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Derivation of effective evolution equations from quantum dynamics.

Goal is to understand emergence from many body quantum dynamics.

I. Introduction

N - particles system: $\psi_N \in L^2(\mathbb{R}^{3N})$.

$|\psi_N(x_1, \dots, x_N)|^2$ probability density. $\Rightarrow \|\psi_N\| = 1$.

In nature $\exists$ 2 kinds of particles: fermions and bosons.

Boson Symmetry: ψ_N symm. w.r.t. permutations.

Time Evolution is described by the N-body Schrödinger Equation:

$i\partial_t \psi_{N,t} = H_N \psi_{N,t}$; H_N is the Hamilton operator self-adjoint on $L^2(\mathbb{R}^{3N})$.

$$H_N = \underbrace{\sum_{j=1}^{N} -\Delta_{x_j}}_{\text{Kinetic}} + \underbrace{\sum_{i<j}^{N} V(x_i - x_j)}_{\text{interactions.}}$$

(we restrict to 2 particle interactions.)

Schrödinger Equation is linear: $\psi_{N,t} = e^{-iH_N t}\psi_N$ $\rightarrow$ global existence uniqueness, ...

In systems of physical interest: $\underset{\text{Dilute Boson Gas}}{1000} < N < \underset{\text{Stars}}{10^{30}}$.

Explicit solution is not so much our interest. We want to understand the macroscopic properties of dynamics, which result in averaging over the particles

II. Mean Field Systems

Every particle interacts with every other particle but interactions are very weak.

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

We are interested in the limit $N \to \infty$.

The $\frac{1}{N}$ factor guarantees the two pieces are of same order.
kinetic involves N terms; potential $\frac{1}{N} \times N^2$ pairs.

Heuristic Discussion

$$\psi_N(\vec{x}) = \prod_{j=1}^{N} \varphi(x_j) \quad ; \quad \psi_N = \varphi^{\otimes N}.$$

Factorization is not preserved due to interaction but we might expect that

$$\psi_{N,t}(\vec{x}) \simeq \prod_{j=1}^{N} \varphi_t(x_j).$$

Then, it is very easy to find an effective equation for φ_t.

$$\frac{1}{N}\sum_{i \neq j} V(x_i - x_j) \simeq \int dy\, |\varphi_t(y)|^2\, V(x_j - y) = (V * |\varphi_t|^2)(x_j)$$

$$\Longrightarrow \quad i\partial_t \varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t.$$

In which sense can we expect the factorization remains?

Marginal Densities

$$\gamma_{N,t} = |\psi_{N,t}\rangle\langle\psi_{N,t}| \quad ; \quad \gamma_{N,t}(\vec{x}_N, \vec{y}_N) = \psi_{N,t}(\vec{x})\,\overline{\psi_{N,t}(\vec{y})} .$$

Density matrix.

For $K = 1, \dots, N$, we define the K-particle marginal density

$$\gamma^{(K)}_{N,t} = T_{(K+1,\dots,N)}\, \gamma_{N,t} .$$

$$\gamma^{(K)}_{N,t}(\vec{x}_K, \vec{y}_K) = \int dx_{K+1} \cdots dx_N \;\gamma_{N,t}(\vec{x}_K, x_{K+1}, \dots, x_N ; \vec{y}_K, x_{K+1}, \dots, x_N).$$

When you take partial traces, you lose information.
Observables that only depend on K particles can be understood.

$$\langle \psi_{N,t}, (J^{(K)} \otimes \mathbb{1}^{N-K})\psi_{N,t}\rangle = \operatorname{tr} J^{(K)} \gamma^{(K)}_{N,t} .$$

