYSTEMS

$\mathbf{x} = (x_1, x_2, \dots, x_N) \in \mathbb{R}^{3N}$ position of the particles.

Symmetric wave function: $\psi_N(x_1, \dots, x_N) \in L^2(\mathbb{R}^{3N})$

$$H_N = \sum_{j=1}^N \left[-\Delta_{x_j} + U(x_j) \right] + \lambda \sum_{i < j} V(x_i - x_j)$$

U is a one-body background (“trapping”) potential

V is the interaction potential

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \quad i\partial_t \gamma_{N,t} = [H, \gamma_{N,t}], \quad [A, B] = AB - BA$$

with $\gamma_{N,t} := |\psi_{N,t}\rangle\langle\psi_{N,t}| = \psi(x_1, x_2 \cdots x_N) \bar{\psi}(x'_1, x'_2 \cdots x'_N)$ density matrix (1 dim. projection).

One particle density matrix:

$$\gamma_\psi^{(1)}(x, y) := \int \psi(x, x_2 \cdots x_N) \bar{\psi}(y, x_2 \cdots x_N) dx_2 \cdots dx_N$$

Time-independent BEC in Scaling Limit

$$H_N = \sum_{j=1}^N \left[-\Delta_{x_j} + U(x_j) \right] + \frac{1}{N} \sum_{i < j} N^3 V(N(x_i - x_j))$$

Approx Dirac delta interaction with range $1/N$ (“hard core”)

[Dyson, Lieb-Seiringer-Yngvason, Lieb-Seiringer]

- Ground state energy is given by the **Gross-Pitaevskii functional**

$$\lim_{N \rightarrow \infty} \inf \text{spec} \frac{H_N}{N} = \inf_{\varphi, \|\varphi\|=1} \mathcal{E}_{GP}(8\pi a_0, \varphi), \quad a_0 = \text{scatt. length of } V$$

$$\mathcal{E}_{GP}(\sigma, \varphi) := \int |\nabla \varphi|^2 + U|\varphi|^2 + \frac{\sigma}{2} |\varphi|^4$$

- **Complete condensation in ground state:**

$$\gamma_N^{(1)}(x; x') \rightarrow \phi(x) \overline{\phi(x')}, \quad \phi = \text{minimizer of } \mathcal{E}_{GP}$$

Time Dependent GROSS-PITAEVSKII (GP) Theory

The GP energy functional also describes the evolution:

$$\gamma_{N,0}^{(1)} \rightarrow \varphi(x)\bar{\varphi}(x') \quad \Longrightarrow \quad \gamma_{N,t}^{(1)} \rightarrow \varphi_t(x)\bar{\varphi}_t(x')$$

The condensate wave fn. evolves according to a NLS

$$i\partial_t\varphi_t = \left[-\Delta + U + 8\pi a_0|\varphi_t|^2 \right]\varphi_t, \quad \varphi_{t=0} = \varphi$$

Many-body effects & corr \rightarrow non-linear on-site self-interaction

Experiments of Bose-Einstein Condensation: Trap Bose gas and observe its evolution after the trap removed.

Dynamics: The ground state of trapped BEC is a highly excited state for the system without traps. GP describes also excited states and their evolution!

Cannot be completely correct. Now set $U = 0$.

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N} \sum_{i < j} V_\beta(x_i - x_j), \quad V_\beta(x) := N^{3\beta} V(N^\beta x), \quad 0 < \beta \leq 1$$

THEOREM: [Erdős-Schlein-Y, 2008] Assume $V \geq 0$ and $V(x) \leq C(1 + |x|)^{-5}$. Suppose the initial state satisfies

$$\gamma_{N,0}^{(1)}(x, y) \rightarrow u_0(x)\bar{u}_0(y), \quad u \in H^1(\mathbb{R}^3)$$

Then for every $k \geq 1$ and $t > 0$ fixed

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

$$i\partial_t u_t = -\Delta u_t + \sigma |u_t|^2 \phi_t, \quad \sigma = \begin{cases} b_0 & \text{if } 0 < \beta < 1 \\ 8\pi a_0 & \text{if } \beta = 1 \end{cases}$$

where a_0 is the scatt. length of V and $b_0 = \int dx V(x) \neq 8\pi a_0$

Adami, Bardos, Golse, Teta: one dim result. Use $\delta \leq -\Delta$ in \mathbb{R} .

SCATTERING LENGTH

$$\left(-\Delta + \frac{1}{2}V(x)\right) (1 - w(x)) = 0 \quad \text{with } w(x) \rightarrow 0 \text{ for } |x| \rightarrow \infty.$$

$$w(x) = \frac{a_0}{|x|} \quad \text{for } |x| \rightarrow \infty \quad \int dx V(x)(1 - w(x)) = 8\pi a_0$$

Dyson's trial function for ground state:

$$W_N(\mathbf{x}) = \prod_{j < k} \left[1 - w(N(x_j - x_k)) \right]$$

States with and without short range structure:

$$\psi_N(\mathbf{x}) = W_N(\mathbf{x}) \prod_{j=1}^N u_0(x_j), \quad \phi_N = \prod_{j=1}^N u_0(x_j)$$

$$\lim_{N \rightarrow \infty} N^{-1} \langle \psi_N, H_N \psi_N \rangle = \int |\nabla u(x)|^2 + 4\pi a_0 |u(x)|^4$$

$$\lim_{N \rightarrow \infty} N^{-1} \langle \phi_N, H_N \phi_N \rangle = \int |\nabla u_0(x)|^2 + \frac{b_0}{2} |u(x)|^4$$

One Body Problem: Fix $\ell \ll N^{-1/3}$. Consider the Neumann problem on $\{x \in \mathbb{R}^3 : |x| \leq \ell\}$:

$$\left(-\Delta + \frac{N^2}{2}V(Nx)\right)(1 - w_\ell(x)) = e_\ell(1 - w(x)).$$

Normalization: $w_\ell(x) = 0$ for $|x| = \ell$.

Lowest eigenvalue: $e_\ell \simeq \frac{a_0}{N\ell^3}$.

Lowest eigenfunction: $1 - w_\ell(x) \simeq 1 - \frac{a_0}{N|x|}$ for $a_0/N \ll |x| \ll \ell_1$

Extend $w(x) = 0$ for $|x| \geq \ell$. Then

$$\left(-\Delta + \frac{1}{2}V_N(x)\right)(1 - w_\ell(x)) = q(x)(1 - w_\ell(x))$$

with

$$q(x) = a\ell^{-3}\chi(|x| \leq \ell)$$

The theorem for $\beta = 1$ holds for ψ_N and ϕ_N .

Our Theorem shows that the local singular structure is preserved by the N -body evolution for initial state ψ_N . For product initial state, it shows that the local structure **emerges** .

$$i\partial_t\phi_{N,t} = H_N\phi_{N,t}, \quad \phi_{N,t=0} = \phi_N$$

$$N^{-1}\langle\phi_{N,t}, H_N\phi_{N,t}\rangle = N^{-1}\langle\phi_N, H_N\phi_N\rangle$$

$$\rightarrow \mathcal{E}_{GP}(b_0, u_0) \neq \mathcal{E}_{GP}(8\pi a_0, u_0) = \mathcal{E}_{GP}(8\pi a_0, u_t)$$

For product initial state, the GP energy functional (with the coupling constant $8\pi a_0$) **does not describe the energy of the N -body system** . But **the time dependent one particle density matrices in a weak limit** is still given by the GP equation with coupling constant $8\pi a_0$.

Mathematically: The convergence of the time dependent density matrices is so weak that the energy does not converge.

Physically: For states with product initial data, the short scale behavior will show the characteristic $1 - w(N(x_i - x_j))$ structure after a short initial layer. This lowers the energy of the system locally. The energy lost was transferred to energy in other scales.

Summary of Lecture 1

$$i\partial_t\psi_{N,t} = H_N\psi_{N,t}, \quad i\partial_t\gamma_{N,t} = [H, \gamma_{N,t}], \quad [A, B] = AB - BA$$

with $\gamma_{N,t} := |\psi_{N,t}\rangle\langle\psi_{N,t}| = \psi(x_1, x_2 \cdots x_N)\bar{\psi}(x'_1, x'_2 \cdots x'_N)$ density matrix (1 dim. projection).

State ψ can also be identified with $\gamma = |\psi\rangle\langle\psi|$, the operator of projection onto $\text{Span}\{\psi\}$ (**pure state**).

In general: $\gamma = \sum_i c_i |\psi_i\rangle\langle\psi_i|$, $0 \leq c_i \leq 1$, $\sum_i c_i = 1$ (**mixed state**).

