

A norm approximation to the boson many body dynamics

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joint work with Chiara Boccato and Benjamin Schlein

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Research line: rigorous derivation of time dependent effective equations approximating many body quantum dynamics, in appropriate limiting regimes

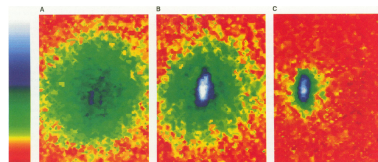
Goals:

- ▶ justify the use of the effective equations, which are often introduced on the basis of heuristics or phenomenological arguments
- ▶ clarify the limits of applicability of the effective theories, providing bounds on the error of the approximation

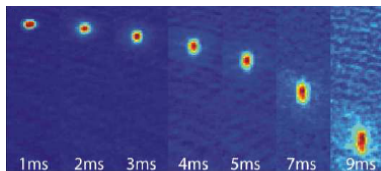
Systems of interest: Bose-Einstein condensates

Statics: describe the appearance of Bose-Einstein condensates in gas of trapped bosons at low temperature.

(→ properties of the ground state of the many-body Hamiltonian)



Anderson et al., BEC in a vapor of Rb-87 (1995)



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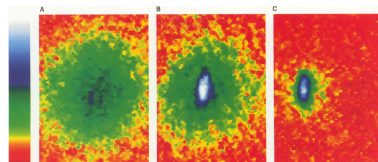
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(→ solve the time-dependent many-body Schrödinger equation)

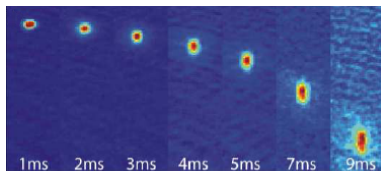
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N bosons in a trap: microscopic description

Wave function $\Psi_{N,0} \in L^2_{sym}(\mathbb{R}^{3N})$ which evolves according to $\Psi_{N,t} = e^{-i H_N t} \Psi_{N,0}$

$$H_N = \sum_{i=1}^N \left(-\Delta_{x_i} + V_{ext}(x_i/L) \right) + \frac{a_0}{R_0^3} \sum_{i < j}^N V((x_i - x_j)/R_0)$$

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$$V_{\text{ext}}(x) \rightarrow \infty \text{ for } |x| \rightarrow \infty$$

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$V \geq 0$, smooth,
short range

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The **scattering length** a_0 is defined through the zero energy cross section

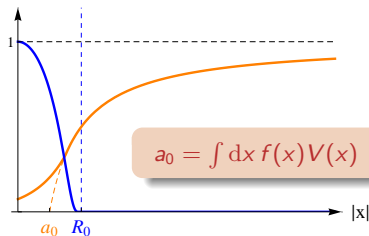
$$\sigma_0 = 4\pi a_0^2 \quad (\text{for hard sphere potentials: } \sigma_0 = 4\pi R_0^2)$$

or the **zero energy scattering function**

$$(-\Delta + W/2)f = 0, \quad f(x) \xrightarrow{|x| \rightarrow \infty} 1$$

If W is a short range potential

$$f(x) = 1 - \frac{a_0}{|x|} \quad \text{for } |x| > R_0$$



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In typical condensates: $N \simeq 10^3 - 10^6$.

How can one investigate the many body quantum dynamics ?

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Key goal:

- ▶ obtain an **approximate macroscopic description** of the system which only takes into account effective interactions in **suitable limiting regimes**

Mean Field limit

A first approximation for the behaviour of Bose condensates: the **mean field scaling limit**

$$H_N^{(MF)} = \sum_{i=1}^N \left(-\Delta_{x_i} + V_{\text{ext}}(x_i) \right) + \underbrace{\frac{1}{N} \sum_{i < j}^N V((x_i - x_j))}_{\text{intensity} \sim N^{-1}, \text{ range} \sim 1}$$

The Mean Field potential describes **many weak collisions**. Correlations among the particles are negligible.

The **ground state wave function** can be approximated for large N by

$$\Psi_N^{(MF)} \simeq \varphi^{\otimes N},$$

with $\varphi \in L^2(\mathbb{R}^3)$ the minimizer of the Hartree functional:

$$\mathcal{E}_{MF}(\varphi) = \int dx \left(|\nabla \varphi(x)|^2 + V_{\text{ext}}(x) |\varphi(x)|^2 + (V \star |\varphi|^2)(x) |\varphi(x)|^2 \right)$$

Gross-Pitaevskii scaling limit

A better approximation: the **Gross-Pitaevskii scaling limit**

$$H_N^{(GP)} = \sum_{i=1}^N (-\Delta_{x_i} + V_{\text{ext}}(x_j)) + \underbrace{\sum_{i < j}^N N^2 V(N(x_i - x_j))}_{\text{intensity} \sim N^2, \text{ range} \sim N^{-1}}$$

Gross-Pitaevskii potential describes **rare but strong collisions**:

- Fix one particle, probability of a collision: $\rho R_0^3 = N \cdot N^{-3} = N^{-2}$
- Average number of collisions: N^{-1}

The potential $N^2 V(Nx)$ has scattering function $f(Nx) = 1 - \frac{a_0}{N|x|}$ and scattering length $a = a_0/N$

Physically relevant: in typical condensates $N \simeq 10^3 - 10^6$ and a is such that $Na \sim 1$.

Gross-Pitaevskii: ground state properties (1)

Correlations among the particles play a crucial role: the ground state energy of the boson gas depends on the scattering length of the interaction potential.