Theorem 1: Under appropriate assumptions on V. Let $\varphi \in H^1(\mathbb{R})$,
$\psi_N = \prod_{j=1}^{N} \varphi_j$. $\psi_{N,t} = e^{-iH_N^{mf} t}\psi_N$. Then $\forall t \in \mathbb{R}$, $\forall K \geq 1$

$$\gamma^{(K)}_{N,t} \xrightarrow[N\to\infty]{} |\varphi_t\rangle\langle\varphi_t|^{\otimes K} ,$$

trace norm sense

where φ_t satisfies

$$\begin{cases} i\partial_t \varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \\ \varphi_{t=0} = \varphi . \end{cases}$$

Note: $$\langle \psi_{N,t}, (J^{(K)} \otimes \mathbb{1}^{(N-K)})\psi_{N,t}\rangle \xrightarrow[N\to\infty]{} \langle \varphi_t^{\otimes K}, J^{(K)} \varphi_t^{\otimes K}\rangle$$

- <u>The BBGKY approach (introduced by Spohn 1980).</u>

This approach starts by studying the evolution of the marginal density

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

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

What happens if we fix k and let $N \to \infty$? Formally, we obtain an infinite hierarchy of equations

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

$\gamma_{\infty,t}^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ solves $(*)$ $\iff$ φ_t solves Hartree Equation

<u>Strategy to show Theorem 1.</u>

- Establish <u>compactness</u> of $\gamma_{N,t}^{(k)}$ w.r.t. some weak topology.
- <u>Convergence</u>: prove that every limit point of $\gamma_{\infty,t}^{(k)}$ satisfies $(*)$
- <u>Uniqueness</u>: prove uniqueness of solution of $(*)$.

Uniqueness ? Bounded V ($\|V\|_\infty < \infty$).

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

drop subscript.

$$\mathcal{U}^{(k)}(t)\,\gamma^{(k)} = e^{i\sum_{j=1}^{k}\Delta_j t}\,\gamma^{(k)}\,e^{-i\sum_{j=1}^{k}\Delta_{x_j} t}$$

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

$\rightsquigarrow$ Duhamel Series :

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

$$\xi_{m,t}^{(k)} = \int_0^t ds_1 \cdots \int_0^{s_{m-1}} ds_m\; \mathcal{U}^{(k)}(t-s_1)\, B^{(k)} \cdots B^{(k+m-1)}\, \mathcal{U}^{(k+m)}(s_m)\, \gamma_0^{(k+m)}$$

$$\eta_{n,t}^{(k)} = \cdots\cdots \qquad \gamma_{s_n}^{(k+n)}.$$

To prove uniqueness, it suffices to show this series converges. So, we need to control the error term η. This turns out to be easy when the potential is bounded.

$$\|B^{(k)}\gamma^{(k+1)}\|_1 \le \cdots \le 2k\,\|V\|_\infty\,\|\gamma^{(k+1)}\|_1$$

$\hookrightarrow$

$$Tr\,|\eta_{n,t}^{(k)}| \le \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n\; k\,(n+1)\cdots(k+n)\,\|V\|_\infty^n = \frac{t^n}{n!}\,\frac{(k+n)!}{n!}\,\|V\|_\infty^n \le 2^k\left(2t\,\|V\|_\infty\right)^k. \implies \text{uniqueness}$$

Uniqueness in Coulomb case.

$$V(x) = \frac{1}{|x|}.$$

$V(x) \le c\,(1-\Delta)$ in the form sense:

$$\int \frac{|\varphi(x)|^2}{|x|} \le C \, \|\varphi\|_{H^1}^2 .$$

<u>Theorem</u> [Erdös - Yau 2000] There is at most one solution of the infinite hierarchy (*) such that

$$\|\gamma_t^{(k)}\|_{H_k^1} = \mathrm{Tr}\, \left| (1-\Delta_{x_1})^{\frac{1}{2}} \cdots (1-\Delta_{x_k})^{\frac{1}{2}} \gamma_t^{(k)} (1-\Delta_{x_k})^{\frac{1}{2}} \cdots (1-\Delta_{x_1})^{\frac{1}{2}} \right|$$

$$\le C^k \quad \forall\ t, k.$$

III Dynamics of Bose-Einstein Condensates

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

$$V_N(x) = N^2 V(Nx) \quad ; \quad V \geq 0 \quad \text{short range}$$

<u>Theorem</u> (Erdos - S - Yau) Suppose $|V(x)| \leq C(1+|x|)^{-\delta/2}$; $\delta > 5$.