Def: Density matrix is a self-adjoint operator γ with $0 \leq \gamma \leq 1$
We will identify it with its (operator) kernel, $\gamma(x; x')$.

$$H_N = \sum_{j=1}^N \left[-\Delta_{x_j} + U(x_j) \right] + \frac{1}{N} \sum_{i < j} N^3 V(N(x_i - x_j))$$

$$\left(-\Delta + \frac{1}{2} V(x) \right) (1 - w(x)) = 0 \quad \text{with } w(x) \rightarrow 0 \text{ for } |x| \rightarrow \infty.$$

$$w(x) = \frac{a_0}{|x|} \quad \text{for } |x| \rightarrow \infty \quad \int dx V(x) (1 - w(x)) = 8\pi a_0$$

In order to obtain the correct coupling constant related to the scattering length, we need short range correlation structure of Dyson type:

$$W_N(\mathbf{x}) = \prod_{j < k} \left[1 - w(N(x_j - x_k)) \right]$$

A good ansatz for states with short range structure:

$$\psi_N(\mathbf{x}) = W_N(\mathbf{x}) \prod_{j=1}^N u(x_j)$$

$$\lim_{N \rightarrow \infty} N^{-1} \langle \psi_N, H_N \psi_N \rangle = \int |\nabla u(x)|^2 + 4\pi a_0 |u(x)|^4$$

One particle density matrix:

$$\gamma_\psi^{(1)}(x, y) := \int \psi(x, x_2 \cdots x_N) \bar{\psi}(y, x_2 \cdots x_N) dx_2 \cdots dx_N$$

Two key open questions for the time indep theory:

[Dyson, Lieb-Seiringer-Yngvason, Lieb-Seiringer]

- Ground state energy is given by the **Gross-Pitaevskii functional**

$$\lim_{N \rightarrow \infty} \inf \text{spec} \frac{H_N}{N} = \inf_{\varphi, \|\varphi\|=1} \mathcal{E}_{GP}(8\pi a_0, \varphi), \quad a_0 = \text{scatt. length of } V$$

$$\mathcal{E}_{GP}(\sigma, \varphi) := \int |\nabla \varphi|^2 + U|\varphi|^2 + \frac{\sigma}{2} |\varphi|^4$$

- Complete condensation in ground state:

$$\gamma_N^{(1)}(x; x') \rightarrow \phi(x)\overline{\phi(x')}, \quad \phi = \text{minimizer of } \mathcal{E}_{GP}$$

It is a dilute limit, not a mean-field limit.

MATHEMATICAL DEFINITION OF BEC

Let γ_N be the ground state or a very low temperature state ($e^{-\beta H_N}$, $\beta \gg 1$) of the interacting Bose-system and recall that $\gamma_N^{(1)}$ is its one-particle density matrix.

Spectral decomposition: $\gamma_N^{(1)} = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$.

DEFINITION: γ_N is a **condensate state** if

$$\liminf_{N \rightarrow \infty} \max_j \lambda_j > 0$$

and γ_N is **a state with a complete condensation** if

$$\liminf_{N \rightarrow \infty} \max_j \lambda_j = 1$$

The corresponding eigenfn. is the **condensate wave function**.

Problem 1: Condensation is expected in $d \geq 3$ for $\beta > \beta_{crit}$ at positive density even without trapping potential. Seems very

hard: there is **no gap** and there are infinitely many low energy states available.

Problem 2. Next order correction to the energy. Prove (or disprove) the Huang-Lee-Yang formula).

Key observation of time dependent theory:

1. States need short range correlation to have the correct scattering length. But even for states without short range correlation evolve according to NLS with correct coefficient given by scattering length.

Expected reason: there is an initial layer so that short range structure forms for arbitrary initial data whose one particle density matrix is a pure state.

2. GP theory is an effective theory in the large scale where all short scale structure is summarized in the scattering length.

3. For product initial state $\phi_N = \prod u_0(x_j)$, the initial energy is given by

$$N^{-1} \langle \phi_N, H_N \phi_N \rangle \rightarrow \mathcal{E}_{GP}(b_0, u_0)$$

After initial layer, the two scale structure was expected to form. For states with two scale structure given by our ansatz, the energy is expected to be $\mathcal{E}_{GP}(8\pi a_0, u_0)$.

However, energy is a conserved quantity in Schrödinger equation and we have a contradiction. Explanation: The ansatz catches short range and long range structures, but not immediate ranges.

Key observation: One can prove one particle density matrix converges to solution of the GP equation, but not its energy.

Outline of the lectures:

1. Mean-field limit and Hartree eq.
2. Sobolev space in “infinite dimension”.
3. Identification of correlations via the second moment of energy.

Connection with wave operator and a new type of Sobolev inequality.

4. Uniqueness of BBGKY hierarchy. Feynman diagram (Combinatorics and Estimates) as a replacement for Strichartz inequality in infinite dimension.

Klainerman-Machedon has a different proof of uniqueness, but no a priori estimate.

II.1. HARTREE EQUATION FROM BOSON DYNAMICS

$$H_N = \sum_{j=1}^N \left[-\Delta_{x_j} + U(x_j) \right] + \frac{1}{N} \sum_{i < j} V(x_i - x_j)$$

EXPECT: If $\Psi_0 = \prod_j \varphi_0(x_j)$, then $\Psi_t \approx \prod_j \varphi_t(x_j)$ as $N \rightarrow \infty$

where
$$i\partial_t \varphi_t = (-\Delta + U)\varphi_t + \left(V \star |\varphi_t|^2 \right) \varphi_t$$

Each particle: subject to the same **mean-field pot.** (LLN for x_j)

$$\frac{1}{N} \sum_{j=1}^N V(x - x_j) |\varphi(x_j)|^2 \approx (V \star |\varphi|^2)(x)$$

Implicitly assumes that the state remains roughly a product (propagation of chaos). This fact needs to be proven.

More precisely, the N -body wavefunction at $t > 0$ cannot be fully described, but its limiting marginals can:

THEOREM: If the initial state is factorized,

$$\gamma_{N,0}(\mathbf{x}, \mathbf{x}') = \prod_{i=1}^N \gamma_0(x_i, x'_i),$$

and $\gamma_{N,t}$ solves $i\partial_t \gamma_{N,t} = [H_N, \gamma_{N,t}]$, then

$$\gamma_t^{(1)} := \lim_{N \rightarrow \infty} \gamma_{N,t}^{(1)}$$

exists and it satisfies the Hartree-equation

$$i\partial_t \gamma_t^{(1)} = \left[-\Delta_x + U + V \star \varrho_t^{(1)}, \gamma_t^{(1)} \right], \quad \gamma_{t=0}^{(1)} = \gamma_0^{(1)}$$

Moreover, **propagation of chaos holds:**

$$\lim_{N \rightarrow \infty} \gamma_{N,t}^{(k)} = \left[\gamma_t^{(1)} \right]^{\otimes k}$$

For pure states, $\gamma^{(1)} = |\varphi\rangle\langle\varphi|$, **Hartree reduces to NLS:**

$$i\partial_t \varphi_t = (-\Delta + U)\varphi_t + \left(V \star |\varphi_t|^2 \right) \varphi_t$$

History of the derivation of NLS/Hartree eq.

- Hepp, 1974. Smooth potential
- Ginibre-Velo, 1979: Special quasifree states
- Spohn, 1980: Bounded potential. Method via BBGKY hierarchy.
- Bardos-Golse-Mauser 2001: weak compactness of BBGKY hierarchy for Coulomb (not enough estimates for uniqueness)
- E-Yau, 2001: Coulomb potential (with uniqueness)
Spohn's BBGKY method + Method of energy moments.
- Schlein-Rodnianski 2008: Coulomb potential with error estimate of order $1/\sqrt{N}$. Base on Ginibre-Velo method.

- Fröhlich-Knowles-Pizzo: $\hbar = \frac{1}{N}$, Wick quantization
- Elgart-Schlein: Pseudorelativistic case, $(1 - \Delta)^{1/2}$, with potential $V(x) = \frac{\lambda}{|x|}$ up to the borderline $\lambda > \lambda_{\text{crit}} = -4/\pi$

$$i\partial_t u_t = (1 - \Delta)^{1/2} u_t + (V * |u_t|^2) u_t$$

There are also proofs for the classical model (probability theory): Kac, McKean, Dobrushin, Spohn.

The problem is **harder** as the interaction **potential becomes more singular**.

V. GENERAL TOOLS FOR N -BODY DYNAMICS

V.1. FUNDAMENTAL DIFFICULTY

What is a good norm/measure for N -particle quantum state?

L^2 -norm is preserved, but it is too strong!

EXAMPLE 1:

$$\psi = f(x_1) \cdots f(x_N), \quad \psi' = g(x_1) \cdots g(x_N). \quad \|\psi\|^2 = \|\psi'\|^2 = 1$$

$$\|\psi - \psi'\|^2 = 2 - 2 \left[\langle f, g \rangle \right]^N \rightarrow 2$$

Any two distinct product states are “almost” orthogonal!

Other norms are hopeless:

$$\|\psi\|_2 = 1 \quad \implies \quad \|\psi\|_p \sim e^{\pm CN}, \quad p \neq 2$$

EXAMPLE 2:

Let f, f', g be orthogonal normalized one body states.

Let $\Psi = \text{Symm}\left[f \otimes \bigotimes_{j=2}^N g\right]$ and $\Psi' = \text{Symm}\left[f' \otimes \bigotimes_{j=2}^N g\right]$

$$\|\Psi - \Psi'\|_{L^2(\mathbb{R}^{3N})}^2 = \|f - f'\|_{L^2(\mathbb{R}^3)}^2 = 2$$

though **only one electron behaves badly**. L^2 norm is too strong.

But $\gamma_{\Psi}^{(1)}(x, x') = \frac{1}{N}\left[f(x)\bar{f}(x') + (N-1)g(x)\bar{g}(x')\right]$

$\text{Tr}\left|\gamma_{\Psi}^{(1)} - \gamma_{\Psi'}^{(1)}\right| = O\left(\frac{1}{N}\right)$ – **controlling only marginals is better.**

EXAMPLE 3: (Fundamental stability question.)

Is there a “norm” so that a change of interaction of order one produces an order one change for typical particle?

Suppose $|V - V'| \sim \varepsilon$ and $\psi'_{N,t}$ is solution with V' . Then

$$\partial_t \|\psi_t - \psi'_t\|^2 \sim \left\langle \psi_t - \psi'_t, \frac{1}{N} \sum_{\ell < j} (V - V')(x_\ell - x_j) \psi_t \right\rangle \sim N\varepsilon$$

But we know $\|\psi_t - \psi'_t\| \leq \|\psi_t\| + \|\psi'_t\| = 2$

This instability makes the analysis of singular potentials very hard: only N -dependent cutoffs are possible.

