Quantum many-body fluctuations around nonlinear Schrödinger dynamics

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N interacting bosons in 3 dimensions

- Hilbert space

$$L^2_s(\mathbb{R}^{3N})$$

- Hamilton operator

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

- Time evolution described by the EXACT N-body Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}$$

Large N: describe the dynamics with an EFFECTIVE evolution equation

N-**body** *linear* Schrödinger equation $\longrightarrow$ **one-body** *non-linear* effective equation

Physical phenomenon: Bose-Einstein condensation

- $N = 10^3 - 10^{10}$
- At very low temperatures: $\psi_N \simeq \varphi^{\otimes N}$ with $\varphi \in L^2(\mathbb{R}^3)$.
- Dynamics:

$$\psi_{N,t} \simeq \varphi_t^{\otimes N}$$

  where φ_t solves the effective Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t .$$

Question: derivation, reliability of the effective equation.

More precisely:

$$H_N = -\sum_{j=1}^{N} \Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} N^{3\beta} V(N^{\beta}(x_i - x_j))$$

- V: repulsive, spherically symmetric interaction potential
- $0 < \beta < 1$: Interpolation between mean field and Gross-Pitaevskii regime.

Dynamics:

- Evolution of the density matrices: establishes the correct effective dynamics
- Study Fluctuations around it: norm approximation of the evolution of the initial state

Previous results on time evolution of density matrices:

- Erdős, Schlein, Yau 2006-2008: if $\langle \psi_N, H_N \psi_N \rangle \leq CN$ and $\gamma_N^{(1)} \to |\varphi\rangle\langle\varphi|$, then

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t|$$

  where φ_t solves

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \qquad \text{for } \beta = 1$$

$$i\partial_t \varphi_t = -\Delta\varphi_t + \left(\int V\right) |\varphi_t|^2 \varphi_t \qquad \text{for } \beta < 1$$

- Spohn 1980; Erdős, Yau 2002; Erdős, Schlein 2008
- Pickl, Knowles 2009; Pickl 2010

With a second quantization method (Ginibre, Velo, Hepp)

- Rodnianski, Schlein 2009; Chen, Lee, Schlein 2011 Mean field regime
- Benedikter, de Oliveira, Schlein 2012 Gross-Pitaevskii regime

Hamiltonian

$$\mathcal{H}_N = \int dx \, \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int dx dy N^{3\beta} V(N^\beta(x-y)) a_x^* a_y^* a_y a_x = \mathcal{K} + \mathcal{V}_N$$

extended to Fock space

$$\mathcal{F} = \bigoplus_{n \geq 0} L_s^2(\mathbb{R}^{3n}, dx_1 \dots dx_n)$$

a_x, a_x^* satisfy CCR

$$[a_x, a_y^*] = \delta(x-y), \qquad [a_x, a_y] = [a_x^*, a_y^*] = 0 \, .$$

Advantage of working in the Fock space → implement a certain structure on the initial data

To describe CORRELATIONS between particles, we consider the scattering equation.

Define $f_{N,\ell}$ as the solution of the eigenvalue problem on the ball of radius ℓ:

$$\left[-\Delta + \frac{1}{2N} N^{3\beta} V(N^\beta x)\right] f_{N,\ell} = \lambda_{N,\ell} f_{N,\ell}$$

associated with the smallest eigenvalue $\lambda_{N,\ell}$, with b.c.:

- $f_{N,\ell} = 1$ for $|x| = \ell$ (normalized)
- $\partial_r f_{N,\ell} = 0$ for $|x| = \ell$

$f_{N,\ell}$ continued to $\mathbb{R}^3$: $f_{N,\ell} = 1$ for all $|x| \geq \ell$
(Neumann problem associated with the potential $V^{3\beta-1} V(N^\beta \cdot)$ on the ball of radius ℓ centered around the origin)