$\psi_N = \varphi^{\otimes N}$, $\varphi \in H^1(\mathbb{R}^3)$, Then $\forall t \in \mathbb{R}$, $k \geq 1$

$$\gamma_{N,t}^{(k)} \xrightarrow[N \to \infty]{} |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$$

where

$$\begin{cases} i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \\ \varphi_{t=0} = \varphi \end{cases}$$

and a_0 = scattering length of V.

Gross-Pitaevskii

$\left\{ \begin{array}{l} b_0 \text{ is 1st Born approximation} \\ \text{to } 8\pi a_0. \end{array} \right.$

<u>Remark</u> Similarity w. H_N^{MF}

$$H_N^{BEC} = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} v_N(x_i - x_j) \quad ; \quad v_N(x) = N^3 V(Nx) \longrightarrow b_0\,\delta(x)$$

$$b_0 = \int V \, dx$$

Formally,

$$i\partial_t \varphi_t = -\Delta\varphi_t + b_0 |\varphi_t|^2 \varphi_t \text{ , so get wrong coupling constant.}$$

$\Longrightarrow$ we must be very careful when we use the mean field heuristics.

We are in an opposite limit.

Nevertheless, we can use the BBGKY hierarchy approach to prove convergence.

The reason $8\pi a_0$ emerges is because there are emerging correlations among particles on the $\frac{1}{N}$ scale.

Uniqueness of Infinite Hierarchy

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

as before ...

<u>but</u>

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

<u>Main Difficulty</u> $\delta(x) \not\leq C\,(1-\Delta)$. as operators

$\Longrightarrow$ Need to use smoothing effects of $\mathcal{U}^{(k)}(t)$.

$\Longrightarrow$ Use Feynman graph representation. ; Use Dispersive properties.

... Feynman graph.

IV Coherent States Approach. (Hepp 1973)

Coherent states are states in the Fock space over $L^2(\mathbb{R}^3)$.

Bosonic Fock space. $\mathcal{F} = \bigoplus_{n\geq 0} \mathcal{F}_n$; $\mathcal{F}_0 = \mathbb{C}$
$\mathcal{F}_n = L^2_s(\mathbb{R}^{3n}) \quad \forall n \geq 1.$

$$\mathcal{F} \ni \psi = \{\psi^{(j)}\}_{j=0}^{\infty} \; ; \quad \psi^{(j)} \in L^2_s(\mathbb{R}^{3j}).$$

$$\tilde{\psi} = \{0, 0, \ldots, \underset{\substack{\uparrow \\ N}}{\psi_N}, 0, \ldots\} \longrightarrow \text{exactly } N\text{-particles.}$$

$$\Omega = \{1, 0, \ldots\} \quad \text{vacuum vector. No particles at all.}$$

Number of particles in a Fock Vector:

$$(\mathcal{N}\psi)^{(n)} = n\,\psi^{(n)}$$

$$(\mathcal{N}\Omega) = 0.$$

$$\mathcal{N}\tilde{\psi} = N\tilde{\psi}.$$

$\forall f \in L^2(\mathbb{R}^3)$, we can define the creation operator

$$(a^*(f)\psi)^{(n)}(x_1, \ldots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\, \psi^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n)$$

$$(a(f)\psi)^{(n)}(x_1, \ldots, x_n) = \sqrt{n+1} \int dx\, \overline{f(x)}\, \psi^{(n+1)}(x, x_1, x_2, \ldots, x_n).$$

$$a^*(f)\Omega = \{0, f, 0, 0, \ldots\}$$

$$a^*(f) = \int dx\, a_x^*\, f(x) \quad ; \quad a(f) = \int dx\, \overline{f(x)}\, a_x.$$

$$\mathcal{N} = \int dx\, a_x^* a_x.$$

This is some formalism. In QM, it is called "2nd Quantization."