L^2 -norm is too strong, it monitors all particles: $\Psi(x_1, \dots, x_N)$ carries info of all particles (too detailed).

As Example 2 shows, the marginals could be better (they carry less information, hence they are less sensitive than the L^2 -norm.)

Keep only information about the k -particle correlations:

$$\gamma_{\Psi}^{(k)}(X_k, X'_k) := \int \Psi(X_k, Y_{N-k}) \overline{\Psi}(X'_k, Y_{N-k}) dY_{N-k}$$

where $X_k = (x_1, \dots, x_k)$. It monitors only k particles.

Recall: it is an operator acting on the k -particle space

Good news: Most physical observables involve only $k = 1, 2$ -particle marginals. Enough to control them.

Bad news: there is no closed equation for them.

III. BASIC TOOL: BBGKY HIERARCHY

$$H = - \sum_{j=1}^N \Delta_j + \frac{1}{N} \sum_{j < k} V(x_j - x_k)$$

$V = V_N$ may depend on N so that $\int V_N = O(1)$.

Take the k -th partial trace of the Schr. eq. $i\partial_t \gamma_{N,t} = [H, \gamma_{N,t}]$

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

A system of N coupled coupled equation. ($k = 1, 2, \dots, N$)

The last one is just the original N -body Schr. eq.

Seems tautological. (?)

$$N = 2$$

$$\begin{aligned} i\partial_t \gamma^{(1)}(x', x) &= i\partial_t \int \bar{\psi}(x', y) \psi(x, y) dy \\ &= \int [\Delta_{x'} - \Delta_x] \bar{\psi}(x', y) \psi(x, y) dy \\ &+ \int [V(x' - y) - V(x - y)] \bar{\psi}(x', y) \psi(x, y) dy \end{aligned}$$

$$i\partial_t \gamma_{N,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{N,t}^{(k)} \right] + \frac{1}{N} \sum_{i < j}^k \left[V(x_i - x_j), \gamma_{N,t}^{(k)} \right] + \frac{N-k}{N} \sum_{j=1}^k \text{Tr}_{x_{k+1}} \left[V(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right]$$

$$i\partial_t \gamma_{N,t}^{(k)} = \left[H_k^0, \gamma_{N,t}^{(k)} \right] + B_k \gamma_{N,t}^{(k+1)} + \varepsilon_k(N), \quad k = 1 \dots N$$

$$H_k^0 := - \sum_{j=1}^k \Delta_j, \quad \varepsilon_k(N) = O\left(\frac{k^2}{N}\right) \quad (\text{negligible})$$

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

B_k is called the **connecting operator**. With kernel notation:

$$(B_k \gamma^{(k+1)})(X_k; X'_k) = \sum_{j=1}^k \int dy \left(V(x_j - y) - V(x'_j - y) \right) \gamma^{(k+1)}(X_k, y; X'_k, y)$$

$[x_{k+1} = x'_{k+1}$ needs to be defined properly !]

Special case: $k = 1$:

$$i\partial_t \gamma_{N,t}^{(1)}(x_1; x'_1) = (-\Delta_{x_1} + \Delta_{x'_1}) \gamma_{N,t}^{(1)}(x_1; x'_1) \\ + \int dx_2 (V(x_1 - x_2) - V(x'_1 - x_2)) \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2) + o(1).$$

To get a closed equation for $\gamma_{N,t}^{(1)}$, we need some relation between $\gamma_{N,t}^{(1)}$ and $\gamma_{N,t}^{(2)}$. Most natural: **independence**

Propagation of chaos: No production of correlations

If initially $\gamma_{N,0}^{(2)} = \gamma_{N,0}^{(1)} \otimes \gamma_{N,0}^{(1)}$, then hopefully $\gamma_{N,t}^{(2)} \approx \gamma_{N,t}^{(1)} \otimes \gamma_{N,t}^{(1)}$

No exact factorization for finite N , but maybe it holds for $N \rightarrow \infty$.

Suppose $\gamma_{\infty,t}^{(k)}$ is a (weak) limit point of $\gamma_{N,t}^{(k)}$ with

$$\gamma_{\infty,t}^{(2)}(x_1, x_2; x'_1, x'_2) = \gamma_{\infty,t}^{(1)}(x_1, x'_1) \gamma_{\infty,t}^{(1)}(x_2; x'_2).$$

$$\begin{aligned}
i\partial_t \gamma_{N,t}^{(1)}(x_1; x'_1) &= (-\Delta_{x_1} + \Delta_{x'_1}) \gamma_{N,t}^{(1)}(x_1; x'_1) \\
&+ \int dx_2 \left(V(x_1 - x_2) - V(x'_1 - x_2) \right) \underbrace{\gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2)}_{\rightarrow \gamma_{\infty,t}^{(1)}(x_1, x'_1) \gamma_{\infty,t}^{(1)}(x_2; x_2)} + o(1)
\end{aligned}$$

With the notation $\varrho_t(x) := \gamma_{\infty,t}^{(1)}(x; x)$, it converges, to

$$\begin{aligned}
i\partial_t \gamma_{\infty,t}^{(1)}(x_1; x'_1) &= (-\Delta_{x_1} + \Delta_{x'_1}) \gamma_{\infty,t}^{(1)}(x_1; x'_1) \\
&+ \left(V * \varrho_t(x_1) - V * \varrho_t(x'_1) \right) \gamma_{\infty,t}^{(1)}(x_1; x'_1)
\end{aligned}$$

\Rightarrow Hartree-Equation for $\gamma_{\infty,t}^{(1)}$

$$i\partial_t \gamma_{\infty,t}^{(1)} = \left[-\Delta + V * \varrho_t, \gamma_{\infty,t}^{(1)} \right],$$

For pure states, $\gamma^{(1)} = |\varphi\rangle\langle\varphi|$, it is just $i\partial_t \varphi = (-\Delta + V * |\varphi|^2) \varphi$

Main technical goal: justify propagation of chaos (Closure).

BUT: $\psi_{N,t} = \prod_j u_t(x_j)$ never solves Schr. eq. with interaction.

Propagation of chaos for interacting systems can hold only as $N \rightarrow \infty$ and only in a weaker form:

$$\lim_N \gamma_N^{(k)} = \lim_N \otimes_1^k \gamma_N^{(1)}$$

for each fixed k .

This indicates to study BBGKY in the $N \rightarrow \infty$ limit instead of Schrödinger.

What kind of equations will $\gamma_\infty^{(k)} := \lim_{N \rightarrow \infty} \gamma_N^{(k)}$ satisfy?

By taking the (formal) limit of the N -particle BBGKY hierarchy, we obtain an infinite hierarchy of coupled equations, called **Hartree (or infinite BBGKY) hierarchy**.

$$i\partial_t \gamma_{N,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{N,t}^{(k)} \right] + \frac{1}{N} \sum_{i < j}^k \left[V(x_i - x_j), \gamma_{N,t}^{(k)} \right] \\ + \frac{N-k}{N} \sum_{j=1}^k \text{Tr}_{x_{k+1}} \left[V(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right]$$

formally converges to ($k = 1, 2, \dots$)

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

i.e.

$$i\partial_t \gamma_{\infty,t}^{(k)} = \left[H_k^0, \gamma_{\infty,t}^{(k)} \right] + B_k \gamma_{\infty,t}^{(k+1)}$$

IV. GENERAL SCHEME TO DERIVE NLS (HARTREE)

$$i\partial_t \gamma_{N,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{N,t}^{(k)} \right] + \frac{1}{N} \sum_{i < j}^k \left[V(x_i - x_j), \gamma_{N,t}^{(k)} \right] + \frac{N-k}{N} \sum_{j=1}^k \text{Tr}_{k+1} \left[V(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right]$$

formally converges to the ∞ Hartree hierarchy: ($k = 1, 2, \dots$)

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

$$\left\{ \gamma_t^{(k)} = \otimes_1^k \gamma_t^{(1)} \right\}_{k=1,2,\dots} \text{ solves } (*) \iff i\partial_t \gamma_t^{(1)} = \left[-\Delta + V * \varrho_t, \gamma_t^{(1)} \right]$$

If we knew that $\left\{ \begin{array}{l} (*) \text{ had a unique solution, and} \\ \lim_N \gamma_{N,t}^{(k)} \text{ exists and satisfies } (*), \end{array} \right.$

then the limit must be **the** factorized one

\implies Propagation of chaos + convergence to Hartree eq.

Step 1: Prove **apriori bound** on $\gamma_{N,t}^{(k)}$ uniformly in N .

Need a good norm and space \mathcal{H} ! (maybe Sobolev)

Step 2: Choose a convergent subsequence: $\gamma_{N,t}^{(k)} \rightarrow \gamma_{\infty,t}^{(k)}$ in \mathcal{H}

Step 3: $\gamma_{\infty,t}^{(k)}$ satisfies the infinite hierarchy (need regularity)

Step 4: Let $\gamma_t^{(1)}$ solve NLHE/NLS. Then $\gamma_t^{(k)} = \otimes \gamma_t^{(1)}$ solves the ∞ -hierarchy in \mathcal{H} . [Trivial]

Step 5: Show that the ∞ -hierarchy has a **unique** solution in \mathcal{H} .

Key mathematical steps: **Apriori bound and uniqueness**

Part I. Apriori bound: use conservation laws
(e.g. H^k is conserved)

Part II. Uniqueness: Expand the BBGKY into **Dyson series**, control the last (error) term by the apriori bound.

IV.1. CASE OF A BOUNDED POTENTIAL (SPOHN 1980)

Part I: Apriori bound. Here it is trivial:

Fact: $\text{Tr}\gamma_{N,t}^{(k)} = 1. \implies$ natural space/norm. $\mathcal{H} =$ trace class.