[Lieb-Seiringer-Yngvason, 2000] Let E_N be the ground state energy of

$$H_N^{(GP)} = \sum_{i=1}^N (-\Delta_{x_i} + V_{\text{ext}}(x_i)) + \sum_{i < j}^N N^2 V(N(x_i - x_j))$$

Then

$$E_N/N \xrightarrow{N \rightarrow \infty} \min_{\varphi \in L^2(\mathbb{R}^3): \|\varphi\|=1} \mathcal{E}_{GP}(\varphi) = \mathcal{E}_{GP}(\varphi_{GP})$$

with $\mathcal{E}_{GP}(\varphi)$ the **Gross-Pitaevskii energy functional**

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

Gross-Pitaevskii: ground state properties (2)

[Lieb-Seiringer, 2002] Let $\Psi_N(x_1, \dots, x_N)$ the ground state of

$$H_N^{(GP)} = \sum_{i=1}^N (-\Delta_{x_i} + V_{\text{ext}}(x_i)) + \sum_{i < j}^N N^2 V(N(x_i - x_j))$$

and $\gamma_N^{(1)}$ be the one particle reduced density associated to $\Psi_N(x_1, \dots, x_N)$

$$\gamma_N^{(1)} := \text{Tr}_{2, \dots, N} |\Psi_N\rangle \langle \Psi_N|$$

Then, in trace norm

$$\gamma_N^{(1)} \xrightarrow{N \rightarrow \infty} |\varphi_{GP}\rangle \langle \varphi_{GP}|$$

where $\varphi_{GP} \in L^2(\mathbb{R}^3)$ the minimizer of the GP functional $\mathcal{E}_{GP}(\varphi)$. This also implies:

$$\gamma_N^{(k)} \xrightarrow{N \rightarrow \infty} |\varphi_{GP}\rangle \langle \varphi_{GP}|^{\otimes k}$$

Complete condensation in the g.s.: the expectation of any k -particle observable in the ground state can be computed using $\varphi_{GP} \otimes \dots \otimes \varphi_{GP}$ instead than Ψ_N .

Gross-Pitaevskii: emergence of correlations

Complete condensation in the GP regime does NOT mean that $\Psi_N \simeq \varphi^{\otimes N}$

$\langle \varphi^{\otimes N}, H_N^{(GP)} \varphi^{\otimes N} \rangle$ (Energy of a factorized state)

$$= N \left[\int dx (|\nabla \varphi(x)|^2 + V_{\text{ext}} |\varphi(x)|^2) + \frac{1}{2} \int dx dy N^3 V(N(x-y)) |\varphi(x)|^2 |\varphi(y)|^2 \right]$$

$$\xrightarrow[N \rightarrow \infty]{} \frac{b_0}{2} \int dx dy \delta(x-y) |\varphi(x)|^2 |\varphi(y)|^2$$

$$\simeq N \int dx \left(|\nabla \varphi(x)|^2 + V_{\text{ext}} |\varphi(x)|^2 + \frac{b_0}{2} |\varphi(x)|^4 \right)$$

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Ground state energy in the Gross-Pitaevskii regime:

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Correlations generated by the strong collisions disappear in $\gamma_N^{(k)}$, but crucially affect the ground state energy.

Between MF and GP scaling limits

Let $0 < \beta < 1$. Intermediate scaling limits between MF and GP are:

$$H_N^{(\beta)} = \sum_{i=1}^N (-\Delta_{x_i} + V_{\text{ext}}(x_j)) + \underbrace{\frac{1}{N} \sum_{i < j}^N N^{3\beta} V(N^\beta(x_i - x_j))}_{\text{intensity} \sim N^{3\beta-1}, \text{ range} \sim N^{-\beta}}$$

For any $0 < \beta < 1$

- the potential $N^{3\beta-1} V(N^\beta x)$ has scattering length $a \simeq N^{-1}$ i.e. particles are correlated up to distances N^{-1}
- the range of the interaction $R_0 \simeq N^{-\beta}$ is much larger than a

Key point: correlations among particles are not negligible, but since $a \ll R_0$ they affect the ground state energy at lowest order with respect to the Gross-Pitaevskii scaling limit.

Dynamics: known results (3d)

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

	$V_N^{(\beta)}(x)$	Effective equation		
Mean Field ($\beta = 0$)	$\frac{1}{N} V(x)$	$i\partial_t \varphi_t = -\Delta \varphi_t + (V \star \varphi_t ^2) \varphi_t$		
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Trace norm convergence: let the initial state Ψ_N be condensate and let $\gamma_{N,t}^{(1)}$ be the reduced density matrix associated to $\Psi_{N,t} = e^{-iH_N^{(\beta)}t} \Psi_N$. Then, $\gamma_{N,t}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$, where φ_t solves the corresponding effective equation.

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Norm approximation: let $\Psi_{N,t} = e^{-iH_N^{(\beta)}t} \Psi_N$. Then,

$$\|\Psi_{N,t} - \Psi_{approx,t}\| \rightarrow 0,$$

where $\Psi_{approx,t}$ depends only on a few degrees of freedom (including φ_t).

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Gross-Pitaevskii ($\beta = 1$)	$N^2 V(Nx)$	$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 \varphi_t ^2 \varphi_t$	Erdős-Schlein-Yau, Pickl, Benedikter et al.	?

Norm approximation: let $\Psi_{N,t} = e^{-iH_N^{(\beta)}t} \Psi_N$. Then,

$$\|\Psi_{N,t} - \Psi_{approx,t}\| \rightarrow 0,$$

where $\Psi_{approx,t}$ depends only on a few degrees of freedom (including φ_t).

Dynamics: known results (3d)

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

	$V_N^{(\beta)}(x)$	Effective equation	Trace Norm	Norm approx
Mean Field ($\beta = 0$)	$\frac{1}{N} V(x)$	$i\partial_t \varphi_t = -\Delta \varphi_t + (V \star \varphi_t ^2) \varphi_t$	Hepp, Ginibre-Velo, Spohn, Erdős-Yau, Rodnianskii-Schlein, Knowles-Pickl	Ginibre-Velo, Grillakis et al., Ben Arous et al.
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Gross-Pitaevskii ($\beta = 1$)	$N^2 V(Nx)$	$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 \varphi_t ^2 \varphi_t$	Erdős-Schlein-Yau, Pickl, Benedikter et al.	?

