Dynamics of Bose-Einstein Condensates

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

 $i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \qquad i\partial_t \gamma_{N,t} = [H, \gamma_{N,t}], \quad [A, B] = AB - BA$ with $\gamma_{N,t} := |\psi_{N,t}\rangle \langle \psi_{N,t}|$ density matrix (1 dim. projection).

One particle density matrix:

$$\gamma_{\psi}^{(1)}(x,y) := \int \psi(x, x_2 \cdots x_N) \overline{\psi}(y, x'_2 \cdots x'_N) dx_2 \cdots dx_N dx'_2 \cdots dx'_N$$

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

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

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

• Complete condensation in ground state:

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

Time Dependent GROSS-PITAEVSKII (GP) Theory

The GP energy functional also describes the evolution:

$$\gamma_{N,0}^{(1)} \to \varphi(x)\bar{\varphi}(x') \implies \gamma_{N,t}^{(1)} \to \varphi_t(x)\bar{\varphi}_t(x')$$

The condensate wave fn. evolves according to a NLS

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

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.

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

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

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

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

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

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

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} and the EY approach.

SCATTERING LENGTH

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

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

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:

$$\psi_N(\mathbf{x}) = W_N(\mathbf{x}) \prod_{j=1}^N u_0(x_j), \qquad \phi_N = \prod_{j=1}^N u_0(x_j)$$
$$\lim_{N \to \infty} N^{-1} \langle \psi_N, H_N \psi_N \rangle = \int |\nabla u(x)|^2 + 4\pi a_0 |u(x)|^4$$
$$\lim_{N \to \infty} N^{-1} \langle \phi_N, H_N \phi_N \rangle = \int |\nabla u_0(x)|^2 + \frac{b_0}{2} |u(x)|^4$$

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.

$$i\partial_t \phi_{N,t} = H_N \phi_{N,t}, \ \phi_{N,t=0} = \phi_N$$
$$N^{-1} \langle \phi_{N,t}, H_N \phi_{N,t} \rangle = N^{-1} \langle \phi_N, H_N \phi_N \rangle$$

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

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.

NONLINEAR HARTREE EQUATION: $\beta = 0, V_{\beta} = V$

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

Hepp: smooth potential, Ginibre-Velo: use coherent state. Schlein-Rodnianski apply to states with fix number of particles with Coulomb potential.

Spohn: bounded potential, BBGKY hierarchy.

Bardos, Golse and Mauser: convergence to hierarchy for Coulomb case, but no uniqueness nor a priori estimates.

Erdos-Y: Uniqueness of Coulomb case and a priori estimate.

bosonic star (Elgart-Schlein, Frohlich-Schwarz)

Fundamental difficulty of N-particle analysis $(N \gg 1)$

There is no good norm. The conserved L^2 -norm is too strong.

Let
$$\Psi = \otimes_1^N f$$
, $\Phi = \otimes_1^N g$, then $\|\Psi - \Phi\|^2 = 2 - 2\langle f, g \rangle^N \approx 2$.

Problem: $\psi(x_1, \ldots x_N)$ carries info of all particles (too detailed).

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.

Quantum analog of the marginals of a probability density.

It is an operator acting on the k-particle space.

$$H = -\sum_{j=1}^{N} \Delta_j + \frac{1}{N} \sum_{j < k} V_{\beta}(x_j - x_k), \qquad i \partial_t \gamma_{N,t} = \left[H, \gamma_{N,t} \right]$$

The BBGKY Hierarchy: The family $\{\gamma_{N,t}^{(k)}\}_{k=1}^N$ satisfies

$$\begin{split} i\partial_t \gamma_{N,t}^{(k)} &= \sum_{j=1}^k \left[-\Delta_{x_j}, \gamma_{N,t}^{(k)} \right] \\ &+ \sum_{j=1}^k \operatorname{Tr}_{k+1} \left[V_\beta(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)} \right] + \text{lower order terms} \,. \\ &\quad \operatorname{Tr}_2 \left[V(x_1 - x_2), \gamma^{(2)} \right] \\ &= \int \mathrm{d}x_2 \left(V(x_1 - x_2) - V(x_1' - x_2) \right) \gamma^{(2)}(x_1, x_2; x_1', x_2) \,. \end{split}$$