Control in trace norm passes to the limit, $\text{Tr}\gamma_{\infty,t}^{(k)} \leq 1.$

Part II: Uniqueness. Hartree hierarchy in integral form:

$$i\partial_t\gamma_t^{(k)} = \left[H_k^0, \gamma_t^{(k)} \right] + B_k\gamma_t^{(k+1)} \implies$$

$$\gamma_t^{(k)} = \mathcal{U}_k(t)\gamma_0^{(k)} - i \int_0^t ds \mathcal{U}_k(t-s)B_k\gamma_s^{(k+1)}$$

$$\mathcal{U}_k(t)\gamma = e^{-itH_k^0}\gamma e^{itH_k^0}$$

Expansion can be continued (Dyson series)

$$\begin{aligned}
\gamma_t^{(k)} &= \mathcal{U}_k(t)\gamma_0^{(k)} - i \int_0^t ds \mathcal{U}_k(t-s)B_k\gamma_0^{(k+1)} \\
&\quad + (-i)^2 \int_0^t ds_1 \int_0^{s_1} ds_2 \mathcal{U}_k(t-s_1-s_2)B_k\mathcal{U}_{k+1}(s_1)B_{k+1}\gamma_{s_2}^{(k+2)} \\
&= \sum_{n=0}^{m-1} \iint_{\sum_k s_k=t} ds_0 \dots ds_n U(s_0)BU(s_1)B \dots BU(s_n)\gamma_0^{(k+n)} \\
&\quad + \iint_{\sum_k s_k=t} ds_0 \dots ds_m U(s_0)BU(s_1)B \dots U(s_{m-1})B\gamma_{s_m}^{(k+m)}
\end{aligned}$$

For uniqueness, only the last term needs to be controlled. Use:

$$\mathrm{Tr}|U\omega| = \mathrm{Tr}|\omega|, \quad |A| := \sqrt{A^*A}$$

$$\mathrm{Tr}|B_k\omega| \leq 2k\|V\|_\infty \mathrm{Tr}|\omega|$$

$$\mathrm{Tr}|\text{last term}| \leq (2\|V\|_\infty)^m k(k+1)\dots(k+m-1) \iint_{\sum_k s_k=t} ds_1 \dots ds_m$$

Note that $\mathrm{Tr}\gamma_{s_m}^{(k+m)} = 1$ was crucially used!

Use that

$$\iint_{\sum_k s_k = t} ds_0 \dots ds_m = \frac{t^m}{m!}$$

$$\begin{aligned} \text{Tr}|\text{last term}| &\leq (2\|V\|_\infty)^m k(k+1)\dots(k+m-1) \iint_{\sum_k s_k = t} ds_1 \dots ds_m \\ &\leq (2t\|V\|_\infty)^m \frac{(k+m-1)!}{(k-1)!m!} \leq 2^k (4t\|V\|_\infty)^m \rightarrow 0 \end{aligned}$$

if $t \leq 1/(4\|V\|_\infty)$.

Gives short time uniqueness in trace norm.

For long time: simply continue, using that the a priori bound gives control on the trace norm **uniformly in time**.

Notice that the $k(k+1)\dots(k+m-1) \sim m!$ from the combinatorics was **exactly compensated** by the time ordered integration to give a geometric series control. (this was noted by Lanford and Hepp earlier)

IV. 2. CASE OF THE COULOMB POTENTIAL (E-YAU 2001)

For **singular potentials: need stronger norm.** E.g. for Coulomb

$$\frac{1}{|x|^2} \leq -\Delta \implies \text{Tr}|B_k \omega| \leq 2k \|\omega\|_{\mathcal{H}^1} \quad (*)$$

with **Sobolev-like** norm

$$\|\omega\|_{\mathcal{H}^1} := \text{Tr}|\nabla \omega \nabla| + \text{Tr}|\omega| \sim \text{Tr}S\omega S, \quad S = \sqrt{1 - \Delta}$$

To see (*),

$$\begin{aligned} \text{Tr}|B_k \omega| &\lesssim \text{Tr} \sqrt{\omega \frac{1}{|x_1 - x_2|^2} \omega} \\ &\leq \text{Tr} \sqrt{\omega S^2 \omega} = \text{Tr} \sqrt{S \omega^2 S} \leq \text{Tr} \sqrt{S \omega S^2 \omega S} = \text{Tr} S \omega S \end{aligned}$$

To close the estimate in H^1 – need **derivatives in each variable:**

$$\|\gamma^{(k)}\|_{\mathcal{H}^k} := \text{Tr} |S_1 \dots S_k \gamma^{(k)} S_k \dots S_1|, \quad S_i = \sqrt{1 - \Delta_{x_i}}$$

For the apriori estimate: Use the conservation of H_N^k

Method of moments (E-Yau, 2001: $V(x) = \pm 1/|x|$):

$$\int |\nabla_1 \cdots \nabla_k \psi_t(x_1, \cdots, x_N)|^2 dx \leq \int \bar{\psi}_t \left(\frac{H + N}{N} \right)^k \psi_t dx$$

Sketch of the proof for $k = 2$: (with $V_{ij} = |x_i - x_j|^{-1}$)

$$(H + N)^2 = \left(\sum_j S_j^2 + \frac{1}{N} \sum_{ij} V_{ij} \right)^2 \geq \sum_{ij} S_i^2 S_j^2 + \frac{1}{N} \sum_{ij} [S_i^2 V_{ij} + V_{ij} S_i^2]$$

(all other terms are positive, e.g. $S_k^2 V_{ij} \geq 0$ if $k \neq i, j$.)

$$S_i^2 V_{ij} + h.c. \geq \nabla_i (\nabla V)_{ij} + \nabla_i^* V \nabla_i \geq -\varepsilon^{-1} S_i^2 - \varepsilon |(\nabla V)_{ij}|^2 \quad (\text{Schwarz})$$

Cutoff V on a short scale ($N^{-1/2}$) then remove by weak stability.

$$|(\nabla V)_{ij}|^2 \sim \frac{1}{|x_i - x_j|^4} \leq \frac{N}{|x_i - x_j|^2} \leq N S_i^2 \quad (\text{Hardy})$$

$$\frac{1}{N} \sum_{ij} [S_i^2 V_{ij} + V_{ij} S_i^2] \geq -\frac{1}{N} \sum_{ij} [\varepsilon^{-1} S_i^2 + \varepsilon N S_i^2] \geq -\frac{1}{\sqrt{N}} \sum_{ij} S_i^2 S_j^2$$

(higher powers are a bit more complicated)

summary:

$$\|\gamma^{(k)}\|_{\mathcal{H}_1} := \text{Tr} |S_1 \dots S_k \gamma^{(k)} S_k \dots S_1|, \quad S_i = \sqrt{1 - \Delta_{x_i}}$$

1. The error term in the Duhamel expansion of BBGKY can be estimated via the \mathcal{H}_1 norm in the Coulomb case—use Hardy inequality.

$$|x|^{-2} \leq -\Delta$$

2. The error term has a combinatoric factor of $m!$. This is cancelled by a $1/m!$ factor from the time integration due to the time ordering.

3. The \mathcal{H}_1 estimate can be obtained via the momentum of energy. The commutator term between $-\Delta$ and V is again controlled by the Hardy inequality.

Method of moments ($V(x) = \pm 1/|x|$):

$$\int |\nabla_1 \dots \nabla_k \psi_t(x_1, \dots, x_N)|^2 d\mathbf{x} \leq \int \bar{\psi}_t \left(\frac{H + N}{N} \right)^k \psi_t d\mathbf{x}$$

IV.3. CASE OF THE MORE SINGULAR POTENTIALS

No Hardy ineq. beyond $|x|^{-2}$. In particular, if $V \rightarrow N^{3\beta}V(N^\beta x)$, $\beta > 0$ (approx. delta function), then $\delta \not\leq -\Delta$.

The following “nonstandard” Sobolev ineq. holds

$$V(x - y) \leq \|V\|_1(1 - \Delta_x)(1 - \Delta_y)$$

$$\implies \delta(x - y) \leq (1 - \Delta_x)(1 - \Delta_y)$$

but after iteration

$$\dots \delta(x_{k-1} - x_k) \delta(x_k - x_{k+1}) \dots \leq \dots (1 - \Delta_k)^2 \dots$$

We would need 4 derivative per variable, but only 2 are available:

$$\begin{aligned} (\text{const})N^2 &\geq \text{Tr } H^2\gamma = \text{Tr} \left[\sum_j (-\Delta_j)^2 + \sum_{i,j} \Delta_j \Delta_i + \dots \right] \gamma \\ &\geq N \text{Tr } \Delta_1^2 \gamma^{(1)} + N^2 \text{Tr } \Delta_1 \Delta_2 \gamma^{(2)} \end{aligned}$$

We will keep H^1 norm and improve on the uniqueness.