- For $0 < \beta < 1$ the many body evolution developes weaker correlations than in the GP regime
  $\longrightarrow$ many body evolution approximated by the NLS, as $N \to \infty$

$$i\partial_t \varphi_t = -\Delta \varphi_t + \left(\int V \right) |\varphi_t|^2 \varphi_t \tag{1}$$

- Two body correlations are anyway relevant in the analysis of fluctuations
  $\longrightarrow$ substitute the NLS with a more precise one

$$i\partial \varphi_t^N = -\Delta \varphi_t^N + (N^{3\beta} V(N^{\beta} .) f_{N,\ell} * |\varphi_t^N|^2) \varphi_t^N \, . \tag{2}$$

In the limit $N \to \infty$, the solution of (2) approaches the solution of (1).

We apply

- Weyl operator $W(\sqrt{N}\varphi) = \exp\left(a^*(\sqrt{N}\varphi) - a(\sqrt{N}\varphi)\right)$
  to obtain a **coherent state** (condensate)
- Bogoliubov transformation $T_{N,t} = \exp\left[\frac{1}{2}\int dxdy \left(k_{N,t}(x,y)a_x^* a_y^* - \text{h.c.}\right)\right]$
  to implement the **two body correlations**

$$\text{kernel:} \qquad k_{N,t}(x,y) = -N(1 - f_{N,\ell}(x-y))\left(\varphi_t^N((x+y)/2)\right)^2$$

Initial data

$$W(\sqrt{N}\varphi)T_{N,0}\xi_N$$

$\longrightarrow$ It has approximately N particles and the effective evolution equation is (2).

Time evolution

$$e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T_{N,0}\xi_N$$

Ansatz: the modified coherent state structure is preserved by the dynamics

Fluctuation dynamics

$$\mathcal{U}_N(t,0) = T^*_{N,t} W^*(\sqrt{N}\varphi_t^N) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T_{N,0}$$

satisfying

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

Goal: Analyse fluctuations around the modified NLS.

- Prove that the fluctuations dynamics has a QUADRATIC GENERATOR IN THE LIMIT $N \to \infty$: approximate $\mathcal{U}_N$ by an evolution $\mathcal{U}_{2,N}$ with a quadratic generator $\mathcal{L}_{2,N}(t)$

$$i\partial_t \mathcal{U}_{2,N}(t;s) = \mathcal{L}_{2,N}(t)\mathcal{U}_{2,N}(t;s) \tag{3}$$

- Use the quadratic fluctuation dynamics to obtain an APPROXIMATION IN NORM of the exact many-body evolution

On fluctuations in mean field regime ($\beta = 0$):

- Hepp 1974; Ginibre, Velo 1979
- Grillakis, Machedon, Margetis 2010, 2011
- Chen 2012
- Lewin, Nam, Serfaty, Solovej 2012
- Ben Arous, Kirkpatrick, Schlein 2013
- Buchholz, Saffirio, Schlein 2014
- Lewin, Nam, Schlein 2014

For $\beta > 0$

- Nam, Napiórkowski 2015: $0 < \beta < 1/3$, with fixed number of particle state
- Kuz 2015: $0 < \beta < 1/2$ second quantization
- Grillakis, Machedon, Margetis 2013, 2015: $0 < \beta < 2/3$ second quantization

Theorem

Let $V \geq 0$ be smooth and compactly supported. Fix $0 < \beta < 1$ and $\ell > 0$. Consider $\xi_N \in \mathcal{F}$ such that

$$\|\xi_N\| = 1 \quad \text{and} \quad \langle \xi_N, \left[\mathcal{N}^2 + \mathcal{K}^2 + \mathcal{V}_N\right] \xi_N \rangle \leq C \quad \text{uniformly in } N.$$

Then there are $C, c_1, c_2 > 0$ such that, for $\alpha = \min(\beta/2, (1-\beta)/2)$,

$$\left\| e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\, T_{N,0}\, \xi_N - e^{-i\int_0^t \eta_N(s)ds}\, W(\sqrt{N}\varphi_t^N)\, T_{N,t}\, \mathcal{U}_{2,N}(t) \xi_N \right\|^2 \leq C N^{-\alpha} \exp(c_1 \exp(c_2|t|))$$

for all $t \in \mathbb{R}$ and all N large enough.