$$\mathcal{H}_N \Big|_{\mathcal{F}_n} = \sum_{j=1}^{n} -\Delta_j + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j)$$

$$\mathcal{H}_N = \int dx \quad \nabla_x a_x^* \nabla_x a_x + \frac{1}{N} \int dx\, dy \; V(x-y)\, a_x^* a_y^* a_y a_x .$$

$$e^{-i\mathcal{H}_N t} \{0, 0, \dots, \psi_N, 0, \dots\} = \{0, \dots, 0, e^{i H_N^{mf} t} \psi_N, 0, \dots\}.$$

Thus, we have not gained anything? But we have more freedom in our choice of initial states!

Coherent states For $f \in L^2(\mathbb{R}^3)$, define the Weyl operator

$$W(f) = e^{a^*(f) - a(f)} .$$

$$\psi(f) = W(f)\Omega = e^{-\|f\|^2/2} \sum_{j=1}^{\infty} \frac{a^*(f)^n \Omega}{n!}$$

coherent state associated to f

This is a linear superposition of different n-particle states. $\psi(f)$ does not have a fixed number of particles.

$$W(f)^* a_x \, W(f) = a_x + f(x)$$

Thus coherent states are eigenfunctions of annihilation operators!

$$a_x \psi(f) = f(x) \psi(f)$$

$$a(g) \psi(f) = \langle g, f \rangle \psi(f).$$

Average number of particles in a coherent state.

$$\langle W(f)\Omega, \mathcal{N} W(f)\Omega \rangle = \|f\|^2.$$

I want to stabilize things and require that the average number of particles is N so that we are considering a mean-field situation.

<u>Theorem</u> (Rodnianski–Schlein) Assume $V^2(x) \le C(1-\Delta)$.

Fix $\varphi \in H^1(\mathbb{R}^3)$, $\|\varphi\|_2 = 1$.

data has expected # of particles N.

$$\psi_{N,t} = e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega$$

Then $\forall t \in \mathbb{R}$

$$\operatorname{Tr}\left| \gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t| \right| \le C_1 \frac{e^{\frac{K}{2}t}}{N}.$$

where φ_t solves the non-linear Hartree equation w. data φ.

<u>Proof</u>

$$\gamma^{(1)}_{N,t}(x,y) = \frac{1}{N}\left\langle e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega,\ a_x^* a_y\, e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega \right\rangle$$

$$= \overline{\varphi_t(x)}\,\varphi_t(y) + \frac{1}{N}\left\langle e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega,\ (a_x^* - \sqrt{N}\overline{\varphi_t(x)})(a_y - \sqrt{N}\varphi_t(y))\, e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega \right\rangle$$

<u>Hepp's Observation:</u>

$$W^*(\sqrt{N}\varphi)\, e^{i\mathcal{H}_N t}\,(a_x^* - \sqrt{N}\,\overline{\varphi_t(x)})\, e^{-i\mathcal{H}_N t}\, W(\sqrt{N}\varphi) = \mathcal{U}^*(t)\, a_x^*\, \mathcal{U}(t)$$

where $\mathcal{U}(t)$ is a linear group with generator $\mathcal{L}(t)$, where

$$\mathcal{L}(t) = \int dx \ \nabla_x a_x^* \nabla a_x + V * |\varphi_t|^2 a_x^* a_x$$

$$+ \iint dx\,dy \ V(x-y)\, \varphi_t(x)\, \overline{\varphi_t(y)}\, a_x^* a_y$$

$$+ \iint dx\,dy \ V(x-y) \left(a_x^* a_y^* \varphi_t(x) \varphi_t(y) + \text{c.c.} \right) a_x$$

$$+ \frac{1}{\sqrt{N}} \iint dx\,dy \ V(x-y)\ a_x^* a_y^* a_y a_x .$$