V. EMERGENCE OF THE SCATTERING LENGTH

$$i\partial_t \gamma_{N,t}^{(1)}(x_1; x'_1) = (-\Delta_{x_1} + \Delta_{x'_1}) \gamma_{N,t}^{(1)}(x_1; x'_1) \\ + \int dx_2 N^3 \left(V(N(x_1 - x_2)) - V(N(x'_1 - x_2)) \right) \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2)$$

Most difficult part: show that, as $N \rightarrow \infty$,

$$\int dx_2 NV_N(x_1 - x_2) \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2), \quad V_N(x) = N^2 V(Nx) \\ \rightarrow 8\pi a_0 \gamma_{\infty,t}^{(2)}(x_1, x_1; x'_1, x_1)$$

Good approximation to the ground state [Dyson]

$$W(\mathbf{x}) = \prod_{i < j} f(N(x_i - x_j)), \quad (-\Delta + V/2)f = 0, \quad f = 1 - w$$

Ansatz for states near the ground state:

$$\psi_N(\mathbf{x}) = \underbrace{W(\mathbf{x})}_{\text{short scale}} \cdot \underbrace{\phi_N(\mathbf{x})}_{\text{large scale}} \quad \text{with} \quad \phi_N(\mathbf{x}) \simeq \prod_{j=1}^N \phi(x_j).$$

If the time evolution preserves the form

$$\psi_{N,t}(\mathbf{x}) = W(\mathbf{x})\phi_{N,t}(\mathbf{x}) \quad \phi_{N,t}(\mathbf{x}) \simeq \prod_{j=1}^N \phi_t(x_j)$$

then $\gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x'_2) \simeq \underbrace{f(N(x_1 - x_2))[x \rightarrow x']}_{\text{short scale corr.}} \underbrace{\gamma_{N,t}^{(1)}(x_1; x'_1)[1 \rightarrow 2]}_{\text{no corr.}}$

$$N^3 \int dx_2 \underbrace{V(N(x_1 - x_2))}_{\text{short scale}} \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2) \rightarrow 8\pi a_0 \gamma_{\infty,t}^{(1)}(x_1; x'_1) \varrho_t^{(1)}(x_1)$$

since $\int V f = 8\pi a_0$ (compare with $\int V = b_0$)

$$\implies i\partial_t \gamma_{\infty,t}^{(1)} = \left[-\Delta + 8\pi a_0 \varrho_t, \gamma_{\infty,t}^{(1)} \right] \quad \text{GPE with } a_0$$

The change of the constant is the signature of the correlation !
 The short scale structure vanishes in trace norm, so propagation of chaos still holds in large scale, but it is relevant in energy norm. It still influences the dynamics by changing b_0 to $8\pi a_0$.

Using $\int V(1-w) = 8\pi a_0$, prove first that

$$\int dx_2 [NV_N(x_1 - x_2)(1 - w_N(x_1 - x_2)) - 8\pi a_0 \delta(x_1 - x_2)] \\ \times (1 - w_N(x_1 - x_2))^{-1} \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2) \rightarrow 0$$

and then use that in the weak limit the factor

$$(1 - w_N(x_1 - x_2))^{-1} \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x_2) \rightarrow \gamma_{\infty,t}^{(2)}(x_1, x_2; x'_1, x_2)$$

\implies In terms of wave function we need **regularity** of

$$\phi_{12}(\mathbf{x}) = (1 - w_N(x_1 - x_2))^{-1} \psi_{N,t}(\mathbf{x}) \quad \text{in} \quad x_1, x_2.$$

VI. APRIORI BOUNDS IN THE GP CASE

We now consider the Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \sum_{i<j} V_N(x_i - x_j), \quad V_N(x) = N^2 V(Nx)$$

that should lead to GP. Scattering length of V_N is $a = O(1/N)$.

$\langle \Psi_t, H^k \Psi_t \rangle$ is still **conserved**, but H^k does **not** control the Sobolev norm; the inequality

$$\langle \Psi, H^k \Psi \rangle \geq (CN)^k \int |\nabla_1 \dots \nabla_k \Psi|^2$$

is **incorrect**, the short scale structure is too singular; $w_N \sim \frac{1}{N|x|+1}$

$$\int \left| \nabla_1 \nabla_2 (1 - w_N(x_1 - x_2)) \right|^2 \geq \int \frac{N^4}{(N|x| + 1)^6} dx = O(N)$$

Solution: Remove the singular part:

VI.1. APRIORI BOUND FOR H^2

Proposition: Suppose that $\varrho := \|V\|_1 + \|V\|_\infty$ is small. Define

$$\Phi_{12}(\mathbf{x}) := \frac{\Psi(\mathbf{x})}{f_N(x_1 - x_2)}, \quad f_N(x) = 1 - w_N(x).$$

Then

$$\langle \Psi, H^2 \Psi \rangle \geq (CN)^2 \int |\nabla_1 \nabla_2 \Phi_{12}|^2$$

(Of course 1,2 can be changed to any $i \neq j$).

It is a remarkable inequality! Finiteness of H^2 **forces** the specific short scale structure since Φ is smoother than Ψ .

Weak limit of (the marginals of) Ψ_N and Φ_N are equal, but Φ_N can be controlled in Sobolev space. Use compactness for Φ_N ! Since the limit Φ_N is smooth, so is the limit of Ψ_N , although Ψ_N 's themselves were not!

HOW CAN H^2 DETECT LOCAL SINGULARITY?

Consider a **one-body model problem**:

$$\mathfrak{h} := -\Delta + N^2V(Nx)$$

$$\mathfrak{h}^2 = \Delta\Delta - \Delta N^2V(Nx) - N^2V(Nx)\Delta + N^4V(Nx)^2$$

Suppose ψ is smooth, then

$$\left\langle \psi, -\Delta N^2V(Nx)\psi \right\rangle = O(N^{-1}) \quad \left\langle \psi, N^4V(Nx)^2\psi \right\rangle = O(N)$$

therefore $\langle \psi, \mathfrak{h}^2\psi \rangle \rightarrow \infty$.

More precisely analysis shows that if $\langle \psi, \mathfrak{h}^2\psi \rangle$ remains finite, then ψ must have a definite singularity structure characterized by the zero energy scattering solution.

Let $f(Nx)$ be the zero energy solution to $\mathfrak{h} = \mathfrak{h}_N$,

$$f(Nx) \sim 1 - \frac{a_0}{N|x|}, \quad |x| \geq O(N^{-1})$$

and write $\psi = f\phi$.

$$\langle \psi, \mathfrak{h}^2 \psi \rangle = \int |\mathfrak{h} f \phi|^2 \geq \int f^2 |\Delta \phi|^2 - \int f^2 (\Delta \log f) |\nabla \phi|^2 + (l.o.t.)$$

$$\text{Hardy inequality} \implies \Delta \log f \sim \frac{a_0}{N|x|^3} \leq \frac{c}{|x|^2}$$

so for small a_0 we have

$$\langle \psi, \mathfrak{h}^2 \psi \rangle \geq C \int f^2 |\Delta \phi|^2 + (l.o.t.) \implies \phi \text{ is regular}$$

Note that $f \rightarrow 1$, so the pointwise limits of ψ and ϕ are the same.

Corollary: If the initial data satisfies the H^2 bound, then

$$\langle \psi_{N,t}, H^2 \psi_{N,t} \rangle = \langle \psi_{N,0}, H^2 \psi_{N,0} \rangle \leq CN^2.$$

$$\implies \int W^2 |\nabla_i \nabla_j \phi_{N,t}|^2 \leq C \quad (\psi_{N,t} = W \phi_{N,t})$$

$$\int |\nabla_i \nabla_j \psi_{N,t}|^2 \leq C \quad \text{is } \mathbf{WRONG!}$$

so one cannot pass to ψ_∞ in the Sobolev space directly.

But our initial data $\langle \psi_{N,0}, H^2 \psi_{N,0} \rangle \rightarrow \infty$.

Corollary: The limiting marginals $\gamma_{\infty,t}^{(k)} := \lim_{N \rightarrow \infty} \gamma_{N,t}^{(k)}$ of Ψ_N satisfy

$$\text{Tr} S_i S_j \gamma_{\infty,t}^{(k)} S_i S_j \leq C, \quad i \neq j$$

one-particle Hamiltonian $\mathfrak{h} = -\Delta + (1/2)V(x)$

Proposition Suppose $V \geq 0$, with $V \in L^1(\mathbb{R}^3)$. Then:

i) (*Existence of the wave operator*). The limit

$$W = \lim_{t \rightarrow \infty} e^{i\mathfrak{h}t} e^{i\Delta t}$$

exists.

ii) (*Completeness of the wave operator*). W is a unitary operator on $L^2(\mathbb{R}^3)$ with

$$W^* = W^{-1} = \lim_{t \rightarrow \infty} e^{-i\Delta t} e^{-i\mathfrak{h}t}$$

iii) (*Intertwining relations*). On $D(\mathfrak{h}) = D(-\Delta)$, we have

$$W^* \mathfrak{h} W = -\Delta \tag{1}$$

iv) (*Yajima's bounds*). Suppose moreover that $V(x) \leq C\langle x \rangle^{-\sigma}$, for some $\sigma > 5$. Then, for every $1 \leq p \leq \infty$, W and W^* map $L^p(\mathbb{R}^3)$ into $L^p(\mathbb{R}^3)$, that is

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

W_N wave op associated with $\mathfrak{h}_N = -\Delta + (1/2)V_N(x)$, with $V_N(x) = N^2V(Nx)$.

Proposition Suppose $V \geq 0$, $V \in L^1(\mathbb{R}^3)$

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

where $W_{N,(i,j)}$ denotes the wave operator W_N acting on the variable $v = x_j - x_i$.

$$W_N^* \psi \sim [1 - w(Nv)]^{-1} \psi$$

Idea: $W^* = \lim_{t \rightarrow \infty} e^{-i\Delta t} e^{-i\mathfrak{h}t}$ eliminates all modes except zero modes to \mathfrak{h} . So $W_{N,v}^* [1 - w(Nv)] \rightarrow 1$.