Under the same hypothesis of the theorem:

Proposition

Let $\mathcal{U}_N$ be the fluctuation dynamics, and $\mathcal{U}_{2,N}$ be the quadratic approximating evolution. Then there exist $C, c_1, c_2 > 0$ such that

$$\left\| \mathcal{U}_N(t;0)\xi_N - e^{-i\int_0^t \eta_N(s)ds}\,\mathcal{U}_{2,N}(t;0)\xi_N \right\|^2 \leq CN^{-\alpha}\exp(c_1\exp(c_2|t|))$$

for all $t \in \mathbb{R}$ and all N large enough.

The theorem is shown if we prove the proposition.

- Full generator of $\mathcal{U}_N(t;0)$:

$$\mathcal{L}_N(t) = \eta_N(t) + \mathcal{L}_{2,N}(t) + \mathcal{V}_N + \mathcal{E}_N(t)$$

  $\mathcal{E}_N(t)$ consists of linear, cubic and quartic terms that are "small".

- The generator of $\mathcal{U}_{2,N}$ is quadratic; it represents the **main part** of the evolution.

$$\begin{aligned}
\mathcal{L}_{2,N}(t) &= (i\partial_t T^*_{N,t})T_{N,t} + \mathcal{L}^{(K)}_{2,N}(t) + \mathcal{L}^{(V)}_{2,N}(t) \\
&\quad + \frac{N}{2}\int dxdy\, \omega_{N,\ell}(x-y) \\
&\qquad \times \Big[\big(\varphi^N_t((x+y)/2)\Delta\varphi^N_t((x+y)/2) + |\nabla\varphi^N_t((x+y)/2)|^2\big)a^*_x a^*_y + \text{h.c.}\Big] \\
&\quad + N\lambda_{\ell,N}\int dxdy\, \mathbf{1}(|x-y|\le \ell)\Big[\big(\varphi^N_t((x+y)/2)\big)^2 a^*_x a^*_y + \text{h.c.}\Big]
\end{aligned}$$

Why a quadratic generator? The approximating dynamics acts on the creation and annihilation operator as a Bogoliubov transformation.

Proof

Step 1: We write

$$\frac{d}{dt}\left\|\mathcal{U}_N(t;0)\xi_N - e^{-i\int_0^t \eta_N(s)ds}\,\mathcal{U}_{2,N}(t;0)\xi_N\right\|^2$$

$$= 2\mathrm{Im}\,\Big\langle \mathcal{U}_N(t,0)\xi_N, \underbrace{(\mathcal{L}_N(t) - \mathcal{L}_{2,N}(t) - \eta_N(t))}_{\mathcal{V}_N+\mathcal{E}_N(t)}\, e^{-i\int_0^t \eta_N(s)ds}\,\mathcal{U}_{2,N}(t;0)\xi_N\Big\rangle$$

Step 2: We estimate

$$|\langle \mathcal{U}_N(t,0)\xi_N, (\mathcal{V}_N + \mathcal{E}_N(t))\,\mathcal{U}_{2,N}(t;0)\xi_N\rangle|$$

$$\leq CN^{-\alpha}e^{K|t|}\Big[\langle \mathcal{U}_N(t;0)\xi_N, (\mathcal{K} + \mathcal{V}_N + \mathcal{N} + 1)\mathcal{U}_N(t;0)\xi_N\rangle$$

$$+ \langle \mathcal{U}_{2,N}(t;0)\xi_N, (\mathcal{K}^2 + \mathcal{N}^2 + 1)\mathcal{U}_{2,N}(t;0)\xi_N\rangle\Big]$$

Step 3: Control expectation values by Gronwall estimates (technical)

Further observations

- Our coherent state modified with a Bogoliubov transformation does not allow us to find an approximation evolving in time with a quadratic generator for $\beta = 1$. Different types of CORRELATIONS are necessary.
- About the GROUND STATE ENERGY: how to construct the correct correlation structure in order to approximate the ground state?