Mean Field case. Fluctuations around Hartree dynamics satisfy a CLT

$$\frac{1}{\sqrt{N}} \sum_{i=1}^N \mathcal{O}_i^{(1)} - \langle \varphi_t, \mathcal{O}^{(1)} \varphi_t \rangle \rightarrow \text{Gauss}(0, \sigma_t^2)$$

and Bogoliubov prediction for the spectrum holds (Seiringer-Grech, Lewin et al.)

Dynamics: known results (3d)

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

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Strategy: apply the method developed by Rodnianski-Schlein, based on

- ▶ a representation of the many boson system on the **Fock space**
- ▶ the study of the time evolution of **coherent states**

Fock space

Idea: **enlarge the set of initial states**, embedding $L_s^2(\mathbb{R}^{3N})$ in the bosonic Fock space:

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} L_s^2(\mathbb{R}^{3n}) = \mathbb{C} \oplus L_s^2(\mathbb{R}^3) \oplus \dots \oplus L_s^2(\mathbb{R}^N) \oplus \dots$$

$$\psi = \{ \psi^{(0)}, \psi^{(1)}, \dots, \psi^{(N)}, \dots \} \in \mathcal{F}$$

- ▶ $\|\psi^{(n)}\|^2 = \text{prob. of having } n \text{ particles in the state } \psi$ ($\sum_n \|\psi^{(n)}\|^2 = 1$)
- ▶ vacuum state: $\Omega = \{1, 0, 0, \dots, 0\}$
- ▶ state with fixed particle number: $\{0, 0, \dots, \psi_N, \dots, 0\}$

Creation and annihilation operators

Creation and annihilation operators: for $f \in L^2(\mathbb{R}^3)$ define

$$a^*(f) : \mathcal{H}^{(n)} \rightarrow \mathcal{H}^{(n+1)}, \quad a(f) : \mathcal{H}^{(n+1)} \rightarrow \mathcal{H}^{(n)}$$

whose action is given by

$$(a^*(f)\psi)^{(n+1)}(x_1, \dots, x_{n+1}) = \frac{1}{\sqrt{n+1}} \sum_{j=1}^{n+1} f(x_j) \psi^{(n)}(x_1, \dots, \cancel{x_j}, \dots, x_{n+1})$$
$$(a(f)\psi)^{(n)}(x_1, \dots, x_n) = \sqrt{n+1} \int dx f(x) \psi^{(n+1)}(x_1, \dots, x_n, x)$$

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

Canonical commutation relations:

$$[a(f), a^*(g)] = \langle f, g \rangle_{L^2}, \quad [a(f), a(g)] = [a^*(f), a^*(g)] = 0$$

Action of a and a^* :

$$a(\varphi)\Omega = 0; \quad \frac{(a^*(\varphi))^N}{\sqrt{N!}}\Omega = \{0, \dots, \varphi^{\otimes N}, \dots, 0\}$$

Fock space Hamiltonian

Operator valued distributions a_x and a_x^* :

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

Number of particle operator: $\mathcal{N} = \int dx a_x^* a_x$

Fock space Gross-Pitaevskii Hamiltonian:

$$\mathcal{H}_N = \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int dx dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x$$

Note that

$$(\mathcal{H}_N \psi)^{(m)} = H_N^{(m)} \psi^{(m)}$$

with

$$H_N^{(m)} = \sum_{j=1}^m -\Delta_{x_j} + N^2 \sum_{i < j}^m V(N(x_i - x_j))$$

Coherent states

For $\varphi \in L^2(\mathbb{R}^3)$ define the **Weyl operator**

$$W(\varphi) = e^{a^*(\varphi) - a(\varphi)}$$

Coherent state with wave function φ :

$$W(\varphi)\Omega = e^{-\|\varphi\|^2/2} \left\{ 1, \varphi, \frac{\varphi^{\otimes 2}}{\sqrt{2!}}, \frac{\varphi^{\otimes 3}}{\sqrt{3!}}, \dots, \frac{\varphi^{\otimes N}}{\sqrt{N!}}, \dots \right\}$$

► Coherent states are normalized: $W^*(\varphi) = W(\varphi)^{-1}$

► Action of the Weyl operator:

$$W^*(\varphi)a_x W(\varphi) = a_x + \varphi(x) \quad \Rightarrow \quad a_x W(\varphi)\Omega = \varphi(x) W(\varphi)\Omega$$

$$W^*(\varphi)a_x^* W(\varphi) = a_x^* + \overline{\varphi(x)}$$

► Expected number of particle: $\langle W(\varphi)\Omega, \mathcal{N} W(\varphi)\Omega \rangle = \|\varphi\|_2^2$

Coherent states

For $\varphi \in L^2(\mathbb{R}^3)$ define the **Weyl operator**

$$W(\varphi) = e^{a^*(\varphi) - a(\varphi)}$$

Initial state with average
particle number N :

$$\Psi_{N,0} = W(\sqrt{N}\varphi)\Omega$$

Coherent state with wave function φ :

$$W(\varphi)\Omega = e^{-\|\varphi\|^2/2} \left\{ 1, \varphi, \frac{\varphi^{\otimes 2}}{\sqrt{2!}}, \frac{\varphi^{\otimes 3}}{\sqrt{3!}}, \dots, \frac{\varphi^{\otimes N}}{\sqrt{N!}}, \dots \right\}$$

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► Expected number of particle: $\langle W(\varphi)\Omega, \mathcal{N} W(\varphi)\Omega \rangle = \|\varphi\|_2^2$

Gross-Pitaevskii regime: coherent state approach

Gross-Pitaevskii Fock space Hamiltonian:

$$\mathcal{H}_N^{(GP)} = \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int dx dy \, N^2 V(N(x-y)) a_x^* a_y^* a_y a_x$$