Notice that

$$|(\nabla_1 \cdot \nabla_2)^2 \psi|^2 \ll |(\nabla_1 \nabla_2)^2 \psi|^2$$

A special Sobolev ineq.:

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

$$|\langle \psi, V(x_1 - x_2) \psi \rangle| \leq C \|V\|_1 \langle \psi, ((\nabla_1 \cdot \nabla_2)^2 - \Delta_1 - \Delta_2 + 1) \psi \rangle$$

Proof

$$\begin{aligned} & N^{-2} \langle \psi, H_N^2 \psi \rangle \\ & \geq \left\langle \psi, \left(-\Delta_1 + \frac{1}{2} V_N(x_1 - x_2) \right) \left(-\Delta_2 + \frac{1}{2} V_N(x_1 - x_2) \right) \psi \right\rangle. \end{aligned}$$

$$u = \frac{x_1 + x_2}{2}, \quad \text{and} \quad v = x_1 - x_2, \quad h_v = -\Delta_v + \frac{1}{2} V_N(v).$$

$$= \left\langle \psi, \left[\left(-\frac{1}{4} \Delta_u + h_v \right)^2 - (\nabla_u \cdot \nabla_v)^2 \right] \psi \right\rangle.$$

Using

$$(\nabla_u \cdot \nabla_v)^2 \leq (-\Delta_u)(-\Delta_v) \leq (-\Delta_u) h_v,$$

we obtain

$$N^{-2} \langle \psi_N, H_N^2 \psi_N \rangle \geq \left\langle \psi, \left(-\frac{1}{4} \Delta_u - h_v \right)^2 \psi \right\rangle.$$

$$= \left\langle W_{N,v}^* \psi_N, \left(\frac{1}{4} \Delta_u - \Delta_v \right)^2 W_{N,v}^* \psi \right\rangle.$$

$$\nabla_1 \cdot \nabla_2 = (1/4) \Delta_u - \Delta_v$$

VII. HIGHER ORDER ENERGY ESTIMATES

Choose $\ell \gg N^{-1}$ with $N\ell^3 \ll 1$ and for $j = 1, \dots, N$ define

$$\theta_j(\mathbf{x}) \simeq \begin{cases} 1 & \text{if } |x_i - x_j| \gg \ell \quad \forall i \neq j \\ 0 & \text{otherwise} \end{cases}$$

Proposition (higher order energy estimates):

$$\langle \psi_N, (H_N + N)^k \psi_N \rangle \geq C^k N^k \int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_k(\mathbf{x}) |\nabla_{x_1} \dots \nabla_{x_k} \psi_N(\mathbf{x})|^2$$

Corollary: we have, uniformly in N and t ,

$$\int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_k(\mathbf{x}) |\nabla_{x_1} \dots \nabla_{x_k} \psi_{N,t}(\mathbf{x})|^2 \leq C^k$$

Proof:

$$\begin{aligned} & \int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_k(\mathbf{x}) |\nabla_{x_1} \dots \nabla_{x_k} \psi_{N,t}(\mathbf{x})|^2 \\ & \leq C^k N^{-k} \langle \psi_{N,t}, (H_N + N)^k \psi_{N,t} \rangle \\ & \leq C^k N^{-k} \langle \psi_N, (H_N + N)^k \psi_N \rangle = C^k \end{aligned}$$

Proposition (higher order energy estimates):

$$\langle \psi_N, (H_N + N)^k \psi_N \rangle \geq C^k N^k \int d\mathbf{x} \theta_1(\mathbf{x}) \dots \theta_k(\mathbf{x}) |\nabla_{x_1} \dots \nabla_{x_k} \psi_N(\mathbf{x})|^2$$

We use

$$\mathrm{Tr}(H_N + N)^k \gamma_{N,t}^{(k)} = \mathrm{Tr}(H_N + N)^k \gamma_{N,0}^{(k)} \leq C^k \quad (*)$$

(Bound on initial data needs to be proven separately, see next section)

Taking the weak limit of $\gamma_N^{(k)}$, from the Proposition and (*) one can derive

Theorem (A priori bound) Let $\gamma_{\infty,t}^{(k)}$ be any weak limit point of $\gamma_{N,t}^{(k)}$, then

$$\|\gamma_{\infty,t}^{(k)}\|_{H_k} := \mathrm{Tr}(1 - \Delta_1)(1 - \Delta_2) \dots (1 - \Delta_k) \gamma_{\infty,t}^{(k)} \leq C^k$$

The actual cutoff function θ is more complicated.

Main trouble with kinetic energy localization

$$|\nabla\theta(x)| \leq (\text{const.})\theta(x)$$

holds for no compactly supported function.

When controlling objects like

$$\int \theta^2 |\nabla\nabla \dots \nabla \Psi|^2 \quad (*)$$

and using integration by parts (as above in the H^2 -proof), one picks up $\nabla\theta$ that cannot be controlled by (*).

However,

$$|\nabla\theta^2| \leq 2\theta|\nabla\theta| \leq (\text{const.})\ell^{-1}\theta$$

if ℓ the lengthscale of θ .

To define our localization function, first define

$$h(x) := \exp\left(-\sqrt{1 + \left(\frac{x}{\ell}\right)^2}\right)$$

$$\begin{aligned} \theta_i(\mathbf{x}) &:= \exp\left(-\frac{1}{\ell^\varepsilon} \sum_{j \neq i} h(x_i - x_j)\right) \\ &= \begin{cases} \approx 1 & \text{if no other particle is near } x_i \\ \text{exp. small} & \text{otherwise} \end{cases} \end{aligned}$$

$$\theta_i^{(n)} := (\theta_n)^{2^n} \quad \implies \quad |\nabla_j \theta_i^{(n)}| \leq C \ell^{-1} \theta_i^{(n-1)}$$

Finally, our localization function for the H^k -analysis:

$$\Theta_k(\mathbf{x}) := \theta_1^{(k)}(\mathbf{x}) \cdot \theta_2^{(k)}(\mathbf{x}) \cdot \dots \cdot \theta_k^{(k)}(\mathbf{x})$$

ensures that there is no particle near x_1, x_2, \dots, x_k .

Choice of ℓ : $N\ell^3 \ll 1$ and $N\ell^2 \gg 1$.

VII.4. REGULARIZATION OF THE INITIAL STATE

In the previous apriori bound, we used that $\text{Tr}(H_N + N)^k \gamma_{N,0}^{(k)} \leq C^k$, which, as it stands, is wrong for product states if $k > 1$, since H_N^2 contains squares of (almost) deltafunctions.

Define the following **regularized initial state**

$$\tilde{\psi}_N := \frac{\chi(\kappa H_N/N)\psi_N}{\|\chi(\kappa H_N/N)\psi_N\|}$$

i.e. cutoff in the energy at threshold $\kappa^{-1}N$. ($\kappa \ll 1$).

Proposition: We have the following facts:

$$\langle \tilde{\psi}_N, H_N^k \tilde{\psi}_N \rangle \leq C^k N^k \kappa^{-k} \quad (1)$$

$$\sup_N \|\psi_N - \tilde{\psi}_N\| \leq \kappa^{1/2} \quad (2)$$

If the asymptotic factorization is satisfied for ψ_N , then the marginals of $\tilde{\psi}_N$ also factorize

$$\tilde{\gamma}_N^{(k)} \rightarrow |\varphi\rangle\langle\varphi|^{\otimes k} \quad (3)$$

Therefore we can run the whole proof for $\tilde{\psi}_N$ since (1) gives the a priori bound. At the end, using the uniform comparison (2), we can let $\kappa \rightarrow 0$ to compare $\gamma_{N,t}^{(k)}$ and $\tilde{\gamma}_{N,t}^{(k)}$, so from (3) the same relation will hold for $\gamma_{N,t}^{(k)}$ as well.

VIII. UNIQUENESS OF THE GP-HIERARCHY IN SOBOLEV NORM

$$i\partial_t \gamma_t^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_t^{(k)} \right] - i\sigma \sum_{j=1}^k \text{Tr}_{x_{k+1}} \left[\delta(x_j - x_{k+1}), \gamma_t^{(k+1)} \right]$$

Recall the Sobolev norm:

$$\|\gamma^{(k)}\|_{H_k} := \text{Tr}(1 - \Delta_1)(1 - \Delta_2) \dots (1 - \Delta_k) \gamma^{(k)}$$

Our goal is to show:

Theorem: Given a family of initial densities, $\{\gamma^{(k)}\}_{k=1,2,\dots}$ with $\|\gamma^{(k)}\|_{H^k} \leq C^k$, then there exists at most one solution $\{\gamma_t^{(k)}\}$ to the hierarchy above with $\gamma_{t=0}^{(k)} = \gamma^{(k)}$ and such that $\|\gamma_t^{(k)}\|_{H^k} \leq C^k$ holds uniformly in t .

$$i\partial_t \gamma_t^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_t^{(k)} \right] - i\sigma \sum_{j=1}^k \text{Tr}_{x_{k+1}} \left[\delta(x_j - x_{k+1}), \gamma_t^{(k+1)} \right]$$

Iterate it in integral form:

$$\begin{aligned} \gamma_t^{(k)} &= \mathcal{U}(t) \gamma_0^{(k)} + \int_0^t ds \mathcal{U}(t-s) B^{(k)} \mathcal{U}(s) \gamma_0^{k+1} + \dots \\ &+ \int_{\sum_k s_k = t} ds_1 \dots ds_n \mathcal{U}(s_1) B^{(k)} \mathcal{U}(s_2) B^{(k+1)} \dots B^{(k+n-1)} \gamma_{s_n}^{k+n} \end{aligned}$$

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

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

Problem 1. $\|B^{(k)} \gamma^{(k+1)}\|_{\mathcal{H}^k} \leq C \|\gamma^{(k+1)}\|_{\mathcal{H}^{k+1}}$ is wrong because $\delta(x) \not\leq (1 - \Delta)$. **Need smoothing from \mathcal{U} !!**

$$\begin{aligned} \gamma_t^{(k)} &= \mathcal{U}(t)\gamma_0^{(k)} + \int_0^t ds \mathcal{U}(t-s)B^{(k)}\mathcal{U}(s)\gamma_0^{k+1} + \dots \\ &+ \int_{\sum_k s_k=t} ds_1 \dots ds_n \mathcal{U}(s_1)B^{(k)}\mathcal{U}(s_2)B^{(k+1)} \dots B^{(k+n-1)}\gamma_{s_n}^{k+n} \end{aligned}$$

Strichartz inequality? Space-time smoothing of $e^{it\Delta}$.

$$\|e^{it\Delta}\psi\|_{L^p(L^q(dx)dt)} = \left[\int dt \left(\int dx |e^{it\Delta}\psi|^q \right)^{p/q} \right]^{1/p} \leq C\|\psi\|_2$$

Problem 2. $B^{(k)}B^{(k+1)} \dots B^{(k+n-1)} \approx n!$, because $B^{(k)} = \sum_1^k [\dots]$.
This can destroy convergence. Gain back from time integral

$$\int_{\sum_k s_k=t} ds_1 \dots ds_n \leq \frac{1}{n!}$$

Here $L^1(ds)$ was critically used, Strichartz destroys convergence.