Derivation of the Hartree equation: $\beta = 0, V_{\beta} = V$ Special case: k = 1:

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

To get a closed equation for $\gamma_{N,t}^{(1)}$, we assume **Propagation of chaos:**

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

Assume that $\gamma_{N,t}^{(1)} \to \omega_t$. With $\varrho_t(x) := \omega_t(x;x)$. We then have the Hartree eq

$$i\partial_t\omega_t = \left[-\Delta + V * \varrho_t, \omega_t\right]$$

The Hartree Hierarchy $\beta = 0$: As $N \to \infty$, the BBGKY hierarchy formally converges to the Hartree hierarchy

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

Remark:

$$\gamma_t^{(k)}(\mathbf{x}_k;\mathbf{x}_k') = \prod_{j=1}^k \phi_t(x_j)\overline{\phi_t}(x_j') \qquad \left(\gamma_t^{(k)} = |\phi_t\rangle\langle\phi_t|^{\otimes k}\right)$$

is a solution of the Hartree hierarchy if ϕ_t satisfies

$$i\partial_t \phi_t = -\Delta \phi_t + (V * |\phi_t|^2) \phi_t$$

Strategy for Rigorous Derivation $\beta = 0$:

- Prove the compactness of $\{\gamma_{N,t}^{(k)}\}_{k=1}^N$ with respect to some weak topology
- Prove that the limit point $\{\gamma_{\infty,t}^{(k)}\}_{k\geq 1}$ is a solution of the infinite Hartree equation.
- Prove the apriori estimate needed for the uniqueness of the hierarchy.
- Prove the uniqueness (well-poseness) of the solution of the infinite Hartree hierarchy.

Main Difficulties for Rigorous Derivation $\beta = 1$:

1. Derive the GP hierarchy: Suppose $\gamma_{N,t}^{(k)} \to \gamma_{\infty,t}^{(k)}$ as $N \to \infty$. Then:

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

Emergence of the scattering length:

Suppose
$$\gamma_{N,t}^{(2)}(x_1, x_2; x_1', x_2) = [1 - w(N(x_1 - x_2))]\gamma_{N,t}^{(1)}(x_1, x_1')\gamma_{N,t}^{(1)}(x_2, x_2),$$

$$\int dx_2 V_{\beta}(x_1 - x_2)[1 - w(N(x_1 - x_2))]f(x_2) = f(x_1) \times \begin{cases} 8\pi a_0 & \text{if } \beta = 1\\ b_0 & \text{if } 0 < \beta < 1 \end{cases}$$



2. Well-poseness of the GP hierarchy in the H_1 class:

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

Tool: Analysis on Feynman diagrams.

3. A priori estimate so that (\dagger) holds. Due to the short scale structure, the estimate

$$\mathsf{Tr} \left(1 - \Delta_{x_1}\right) \dots \left(1 - \Delta_{x_k}\right) \gamma_{N,t}^{(k)} \leq C^k$$

is wrong.

Only after taking the weak limit so that the short scale structure disappears, can such bounds hold.

Klainerman-Machedon: Uniqueness via space-time norm.

Method of Moments of Energy—the second moment

Proposition: For any wave function ψ_N :

$$\langle \psi_N, H_N^2 \psi_N \rangle \ge C N^2 \int \mathrm{d}\mathbf{x} |\nabla_1 \nabla_2 \phi_{12}|^2$$

with $\phi_{12}(\mathbf{x}) = [1 - w(N(x_1 - x_2))]^{-1}\psi_N(\mathbf{x}).$

Consequence: any eigenfunction with energy $\simeq N$ must have the short scale structure $[1 - w(N(x_1 - x_2))]$ when x_1 is near x_2 .

- BEC for ground state ψ without scaling: Off-diagonal long range order (Yang)
- How to interpret systems with negative scattering length?

$$\inf_{u} \int |\nabla u|^2 \mathrm{d}x + \int U|u|^2 - 4\pi a_0 \int |u|^4 \mathrm{d}x = -\infty$$

The BEC cannot be the ground state! BEC for system with negative correlation length is a metastable state.

• fermi systems