Remark

- It is possible to define a quadratic fluctuation dynamics $\mathcal{U}_{2,\infty}(t)$ independent on N, satisfying
$$i\partial_t \mathcal{U}_{2,\infty}(t;s) = \mathcal{L}_{2,\infty}(t)\mathcal{U}_{2,\infty}(t;s)$$
and to prove
$$\left\| e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T_{N,0}\xi_N - e^{-i\int_0^t \eta_N(s)ds} W(\sqrt{N}\varphi_t^N) T_{N,t}\,\mathcal{U}_{2,\infty}(t)\xi_N \right\|^2 \le CN^{-\alpha} \exp(c_1 \exp(c_2|t|))$$

On the GROUND STATE:

- Lieb, Seiringer, Yngvason 2000: for $\beta = 1$, as $N \to \infty$,
  $\frac{E_N}{N} \longrightarrow \min_{\varphi \in L^2(\mathbb{R}^3), ||\varphi||=1} \mathcal{E}_{GP}$, where

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

  a_0 is the scattering length of V

- Lieb, Seiringer 2002: for $\beta = 1$, as $N \to \infty$,

$$\gamma_N^{(1)} = \mathrm{Tr}_{2,\dots,N} |\Psi_N\rangle\langle\Psi_N| \to |\varphi_{GP}\rangle\langle\varphi_{GP}|$$

  where Ψ_N is the ground state and φ_{GP} is the minimizer of $\mathcal{E}_{GP}$

- Lewin, Nam, Serfaty, Solovej 2012: $\beta = 0$, energy spectrum
- Erdős, Schlein, Yau 2008: second order correction to the energy, soft potential
- Lewin, Nam, Rougerie 2015: Nonlinear Schrödinger energy functional

Between mean-field and Gross-Pitaevskii regime

$\beta = 1/3$: threshold between mean-field behaviour and GP

$$\frac{1}{N}\sum_{i<j}^{N} N^{3\beta} V(N^{\beta}(x_i - x_j))$$

- Particles interact when they are at a distance of the order $N^{-\beta}$ (Range of the potential)
- In a box of size 1, the mean interparticle distance is $N^{-1/3}$
- $\beta < 1/3$: mean-field behaviour prevails
- When $\beta > 1/3$ the interaction gets more singular

$\beta = 1$: Rare but strong collisions

- Probability of a collision: $N \cdot N^{-3\beta} = N^{-3\beta+1}$
- Intensity of the interaction: $N^{3\beta-1}$

Reduced density matrices

Density matrix

$$\gamma_N = |\psi_N\rangle\langle\psi_N|$$

k-particle marginal density associated with ψ_N: partial trace over $N-k$ particles

$$\gamma^{(k)}_{N,t} = \mathrm{Tr}_{k+1,\dots,N}\gamma_{N,t}$$

The expectation value of k-particle observable A can be computed using only $\gamma^{(k)}_{N,t}$

$$\langle\psi_{N,t}|(A_{[1,\dots,k]}\otimes 1^{(N-k)})|\psi_{N,t}\rangle = \mathrm{Tr}\,\gamma^{(k)}_{N,t}A_{[1,\dots,k]}$$

Convergence towards the effective dynamics:

$$\gamma^{(k)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \tag{4}$$

in the trace norm topology

$$\mathrm{Tr}\,|\gamma^{(k)}_{N,t} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k}| \longrightarrow 0 \qquad \text{as} \qquad N\to\infty \tag{5}$$