We expand it into **Feynman graphs** and do all integrals carefully.

VIII.1 FEYNMAN GRAPHS

Iteration of the ∞ -hierarchy: $\gamma_{\infty,t} = \mathcal{U}_t \gamma_0 + \int_0^t ds \mathcal{U}_{t-s} B \gamma_{\infty,s}$

$$\gamma_{\infty,t}^{(k)} = \sum_{m=0}^n \Xi_m^{(k)}(t) + \Omega_n^{(k)}(t)$$

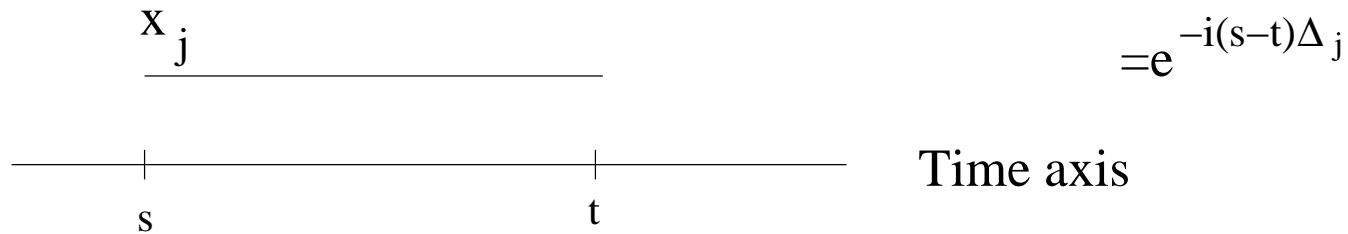
$$\Omega_n^{(k)} = \int \dots \int ds_1 ds_2 \dots ds_n \mathcal{U}_{t-s_1} B \mathcal{U}_{s_1-s_2} B \dots \mathcal{U}_{s_{n-1}-s_n} B \gamma_{\infty,s_n}^{(k+n)}$$

$\Xi_m^{(k)}$ are similar but with the initial condition γ_0 at the end.

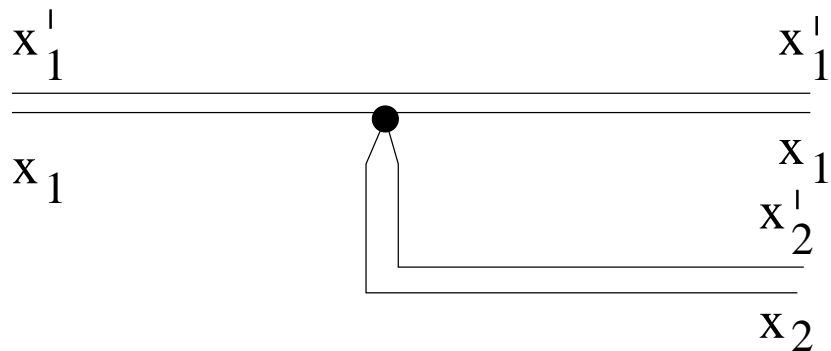
Feynman graphs: convenient representation of Ξ and Ω .

Lines represent **free propagators**.

E.g. the propagator line of the j -th particle between times s and t represent $\exp[-i(s-t)\Delta_j]$:

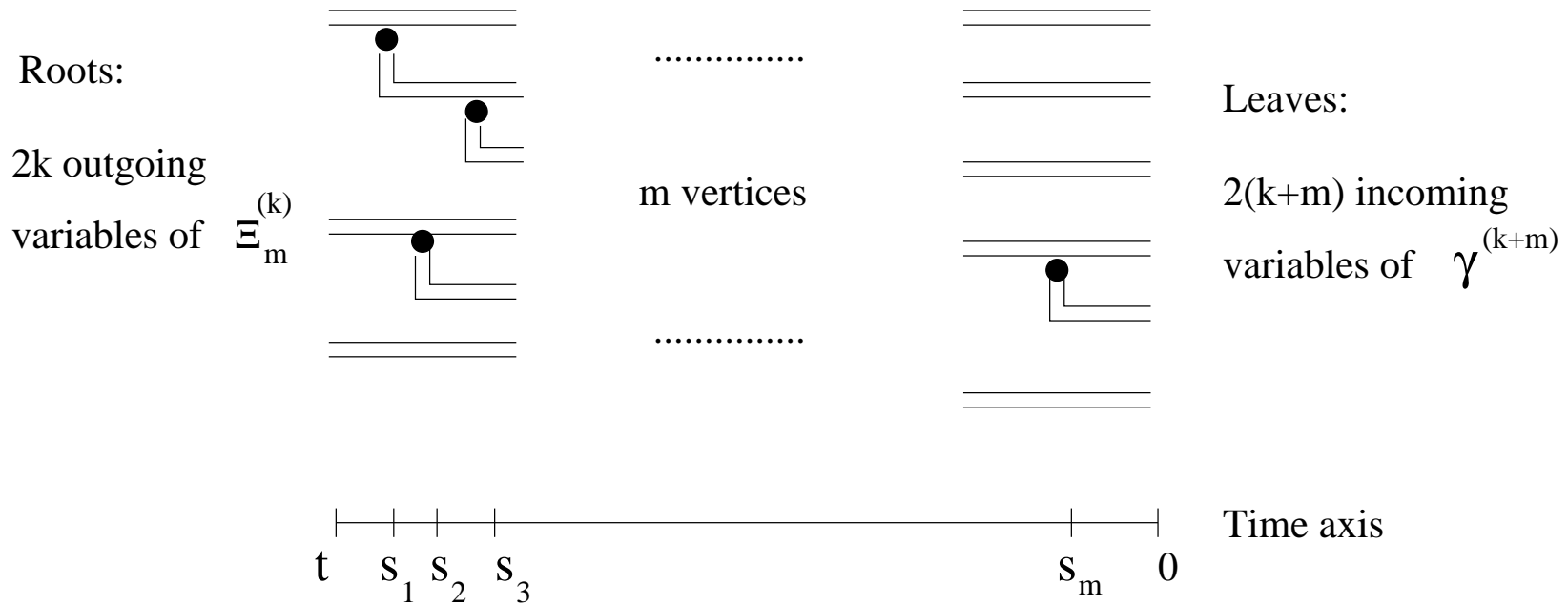


Vertices represent B , e.g. $V(x_1 - x_2)\gamma(x_1, x_2; x'_1, x'_2)\delta(x_2 - x'_2)$



$$\Xi_m^{(k)} = \int \dots \int ds_1 ds_2 \dots ds_m \mathcal{U}_{t-s_1} B \mathcal{U}_{s_1-s_2} B \dots \mathcal{U}_{s_{m-1}-s_m} B \mathcal{U}_{s_m} \gamma_{\infty,0}^{(k+m)}$$

corresponds to summation over all graphs Γ of the form:



$$\text{Tr } \mathcal{O} \Xi_m^{(k)} = \sum_{\Gamma} \text{val}(\Gamma)$$

Value of a graph Γ in momentum space

$$\text{Val}(\Gamma) = \int \int \prod_{e \in E} d\alpha_e dp_e \prod_e \frac{1}{\alpha_e - p_e^2 + i\eta_e} \prod_{v \in V} \delta\left(\sum_{e \in v} \alpha_e\right) \delta\left(\sum_{e \in v} p_e\right) \\ \times e^{-it \sum_{e \in \text{Root}} (\alpha_e - i\eta_e)} \mathcal{O}(p_e : e \in \text{Root}) \gamma_0(p_e : e \in \text{Leaves})$$

$p_e \in \mathbb{R}^3$ is the momentum on edge e

$\alpha_e \in \mathbb{R}$ variable dual to time running on the edge e .

$\eta_e = O(1)$ regularizations satisfying certain compatibility cond.

Two main issues to look at

- What happens to the **$m!$ problem** (combinatorial complexity of the BBGKY hierarchy)?

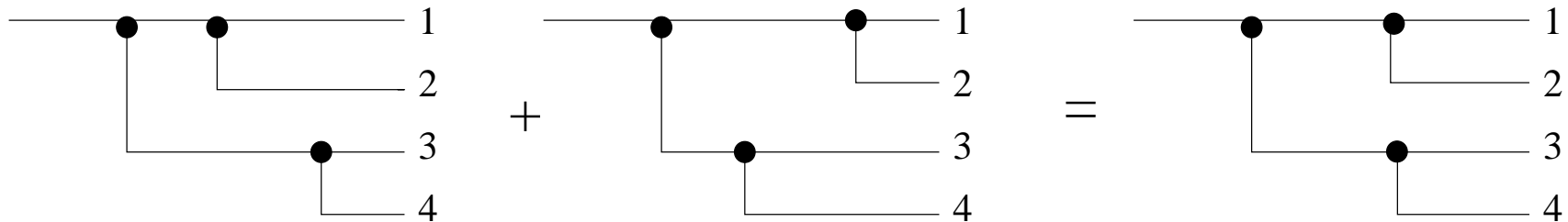
- What happens to the singular interaction = **large p problem**

In other words: why is $\text{Val}(\Gamma)$ UV-finite?