First idea: we assume the evolution of a coherent state to be approximately coherent with φ_t solution of GP equation:

$$e^{-it\mathcal{H}_N^{GP}} W(\sqrt{N}\varphi)\Omega \simeq W(\sqrt{N}\varphi_t)\Omega$$

Then

$$\begin{aligned} N\gamma_{N,t}^{(1)}(x,y) &= \langle e^{-i\mathcal{H}_N^{MF}t} W(\sqrt{N}\varphi)\Omega, a_y^* a_x e^{-i\mathcal{H}_N^{MF}t} W(\sqrt{N}\varphi)\Omega \rangle \\ &\simeq \langle W(\sqrt{N}\varphi_t)\Omega, a_y^* a_x W(\sqrt{N}\varphi_t)\Omega \rangle \\ &= \langle \Omega, (a_y^* + \sqrt{N}\overline{\varphi_t(y)}) (a_x + \sqrt{N}\varphi_t(x)) \Omega \rangle \\ &= N \overline{\varphi_t(y)} \varphi_t(x) \end{aligned}$$

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Rigorous approach: define

$$e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi)\Omega := W(\sqrt{N}\varphi_t) \mathcal{U}_N(t)\Omega$$

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Rigorous approach: define

$$W(\sqrt{N}\varphi_t) W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) \Omega := W(\sqrt{N}\varphi_t) \mathcal{U}_N(t) \Omega$$

where

$$\mathcal{U}_N(t) = W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi)$$

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$$\mathcal{U}_N(t) = W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi)$$

One obtains:

$$\mathrm{Tr} |\gamma_{N,t}^{(1)}(x,y) - |\varphi_t\rangle\langle\varphi_t|| \leq \frac{C}{\sqrt{N}} \langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega \rangle$$

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The problem reduces to **control of the number of fluctuations**: is it possible to show that

$$\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega \rangle \leq D(t) \quad ?$$

Gross-Pitaevskii regime: coherent state approach

$$\frac{d}{dt} \langle \mathcal{U}_N(t) \Omega, \mathcal{N} \mathcal{U}_N(t) \Omega \rangle \leq | \langle \mathcal{U}_N(t) \Omega, [\mathcal{L}_N(t), \mathcal{N}] \mathcal{U}_N(t) \Omega \rangle |$$

with $i\partial_t \mathcal{U}_N(t) = \mathcal{L}_N(t) \mathcal{U}_N(t)$

$$\begin{aligned} \mathcal{L}_N(t) = & \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{N} \int dx dy N^3 V(N(x-y)) a_x^* a_y^* a_x a_y \\ & + \sqrt{N} \int dx dy N^3 V(N(x-y)) (1 - f(N(x-y))) \left[|\varphi_t^{(N)}(y)|^2 \varphi_t^{(N)}(x) a_x^* + \text{h.c.} \right] \\ & + \frac{1}{2} \int dx dy N^3 V(N(x-y)) \left(\varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x^* + \text{h.c.} \right) \\ & + \int dx dy N^3 V(N(x-y)) \left(|\varphi_t^{(N)}(x)|^2 a_y^* a_y + \varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x \right) \\ & + \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \left(\overline{\varphi_t^{(N)}(y)} a_x^* a_x a_y + \text{h.c.} \right) \end{aligned}$$

Gross-Pitaevskii regime: coherent state approach

$$\frac{d}{dt} \langle \mathcal{U}_N(t) \Omega, \mathcal{N} \mathcal{U}_N(t) \Omega \rangle \leq |\langle \mathcal{U}_N(t) \Omega, [\mathcal{L}_N(t), \mathcal{N}] \mathcal{U}_N(t) \Omega \rangle| \sim \sqrt{N}$$

with $i\partial_t \mathcal{U}_N(t) = \mathcal{L}_N(t) \mathcal{U}_N(t)$

$$\begin{aligned} \mathcal{L}_N(t) = & \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{N} \int dx dy N^3 V(N(x-y)) a_x^* a_y^* a_x a_y \\ & + \sqrt{N} \int dx dy N^3 V(N(x-y)) (1 - f(N(x-y))) \left[|\varphi_t^{(N)}(y)|^2 \varphi_t^{(N)}(x) a_x^* + \text{h.c.} \right] \\ & + \frac{1}{2} \int dx dy N^3 V(N(x-y)) \left(\varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x^* + \text{h.c.} \right) \\ & + \int dx dy N^3 V(N(x-y)) \left(|\varphi_t^{(N)}(x)|^2 a_y^* a_y + \varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x \right) \\ & + \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \left(\overline{\varphi_t^{(N)}(y)} a_x^* a_x a_y + \text{h.c.} \right) \end{aligned}$$

Heuristically, $e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi)\Omega$ **develops singular correlations**, which are not captured by the approximate evolution $W(\sqrt{N}\varphi_t)\Omega$.

Gross-Pitaevskii regime: squeezed coherent states

- Define a **correlation structure**:

$$k_t(x, y) = -N(1 - f(N(x - y)))\varphi_t(x)\varphi_t(y) \quad (\|k_t\|_{L^2 \times L^2} \leq C)$$

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- Implement correlations** using a Bogoliubov transformation

$$T(k_t) := e^{\frac{1}{2} \int dx dy (k_t(x, y) a_x^* a_y^* - \bar{k}_t(x, y) a_x a_y)}$$

whose action is

$$T^*(k_t) a(f) T(k_t) = a(\cosh_{k_t}(f)) + a^*(\sinh_{k_t}(\bar{f})) \simeq a(f) + a^*(k_t \bar{f})$$

$$T^*(k_t) a^*(f) T(k_t) = a^*(\cosh_{k_t}(f)) + a(\sinh_{k_t}(\bar{f})) \simeq a^*(f) + a(k_t \bar{f})$$

$$\text{with } \cosh_{k_t} = \sum_{j=0}^{\infty} \frac{(k_t \bar{k}_t)^j}{2^j j!} \quad \text{and} \quad \sinh_{k_t} = k_t + \sum_{j=1}^{\infty} \frac{(k_t \bar{k}_t)^j}{(2j+1)!}$$