Properties of the Weyl operator

$$W(\varphi)^* a(f) W(\varphi) = a(f) + \langle f, \varphi \rangle$$

and

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

Properties of the Bogoliubov transformation

$$T^*_{N,t} a(f) T_{N,t} = a(\cosh_{k_{N,t}} f) + a^*(\sinh_{k_{N,t}} \overline{f})$$
$$T^*_{N,t} a^*(f) T_{N,t} = a^*(\cosh_{k_{N,t}} f) + a(\sinh_{k_{N,t}} \overline{f})$$

Generator $\mathcal{L}_{2,N}$

$$\mathcal{L}_{2,N}(t) = (i\partial_t T^*_{N,t})T_{N,t} + \mathcal{L}^{(K)}_{2,N}(t) + \mathcal{L}^{(V)}_{2,N}(t) \tag{6}$$

$$+ \frac{N}{2}\int dxdy\, \omega_{N,\ell}(x-y) \tag{7}$$

$$\times \left[(\varphi^N_t((x+y)/2)\Delta\varphi^N_t((x+y)/2) + |\nabla\varphi^N_t((x+y)/2)|^2)a^*_x a^*_y + \text{h.c.}\right] \tag{8}$$

$$+ N\lambda_{\ell,N}\int dxdy\, \mathbf{1}(|x-y|\le \ell)\left[(\varphi^N_t((x+y)/2))^2 a^*_x a^*_y + \text{h.c.}\right] \tag{9}$$

$$\begin{aligned}\eta_N(t) = \; & N \int dxdy N^{3\beta} V(N^\beta(x-y))(1/2 - f_{N,\ell}(x-y))|\varphi_t^N(x)|^2|\varphi_t^N(y)|^2 \\ & + \int dxdy |\nabla_x \sinh_{k_{N,t}}(x,y)|^2 + \int dx (N^{3\beta} V(N^\beta .) * |\varphi_t^N|^2)(x) \langle s_x^N, s_x^N \rangle \\ & + \int dxdy N^{3\beta} V(N^\beta(x-y)) \varphi_t^N(x) \bar{\varphi}_t^N(y) \langle s_x^N, s_y^N \rangle \\ & + \mathrm{Re} \int dxdy \, N^{3\beta} V(N^\beta(x-y)) \varphi_t^N(x) \varphi_t^N(y) \langle s_x^N, c_y^N \rangle \\ & + \frac{1}{2N} \int dxdy N^{3\beta} V(N^\beta(x-y)) \Big[|\langle s_x^N, c_y^N \rangle|^2 + |\langle s_x^N, s_y^N \rangle|^2 + \langle s_y^N, s_y^N \rangle \langle s_x^N, s_x^N \rangle \Big] \end{aligned} \tag{10}$$

$$
\begin{aligned}
\mathcal{L}_{2,N}^{(V)}(t) = & \int dx \, (N^{3\beta} V(N^{\beta}.) * |\varphi_t^N|^2)(x) \\
& \qquad \times \left[a^*(c_x^N) a(c_x^N) + a^*(s_x^N) a(s_x^N) + a^*(c_x^N) a^*(s_x^N) + a(s_x^N) a(c_x^N) \right] \\
& + \int dx dy N^{3\beta} V(N^{\beta}(x-y)) \varphi_t^N(x) \bar{\varphi}_t^N(y) \\
& \qquad \times \left[a^*(c_x^N) a(c_y^N) + a^*(s_y^N) a(s_x^N) + a^*(c_x^N) a^*(s_y^N) + a(s_x^N) a(c_y^N) \right] \\
& + \frac{1}{2} \int dx dy N^{3\beta} V(N^{\beta}(x-y)) \varphi_t^N(x) \varphi_t^N(y) \\
& \qquad \times \left[a^*(c_x^N) a(s_y^N) + a^*(c_y^N) a(s_x^N) + a(s_x^N) a(s_y^N) \right] \\
& + \frac{1}{2} \int dx dy N^{3\beta} V(N^{\beta}(x-y)) \bar{\varphi}_t^N(x) \bar{\varphi}_t^N(y) \\
& \qquad \times \left[a^*(s_y^N) a(c_x^N) + a^*(s_x^N) a(c_y^N) + a^*(s_x^N) a^*(s_y^N) \right] \\
& + \frac{1}{2} \int dx dy N^{3\beta} V(N^{\beta}(x-y)) \varphi_t^N(x) \varphi_t^N(y) \left[a^*(p_x^N) a_y^* + a^*(c_x^N) a^*(p_y^N) \right] \\
& + \frac{1}{2} \int dx dy N^{3\beta} V(N^{\beta}(x-y)) \bar{\varphi}_t^N(x) \bar{\varphi}_t^N(y) \left[a(p_x^N) a_y + a(c_x^N) a(p_y^N) \right]
\end{aligned}
\tag{11}
$$