VIII.2 COMBINATORIAL RESUMMATION

Let $k = 1$ for simplicity, i.e. we have a tree (not a forest).

The Duhamel expansion keeps track of the full time ordering and it counts the following two graphs separately:



Number of graphs on m vertices **with** time ordering: $m!$
 (the j -th new vertex can join each of the $(j - 1)$ earlier ones)

Number of graphs on m vertices **without** time ordering = Number of binary trees = Catalan numbers $\frac{1}{m+1} \binom{2m}{m} \leq C^m$.

The resummation reduced $m!$ to C^m . **The factorial was fake!**

VIII.3. ULTRAVIOLET REGIME: FINITENESS OF VAL(Γ)

$$|\text{Val}(\Gamma)| \leq \int \int \prod_{e \in E} d\alpha_e dp_e \prod_e \frac{1}{\langle \alpha_e - p_e^2 \rangle} \prod_{v \in V} \delta\left(\sum_{e \in v} \alpha_e\right) \delta\left(\sum_{e \in v} p_e\right) \\ \times \mathcal{O}(p_e : e \in \text{Root}) \gamma_0(p_e : e \in \text{Leaves})$$

$\|\gamma_0\|_{\mathcal{H}^{(m+1)}}$ guarantees a $\langle p_e \rangle^{-5/2}$ decay on each leaf.

Perform integration over all α and p , starting from the leaves and moving towards the roots. At each vertex, we **propagate the decay** from the son-edges to the father-edge.

Typical example.

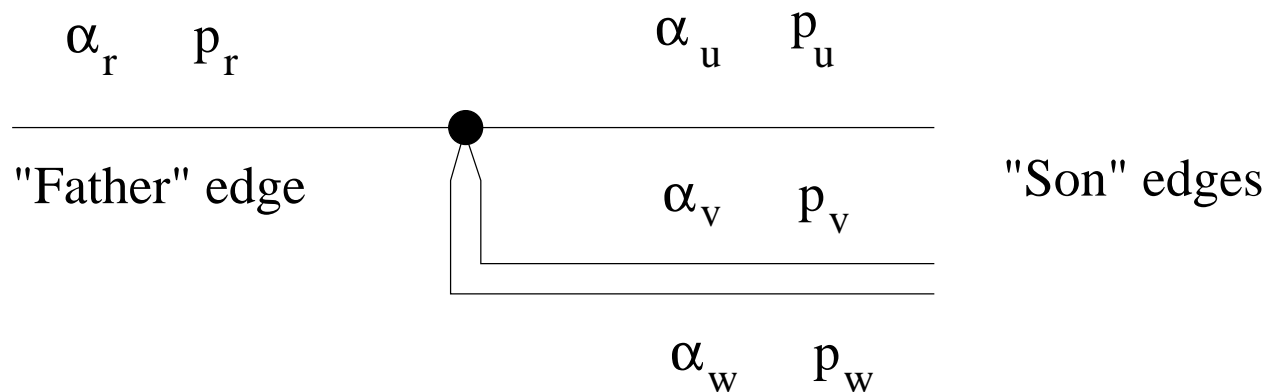
Integrate first the α -variables of the son-edges

$$\int d\alpha_u d\alpha_v d\alpha_w \frac{\delta(\alpha_r = \alpha_u + \alpha_v - \alpha_w)}{\langle \alpha_u - p_u^2 \rangle \langle \alpha_v - p_v^2 \rangle \langle \alpha_w - p_w^2 \rangle} \leq \frac{\text{const}}{\langle \alpha_r - p_u^2 - p_v^2 + p_w^2 \rangle^{1-\varepsilon}}$$

Then integrate over the momenta of the son-edges

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

Momentum decay propagated!



$$|\text{Val}(\Gamma)| \leq \int \int \prod_{e \in E} d\alpha_e dp_e \prod_e \frac{1}{\langle \alpha_e - p_e^2 \rangle} \prod_{v \in V} \delta\left(\sum_{e \in v} \alpha_e\right) \delta\left(\sum_{e \in v} p_e\right) \\ \times \mathcal{O}(p_e : e \in \text{Root}) \gamma_0(p_e : e \in \text{Leaves})$$

Power counting ($k = 1$, one root case).

of edges = $3m + 2$, no. of leaves = $2m + 2$

of effective p_e (and α_e) variables: $(3m + 2) - m = 2m + 2$

$2m + 2$ propagators are used for the convergence of α_e integrals

Remaining m propagators give $\langle p^2 \rangle$ decay each.

Total p -decay: $\frac{5}{2}(2m + 2) + 2m = 7m + 5$ in $3(2m + 2)$ dim.

There is some room, but each variable must be checked. We follow the momentum decay on legs as we successively integrate out each vertex. There are 7 types of edges, 12 types of vertex integrations that form a closed system. \square

IX. CONCLUSIONS

- We derived the **GP equation** from many-body Ham. with interaction on scale $1/N$. Coupling const. = **scattering length**. GP theory is also valid far from equilibrium/ground state
- A specific short scale correlation structure is preserved or even **emerges** along the dynamics. In the $N \rightarrow \infty$ limit, this structure is negligible in L^2 sense (ensuring a closed eq. for the orbitals) but not in energy sense, thus it influences the dynamics via the emergence of the scatt. length.
- For interaction on scale $1/N^\beta$, $\beta < 1$, the coupling constant is the **Born approximation** to scattering length.
- **Conservation** of H^k can imply bounds in Sobolev space
- Strichartz can be strengthened with Feynman diagrams in many body problems

X. OPEN PROBLEMS

- Remove the positivity condition on V
- What happens for negative scattering length? Metastability?
- Understand the mesoscopic scales. What happened to the excess energy for the product initial state?
- Fermi systems (bound pairs of fermions are bosons)
- Combine many-body and random potential

II.2. VLASOV EQUATION FROM FERMION DYNAMICS (DETOUR)

Trapped fermions have energy/particle $\approx N^{2/3}$

Time scale $\approx N^{-1/3}$

Wavelength $\approx N^{-1/3} \ll$ potential lengthscale $\approx O(1) \implies$ SC

$$i\varepsilon\partial_t\Psi = \left[-\varepsilon^2 \sum_j \Delta_j + \frac{1}{N} \sum_{k < j} V(x_k - x_j) \right] \Psi, \quad \varepsilon := N^{-1/3}$$

Typical **semiclassical fermionic state**

$$\Psi = \bigwedge_j \varphi_j, \quad \varphi_j(x) = e^{ik_j x} g(x), \quad |k_j| \lesssim N^{1/3}$$

and $\gamma^{(1)}(x; x')$ is supported near $|x - x'| \sim \varepsilon$.

Wigner transform of $\gamma^{(1)}$ **at scale** ε

$$W_\varepsilon^{(1)}(x, v) := \int \gamma^{(1)}(x + \varepsilon\eta, x - \varepsilon\eta) e^{i\eta v} dv$$

Similarly for k -particle density matrices, $\gamma^{(k)}(x_1, \dots, x_k; x'_1, \dots, x'_k)$

$$i\varepsilon\partial_t\Psi = \left[-\varepsilon^2 \sum_j \Delta_j + \frac{1}{N} \sum_{k<j} V(x_k - x_j) \right] \Psi, \quad \varepsilon := N^{-1/3}$$

THEOREM: If the initial state asymptotically factorizes,
 $W_{N,\varepsilon}^{(k)} \approx \otimes_1^k W$, then $W_{N,\varepsilon}^{(k)}(t) \approx \otimes_1^k W_t$ (propagation of chaos)

Then the weak limit $W_t = \lim W_{N,\varepsilon}^{(1)}(t)$ satisfies

$$\partial_t W_t(x, v) + v \cdot \nabla_x W_t(x, v) = \nabla_x (V * \varrho_t) \cdot \nabla_v W_t(x, v)$$

$$\varrho_t(x) := \int W_t(x, v) dv$$

Limit equation is classical (nonlinear Vlasov equation)
 (Unlike Hartree/NLS for bosons that are quantum equations.)

[Narnhofer-Sewell]: V is analytic, [Spohn]: $V \in C^2$

NL Vlasov equation is the SC limit of the Hartree eq.

$$i\varepsilon\partial_t\varphi_t^\varepsilon = -\varepsilon^2\Delta\varphi_t^\varepsilon + \left(V \star |\varphi_t^\varepsilon|^2\right)\varphi_t^\varepsilon$$

$$i\varepsilon\partial_t\gamma_t^\varepsilon = \left[-\varepsilon^2\Delta + V \star \varrho_t^\varepsilon, \gamma_t^\varepsilon\right], \quad \varrho_t^\varepsilon(x) := \gamma_t^\varepsilon(x, x)$$

Let $\widetilde{W}^\varepsilon(t, x, v)$ be the rescaled Wigner transform of γ_t^ε .

THEOREM [Elgart-E-Schlein-Yau]: V analytic

Suppose for $k \leq 2 \log N$ and bounded k -body observables $O^{(k)}$,

$$\left| \left\langle O^{(k)}, W_{N,\varepsilon}^{(k)}(0) - \bigotimes_{j=1}^k W^{(1)}(0) \right\rangle \right| \leq \frac{1}{N}$$

Then for short time

$$\left| \left\langle O^{(k)}, W_{N,\varepsilon}^{(k)}(t) - \bigotimes_{j=1}^k \widetilde{W}^\varepsilon(t) \right\rangle \right| \leq \frac{1}{N}$$

Hartree eq. exact up to $O(\varepsilon^3)$. Open: remove analyticity.