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- Add short-scale correlations.** New initial data:

$$\psi_{N,0} = W(\sqrt{N}\varphi) T(k_0) \Omega \quad (\text{squeezed coherent state})$$

Gross-Pitaevskii regime: modified fluctuation dynamics

Gross-Pitaevskii Hamiltonian:

$$\mathcal{H}_N^{(GP)} = \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int dx dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x$$

We assume

$$e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) T(k_0) \Omega \simeq W(\sqrt{N}\varphi_t) T(k_t) \Omega$$

Gross-Pitaevskii regime: modified fluctuation dynamics

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We define **a new fluctuation operator** $\tilde{\mathcal{U}}_N(t)$:

$$e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) T(k_0) \Omega := W(\sqrt{N}\varphi_t) T(k_t) \tilde{\mathcal{U}}_N(t) \Omega$$

where

$$\tilde{\mathcal{U}}_N(t) = T^*(k_t) W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) T(k_0)$$

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where

$$\tilde{\mathcal{U}}_N(t) = T^*(k_t) W^*(\sqrt{N}\varphi_t) e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) T(k_0)$$

As before:

$$\mathrm{Tr} |\gamma_{N,t}^{(1)}(x, y) - |\varphi_t\rangle\langle\varphi_t|| \leq \frac{C}{\sqrt{N}} \langle \tilde{\mathcal{U}}_N(t) \Omega, \mathcal{N} \tilde{\mathcal{U}}_N(t) \Omega \rangle$$

The number of fluctuations w.r.t. the new dynamics stays of order one

$$\langle \tilde{\mathcal{U}}_N(t) \Omega, \mathcal{N} \tilde{\mathcal{U}}_N(t) \Omega \rangle \leq e^{c_1 \exp(c_2)|t|}$$

Gross-Pitaevskii regime: modified fluctuation dynamics

The generator of $\tilde{\mathcal{U}}_N(t) = T^*(k_t)W^*(\sqrt{N}\varphi_t)e^{-i\mathcal{H}_N^{(GP)}t}W(\sqrt{N}\varphi)T(k_0)$ is:

$$\begin{aligned}\tilde{\mathcal{L}}_N(t) = & [i\partial_t T^*(k_t)]T(k_t) \\ & + T^*(k_t) \left[\int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{N} \int dx dy N^3 V(N(x-y)) a_x^* a_y^* a_x a_y \right. \\ & + \sqrt{N} \int dx dy N^3 V(N(x-y))(1 - f(N(x-y))) \left[|\varphi_t^{(N)}(y)|^2 \varphi_t^{(N)}(x) a_x^* + \text{h.c.} \right] \\ & + \frac{1}{2} \int dx dy N^3 V(N(x-y)) \left(\varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x^* + \text{h.c.} \right) \\ & + \int dx dy N^3 V(N(x-y)) \left(|\varphi_t^{(N)}(x)|^2 a_y^* a_y + \varphi_t^{(N)\bar{}}(x) \varphi_t^{(N)}(y) a_y^* a_x \right) \\ & \left. + \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \left(\overline{\varphi_t^{(N)}(y)} a_x^* a_x a_y + \text{h.c.} \right) \right] T(k_t)\end{aligned}$$

Gross-Pitaevskii regime: modified fluctuation dynamics

The generator of $\tilde{\mathcal{U}}_N(t) = T^*(k_t) W^*(\sqrt{N}\varphi_t) e^{-i\mathcal{H}_N^{(GP)}t} W(\sqrt{N}\varphi) T(k_0)$ is:

$$\begin{aligned} \tilde{\mathcal{L}}_N(t) = & [i\partial_t T^*(k_t)] T(k_t) \\ & + T^*(k_t) \left[\int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{N} \int dx dy N^3 V(N(x-y)) a_x^* a_y^* a_x a_y \right. \\ & + \sqrt{N} \int dx dy N^3 V(N(x-y)) (1 - f(N(x-y))) \left[|\varphi_t^{(N)}(y)|^2 \varphi_t^{(N)}(x) a_x^* + \text{h.c.} \right] \\ & + \frac{1}{2} \int dx dy N^3 V(N(x-y)) \left(\varphi_t^{(N)}(x) \varphi_t^{(N)}(y) a_y^* a_x^* + \text{h.c.} \right) \\ & + \int dx dy N^3 V(N(x-y)) \left(|\varphi_t^{(N)}(x)|^2 a_y^* a_y + \varphi_t^{(N)\bar{}}(x) \varphi_t^{(N)}(y) a_y^* a_x \right) \\ & \left. + \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \left(\overline{\varphi_t^{(N)}(y)} a_x^* a_x a_y + \text{h.c.} \right) \right] T(k_t) \end{aligned}$$

Key point. The action of Bogoliubov transformation destroys normalorder:

$$\begin{aligned} T^*(k_t) (\sqrt{N} a^\# + \frac{1}{\sqrt{N}} a^\# a^\# a^\#) T(k_t) &= \sqrt{N}(\text{linear}) + \frac{1}{\sqrt{N}}(\text{cubic, not normalorder}) \\ &= \sqrt{N}(\text{linear}) - \sqrt{N}(\text{linear}) + \frac{1}{\sqrt{N}}(\text{cubic, normalorder}) \end{aligned}$$

Gross-Pitaevskii regime: rate of convergence

Theorem [Benedikter-de Oliveira-Schlein, 2012] Let $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$, $V \geq 0$ and

$$\mathcal{H}_N^{(GP)} = \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2} \int dx dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x$$

- Let $\gamma_{N,t}^{(1)}$ be the reduced density of

$$\Psi_{N,t} = e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi) T(k_0)\Omega$$

- Let φ_t solve the Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t, \quad \text{with initial data } \varphi_0 = \varphi$$

Then

$$\text{Tr} \left| \gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t| \right| \leq CN^{-1/2} e^{c_1 \exp(c_2|t|)}$$

- The class of initial data $\Psi_{N,0} = W(\sqrt{N}\varphi) T(k_0)\Omega$ has expected particle number N and “correct energy”: $\langle \Psi_{N,0}, \mathcal{H}_N^{(GP)} \Psi_{N,0} \rangle = N\mathcal{E}_{GP}(\varphi) + \mathcal{O}(1)$
- The same strategy can be applied for any $0 < \beta < 1$.