$$
\begin{aligned}
\mathcal{L}^{(K)}_{2,N}(t) = & \int dx \nabla_x a^*_x \nabla_x a_x \\
& + \int dx \Big[a^*_x a(-\Delta_x p^N_x) + a^*(-\Delta_x p^N_x) a_x + a^*(\nabla_x p^N_x) a(\nabla_x p^N_x) \\
& \quad + \nabla_x a^*(k_x) \nabla_x a(k_x) + a^*(-\Delta_x r^N_x) a(k_x) + a^*(s^N_x) a(-\Delta_x r^N_x) \\
& \quad + a^*(-\Delta_x p^N_x) a^*(k_x) + a(k_x) a(-\Delta p^N_x) + a^*_x a^*(-\Delta_x r^N_x) \\
& \quad + a(-\Delta_x r^N_x) a_x + a^*(p^N_x) a^*(-\Delta_x r^N_x) + a(-\Delta_x r^N_x) a(p^N_x) \Big]
\end{aligned}
\tag{12}
$$

Step 2:

- For $|\langle \mathcal{U}_N(t,0)\xi_N, \mathcal{V}_N \mathcal{U}_{2,N}(t;0)\xi_N\rangle|$ we use the estimate

$$\langle \mathcal{U}_N(t,0)\xi_N, \mathcal{V}_N \mathcal{U}_{2,N}(t;0)\xi_N\rangle \leq \frac{C}{N^{1/2}} \langle \mathcal{U}_N(t,0)\xi_N, \mathcal{V}_N \mathcal{U}_N(t;0)\xi_N\rangle^{1/2} \times \left(\int dxdy N^{3\beta} V(N^\beta(x-y)) \langle \mathcal{U}_N(t,0)\xi_N, a_x^* a_y^* a_x a_y \mathcal{U}_N(t;0)\xi_N\rangle\right)^{1/2}$$

  together with

$$\int dxdy N^{3\beta} V(N^\beta(x-y)) \|a_x a_y \psi\|^2 \leq C \int dxdy \|\nabla_x a_x \nabla_y a_y \psi\|^2 + C \int dxdy \|\nabla_x a_x a_y \psi\|^2$$

- With similar methods

$$|\langle \psi_1, \mathcal{E}_N(t)\psi_2\rangle| \leq CN^{-\alpha} e^{K|t|} \left[\langle \psi_1, (\mathcal{K} + \mathcal{N} + 1)\psi_1\rangle + \langle \psi_2, (\mathcal{K}^2 + (\mathcal{N}+1)^2)\psi_2\rangle\right]$$

Remark: Only the estimate for $\langle \mathcal{U}_N(t;0)\xi_N, (\mathcal{K} + \mathcal{V}_N + \mathcal{N} + 1)\mathcal{U}_N(t;0)\xi_N\rangle$ is not enough for the fluctuation dynamics