A norm approximation result

[Boccato-C.-Schlein, 2015] Let $0 < \beta < 1$

$$\mathcal{H}_N^{(\beta)} = \int dx \nabla_x a_x^* \nabla_x a_x + N^{3\beta-1} \int dx dy V(N^\beta(x-y)) a_x^* a_y^* a_y a_x$$

with V smooth, positive, spherically symmetric and with compact support, and $T(k_t) = \exp(\int k_t(x, y) a_x^* a_y^* - \text{h.c.})$ with correlation kernel

$$k_t(x, y) = -N (1 - f_{\ell, N}(x - y)) \varphi_t^2((x+y)/2)$$

with a “modified” scattering function $f_{\ell, N}$ satisfying

$$\begin{cases} (-\Delta + \frac{1}{2} N^{3\beta-1} V(N^\beta x)) f_{\ell, N}(x) = \lambda_{\ell, N} f_{\ell, N}(x), & |x| \leq \ell \\ f_{\ell, N}(\ell) = 1, \quad \partial_r f_{\ell, N}(\ell) = 0 \end{cases}$$

and φ_t solution of $i\partial_t \varphi_t = -\Delta \varphi_t + (\int V) |\varphi_t|^2 \varphi_t$. Then

$$\| (e^{-it\mathcal{H}_N^{(\beta)}} W(\sqrt{N}\varphi) T(k_0) \Omega - W(\sqrt{N}\varphi_t) T(k_t) \mathcal{U}_2 \Omega) \| \xrightarrow{N \rightarrow \infty} 0$$

Remarks

$$\| (e^{-it\mathcal{H}_N^{(\beta)}} W(\sqrt{N}\varphi) T(k_0)\Omega - W(\sqrt{N}\varphi_t) T(k_t)\mathcal{U}_2\Omega) \| \leq C N^{-\gamma} e^{c_1 \exp(c_2|t|)}$$

$$\gamma = \min(\beta/4, (1 - \beta)/4)$$

Limit dynamics. \mathcal{U}_2 has a quadratic generator, as a consequence it depends only on few parameters (\rightarrow great simplification)

Initial data. The theorem also holds for initial data of the form $W(\sqrt{N}\varphi) T(k_0)\psi$ with $\psi \in \mathcal{F}$ satisfying

$$\langle \psi, (\mathcal{N}^2 + \mathcal{K}^2 + \mathcal{H}_N^{(\beta)}) \psi \rangle \leq C$$

Comparison with Mean Field. Similar result without introducing correlations:

$$\| (e^{-it\mathcal{H}_N^{(MF)}} W(\sqrt{N}\varphi)\Omega - W(\sqrt{N}\varphi_t) \mathcal{U}_2^{(MF)}\Omega) \| \leq C N^{-1/2} e^{k|t|}$$

Strategy of the proof

Our goal is to prove that:

$$\| \underbrace{e^{-it\mathcal{H}_N^{(\beta)}} W(\sqrt{N}\varphi) T(k_0)\Omega}_{W(\sqrt{N}\varphi_t) T(k_t) \tilde{\mathcal{U}}_N(t)\Omega} - W(\sqrt{N}\varphi_t) T(k_t) \mathcal{U}_2(t)\Omega \|^2 \leq \frac{C(t)}{N^\gamma}$$

It is sufficient to show that

$$\|(\tilde{\mathcal{U}}_N(t) - \mathcal{U}_2(t))\Omega\|^2 \leq \frac{C(t)}{N^\gamma}$$

One uses

$$\frac{d}{dt} \|(\tilde{\mathcal{U}}_N(t) - \mathcal{U}_2(t))\Omega\|^2 = \text{Im} \langle \tilde{\mathcal{U}}_N\Omega, (\tilde{\mathcal{L}}_N - \mathcal{L}_2)\mathcal{U}_2\Omega \rangle$$

Goal: show that $|\langle \tilde{\mathcal{U}}_N\Omega, (\tilde{\mathcal{L}}_N - \mathcal{L}_2)\mathcal{U}_2\Omega \rangle| \leq C(t)N^{-\gamma}$

Strategy of the proof

One finds:

$$|\langle \tilde{\mathcal{U}}_N \Omega, (\tilde{\mathcal{L}}_N - \mathcal{L}_2) \mathcal{U}_2 \Omega \rangle| \leq \frac{C(t)}{N^{-\delta}} \left[\langle \tilde{\mathcal{U}}_N \psi, \mathcal{V}_N + \mathcal{K} + \mathcal{N} + 1, \tilde{\mathcal{U}}_N \psi \rangle + \langle \mathcal{U}_2 \psi, (\mathcal{K} + \mathcal{N} + 1)^2, \mathcal{U}_2 \psi \rangle \right]$$