Step 3: We use now the Gronwall estimates

$$\langle \mathcal{U}_N(t;0)\psi, \mathcal{N}\mathcal{U}_N(t;0)\psi\rangle \leq C\exp(c_1\exp(c_2|t|))\langle\psi, \left(\mathcal{N}+\mathcal{N}^2/N+\mathcal{H}_N\right)\psi\rangle$$

$$|\langle \mathcal{U}_N(t;0)\psi, (\mathcal{L}_N(t)-\eta_N(t))\mathcal{U}_N(t;0)\psi\rangle| \leq C\exp(c_1\exp(c_2|t|))\langle\psi, \left(\mathcal{N}+\mathcal{N}^2/N+\mathcal{H}_N\right)\psi\rangle$$

and

$$\langle \mathcal{U}_{2,N}(t;0)\psi, \mathcal{N}\mathcal{U}_{2,N}(t;0)\psi\rangle \leq C\exp(c_1\exp(c_2|t|))\langle\psi,(\mathcal{N}+1)\psi\rangle$$

$$\langle \mathcal{U}_{2,N}(t;0)\psi, \mathcal{N}^2\mathcal{U}_{2,N}(t;0)\psi\rangle \leq C\exp(c_1\exp(c_2|t|))\langle\psi,(\mathcal{N}+1)^2\psi\rangle$$

$$\langle \mathcal{U}_{2,N}(t;0)\psi, \mathcal{L}^2_{2,N}(t)\mathcal{U}_{2,N}(t;0)\psi\rangle \leq C\exp(c_1\exp(c_2|t|))\langle\psi,(\mathcal{K}+\mathcal{N}+1)^2\psi\rangle$$

We obtain

$$\frac{d}{dt}\left\|\mathcal{U}_N(t;0)\xi_N - e^{-i\int_0^t \eta_N(s)ds}\,\mathcal{U}_{2,N}(t;0)\xi_N\right\|^2$$
$$\leq C\exp(c_1\exp(c_2|t|))N^{-\alpha}\langle\xi_N, (\mathcal{N}^2+\mathcal{K}^2+\mathcal{V}_N)\xi_N\rangle$$

Integrating over time, we obtain

$$\left\|\mathcal{U}_N(t;0)\xi_N - e^{-i\int_0^t \eta_N(s)ds}\,\mathcal{U}_{2,N}(t;0)\xi_N\right\|^2 \leq CN^{-\alpha}\exp(c_1\exp(c_2|t|))$$

To get the norm approximation:

$$\begin{aligned}
&\left\| e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T_{N,0}\xi_N - e^{-i\int_0^t \eta_N(s)ds} W(\sqrt{N}\varphi_t^N) T_{N,t}\mathcal{U}_{2,N}(t;0)\xi_N \right\|^2 \\
&= \left\| W(\sqrt{N}\varphi_t^N) T_{N,t} \left[\mathcal{U}_N(t;0) - e^{-i\int_0^t \eta_N(s)ds} \mathcal{U}_{2,N}(t;0) \right] \xi_N \right\|^2 \\
&= \left\| \left[\mathcal{U}_N(t;0) - e^{-i\int_0^t \eta_N(s)ds} \mathcal{U}_{2,N}(t;0) \right] \xi_N \right\|^2 \leq C N^{-\alpha} \exp(c_1 \exp(c_2 |t|))
\end{aligned}$$

Let V be smooth, positive, spherically symmetric and compactly supported with $b_0 = \int V dx$. Let $f_{N,\ell}$ be the ground state of the Neumann problem

$$\left(-\Delta + \frac{1}{2} N^{3\beta-1} V(N^\beta \cdot)\right) f_{N,\ell} = \lambda_{N,\ell} f_{N,\ell} \tag{13}$$

on the sphere of radius ℓ, with the boundary conditions

$$f_{N,\ell}(x) = 1 \qquad \partial_r f_{N,\ell}(x) = 0$$

for all $x \in \mathbb{R}^3$ with $|x| = \ell$. For N sufficiently large (such that $RN^{-\beta} < \ell$) we have:

I)

$$\left| \lambda_{N,\ell} - \frac{3b_0}{8\pi N \ell^3} \right| \leq \frac{C}{N^{2-\beta}} \tag{14}$$

II) There is a constant $0 < c_0 < 1$ such that, for all $|x| \leq \ell$,

$$c_0 \leq f_{N,\ell}(x) \leq 1 \tag{15}$$

III) Let $\omega_{N,\ell} = 1 - f_{N,\ell}$. There exists a constant $C > 0$ such that, for all $|x| \leq \ell$,

$$\omega_{N,\ell}(x) \leq \frac{C}{N(|x| + N^{-\beta})} \qquad |\nabla \omega_{N,\ell}(x)| \leq \frac{C}{N(|x|^2 + N^{-2\beta})} \tag{16}$$

Proposition (Propagation of regularity for the NLS and modified NLS)

Let V be non-negative, smooth and spherically symetric. Let $\varphi \in H^1(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$.

I) *There exist unique global solutions $\varphi_.^N$ and $\varphi_.$ in $C(\mathbb{R}; H^1(\mathbb{R}^3))$ of (MGP) and, respectively, of (GP) with initial data φ. The solutions are such that $\|\varphi_t\|_2 = \|\varphi_t^N\|_2 = \|\varphi\|_2 = 1$ and*

$$\|\varphi_t\|_{H^1}, \|\varphi_t^N\|_{H^1} \leq C$$

for a constant $C > 0$ and all $t \in \mathbb{R}$.

II) *Under the additional assumption that $\varphi \in H^n(\mathbb{R}^3)$, for an integer $n \in \mathbb{N}$, then $\varphi_t, \varphi_t^N \in H^n(\mathbb{R}^3)$ for all $t \in \mathbb{R}$ and there exist constants $C > 0$ (depending on $\|\varphi\|_{H^n}$ and on n) and $K > 0$ (depending only on $\|\varphi\|_{H^1}$ and on n) such that*

$$\|\varphi_t\|_{H^n}, \|\varphi_t^N\|_{H^n} \leq Ce^{K|t|}$$

for all $t \in \mathbb{R}$.

III) *Let $\varphi \in H^4(\mathbb{R}^3)$. Then there exists $C > 0$ (depending on $\|\varphi\|_{H^4}$) and $K > 0$ (depending only on $\|\varphi\|_{H^1}$) such that*

$$\|\dot{\varphi}_t\|_{H^2}, \|\ddot{\varphi}_t\|_2 \leq Ce^{K|t|}$$

Proposition (Convergence of the NLS to the modified NLS)

Under the same hypothesis as before:

i) *Let* $\varphi \in H^2(\mathbb{R}^3)$*. Then there exist constants* $C, c_1 > 0$ *(depending on* $\|\varphi\|_{H^2}$*) and* $c_2 > 0$ *(depending only on* $\|\varphi\|_{H^1}$*) such that*

$$\|\varphi_t - \varphi_t^N\|_2 \leq CN^{-\gamma} \exp(c_1 \exp(c_2|t|)) \qquad \textit{with } \gamma = \min(\beta, 1-\beta).$$

ii) *Let* $\varphi \in H^4(\mathbb{R}^3)$*. Then there exist constants* $C, c_1 > 0$ *(depending on* $\|\varphi\|_{H^4}$*) and* $c_2 > 0$ *(depending only on* $\|\varphi\|_{H^1}$*) such that*

$$\|\varphi_t - \varphi_t^N\|_{H^2}, \|\dot{\varphi}_t - \dot{\varphi}^N{}_t\|_2 \leq CN^{-\gamma} \exp(c_1 \exp(c_2|t|)) \qquad \textit{with } \gamma = \min(\beta, 1-\beta)$$