The problem ends up in

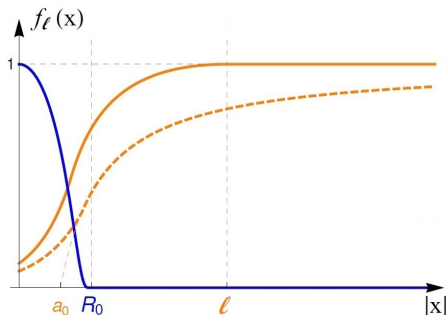
- controlling the growth of \mathcal{N} , \mathcal{V}_N and \mathcal{K} w.r.t. the full dynamics $\tilde{\mathcal{U}}_N$: similar to what done in [\[Benedikter- de Oliveira-Schlein, 12\]](#)
- controlling the growth of \mathcal{N}^2 and \mathcal{K}^2 w.r.t. the limiting dynamics \mathcal{U}_2 : **this step requires a careful choice of the correlation kernel**

Correlation structure

We denote with $f_{\ell,N}$ the ground state solution of the Neumann problem:

$$\begin{cases} (-\Delta + \frac{1}{2}N^{3\beta-1}V(N^\beta x))f_{\ell,N}(x) \\ \quad = \lambda_{\ell,\beta}f_{\ell,N}(x), \quad |x| \leq \ell \\ f_{\ell,N}(\ell) = 1, \quad \partial_r f_{\ell,N}(\ell) = 0 \end{cases}$$

with $a_0 \sim N^{-1}$, $R_0 \sim N^{-\beta}$ and $\ell \sim 1$.

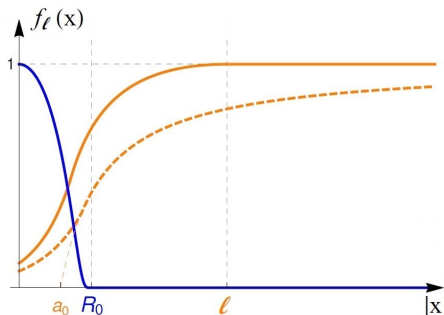


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Idea: particles are correlated up to distances of order 1.

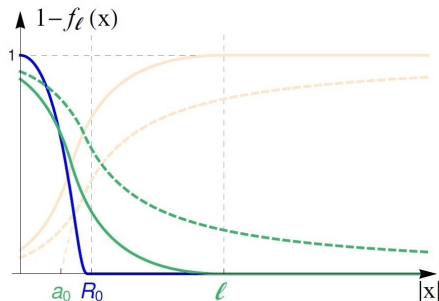
$$k_t(x, y) = -N (1 - f_{\ell,N}(x - y)) \varphi_t^2(x+y/2)$$

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$$\begin{cases} (-\Delta + \frac{1}{2}N^{3\beta-1}V(N^\beta x))f_{\ell,N}(x) = \lambda_{\ell,\beta}f_{\ell,N}(x), & |x| \leq \ell \\ f_{\ell,N}(\ell) = 1, \quad \partial_r f_{\ell,N}(\ell) = 0 \end{cases}$$

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Idea: particles are correlated up to distances of order 1.

$$k_t(x, y) = -N(1 - f_{\ell,N}(x - y))\varphi_t^{2(x+y/2)}$$

Extension to the Gross-Pitaevskii regime

Goal: show that $|\langle \tilde{\mathcal{U}}_N \Omega, (\tilde{\mathcal{L}}_N(t) - \mathcal{L}_2(t)) \mathcal{U}_2 \Omega \rangle| \leq C(t) N^{-\gamma}$, $\gamma > 0$

For $\beta = 1$ consider the following cubic term belonging to $\tilde{\mathcal{L}}_N$:

$$C = \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \varphi_t(y) a_x^* a_y^* a_x$$

Then

$$\langle \tilde{\mathcal{U}}_N \Omega, C \mathcal{U}_2 \Omega \rangle = \frac{1}{\sqrt{N}} \int dx dy N^3 V(N(x-y)) \varphi_t(y) \langle \underbrace{a_x a_y \tilde{\mathcal{U}}_N \Omega}_{\Psi_N(x,y)}, \underbrace{a_x \mathcal{U}_2 \Omega}_{h(x)} \rangle$$

If $\Psi_N(x, y) = \sqrt{N} g(N(x-y))$ we have by scaling

$$\langle \tilde{\mathcal{U}}_N \Omega, C \mathcal{U}_2 \Omega \rangle = \int dx dy V(x-y) g(x-y) h(x) \varphi_t(x-y/N) \simeq O(1)$$

This singular state is compatible with the condition $\langle \tilde{\mathcal{U}}_N \Omega, \mathcal{H}_N \tilde{\mathcal{U}}_N \Omega \rangle \sim O(1)$

Extension to the Gross-Pitaevskii regime & perspectives

In the Gross-Pitaevskii scaling, for initial data of the form $W(\sqrt{N}\varphi)T(k_0)\Omega$, fluctuations cannot be described by a quadratic generator

$$\| (e^{-it\mathcal{H}_N^{(GP)}} W(\sqrt{N}\varphi)T(k_0)\Omega - W(\sqrt{N}\varphi_t)T(k_t)\mathcal{U}_2\Omega) \| \not\rightarrow 0$$

- Understand the role of cubic correlations, starting from the statics.

Cubic correlations seem to play a role in proving the **Lee-Huang-Yang second order correction** to the ground state energy of the bose gas:

$$\lim_{\substack{N \rightarrow \infty \\ \rho = \text{const.}}} \frac{E_N}{N} = 4\pi\rho a \left[1 + \frac{128}{15\pi} (\rho a^3)^{1/2} + \dots \right],$$

see Erdős-Schlein-Yau (2008) and Yau-Yin (2013)

The limiting generator

The limit dynamics $\mathcal{U}_2(t)$ has quadratic generator:

$$\begin{aligned}\mathcal{L}_2(t) = & (i\partial_t T_t^*) T_t + \frac{1}{2} \int dx \nabla_x a_x^* \nabla_x a_x \\ & + \frac{1}{2} \int dx \left(2a_x^* a(-\Delta_x p_x) + a^*(\nabla_x p_x) a(\nabla_x p_x) + a^*(s_x) a(-\Delta_x s_x) \right) \\ & + \int dx \left(a^*(c_x) a^*(-\Delta_x r_x) + a^*(p_x) a^*(-\Delta_x k_x) \right) \\ & + \frac{1}{4} \int dx dy (1 - f_\ell(x - y)) \left(\Delta_{\frac{x+y}{2}} \varphi_t^2((x+y)/2) \right) a_x^* a_y^* \\ & + \frac{3a_0}{\ell^3} \int dx dy \chi(|x - y| \leq \ell) \varphi_t^2((x+y)/2) a_x^* a_y^* \\ & + 4\pi a_0 \int dx \varphi_t^2(x) \left(a^*(c_x) a^*(p_x) + a_x^* a^*(p_x) + 2a^*(c_x) a(s_x) + a(s_x) a(s_x) \right) \\ & + b_0 \int dx |\varphi_t(x)|^2 \left(a^*(c_x) a(c_x) + 2a^*(c_x) a^*(s_x) + a^*(s_x) a(s_x) \right)\end{aligned}$$

with $c(k_t) := \sum_{j=0}^{\infty} \frac{(k_t \bar{k}_t)^n}{2n!} = 1 + p(k_t)$; $s(k_t) := k_t + \sum_{j=1}^{\infty} \frac{(k_t \bar{k}_t)^n k_t}{(2n+1)!} = k_t + r(k_t)$.

Limit dynamics and Bogoliubov transformation

For every $t \in \mathbb{R}$ there exist $u_t, v_t : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ such that

$$\begin{aligned}\mathcal{U}_2^*(t) a(f) \mathcal{U}_2(t) &= a(u_t f) + a^*(v_t f) := b(f) \\ \mathcal{U}_2^*(t) a^*(f) \mathcal{U}_2(t) &= a(v_t f) + a^*(u_t f) := b^*(f)\end{aligned}$$

with $b(f)$ and $b^*(g)$ satisfying canonical commutation relations.

The limit dynamics has three degrees of freedom: (φ_t, u_t, v_t)

If we define $\Theta_t = \begin{pmatrix} u_t & v_t \\ v_t & u_t \end{pmatrix}$ than $i\partial_t \Theta_t = D(t)\Theta_t$ with

$$D(t) = \begin{pmatrix} -\Delta + A_1 & A_2 \\ A_2 & -\Delta + A_1 \end{pmatrix}$$

and A_1 and A_2 operators on $L^2(\mathbb{R}^3)$, whose kernel can be explicitly written.
 $\rightarrow (u_t, v_t)$ are determined by a partial differential equation on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$

Correlation structure

$$\| (e^{-it\mathcal{H}_N^{(\beta)}} W(\sqrt{N}\varphi) T(k_0)\Omega - W(\sqrt{N}\varphi_t) T(k_t)\mathcal{U}_2\Omega) \| \leq C N^{-\gamma} e^{c_1 \exp(c_2|t|)}$$

Remark. The upper bound for the ground state energy of a Bose gas [Dyson 1957, Lieb-Seiringer-Yngvason 2000]

$$e_0(\rho) < 4\pi\rho a_0(1 + O(\rho a_0^3))$$

can be obtained using a trial function of the form

$$\Psi_N(x_1, \dots, x_N) = \prod_{i < j} f_\ell(|x_i - x_j|)$$

where $f_\ell(x)$ is a solution of the scattering equation

$$(-\Delta + \tfrac{1}{2}V)f_\ell(x) = 0 \quad \forall |x| \leq \ell$$

with boundary condition $f_\ell(\ell) = 1$. For the proof to be valid we need

$$\frac{4}{3}\pi\ell^3\rho = 1$$

Correlations affect the GP dynamics

Evolution of $\gamma_{N,t}^{(1)}$:

$$i\partial_t \gamma_{N,t}^{(1)} = [-\Delta, \gamma_{N,t}^{(1)}] + (N-1) \text{Tr}_2[N^2 V(N(x_1 - x_2)), \gamma_{N,t}^{(2)}]$$

In terms of the operator kernels:

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

The ansatz

$$\begin{aligned} \gamma_{N,t}^{(1)}(x_1; x_2) &= \varphi_t(x_1) \overline{\varphi_t(x_2)} \\ \gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x'_2) &= \varphi_t(x_1) \varphi_t(x_2) \overline{\varphi_t(x'_1)} \overline{\varphi_t(x'_2)} \end{aligned}$$

leads to

$$\begin{aligned} i\partial_t \varphi_t(x_1) &= -\Delta \varphi_t(x_1) + \int dx_2 (N-1) N^2 V(N(x_1 - x_2)) |\varphi_t(x_2)|^2 \varphi_t(x_1) \\ &\xrightarrow{N \rightarrow \infty} -\Delta \varphi_t(x_1) + b_0 |\varphi_t(x_1)|^2 \varphi_t(x_1) \end{aligned}$$

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The ansatz

$$\gamma_{N,t}^{(1)}(x_1; x_2) = \varphi_t(x_1) \overline{\varphi_t(x_2)}$$

$$\gamma_{N,t}^{(2)}(x_1, x_2; x'_1, x'_2) = f(N(x_1 - x_2)) f(N(x'_1 - x'_2)) \varphi_t(x_1) \varphi_t(x_2) \overline{\varphi_t(x'_1)} \overline{\varphi_t(x'_2)}$$

leads to

$$\begin{aligned} i\partial_t \varphi_t(x_1) &= -\Delta \varphi_t(x_1) + \int dx_2 (N-1) N^2 V(N(x_1 - x_2)) f(N(x_1 - x_2)) |\varphi_t(x_2)|^2 \varphi_t(x_1) \\ &\xrightarrow{N \rightarrow \infty} -\Delta \varphi_t(x_1) + 8\pi a_0 |\varphi_t(x_1)|^2 \varphi_t(x_1) \end{aligned}$$