Derivation of the NLS

Consider an interacting Bose gas with the interaction V_N^β with the Hamiltonian

$$H = \sum_{j=1}^{N} -\Delta_j + \sum_{j \neq k} V_N^\beta (x_j - x_k)$$

→ β stands for the scaling behavior of the interaction.

→ V_N^β scaled in N in such a way that the interaction energy per particle is of order 1.

We treat interaction taking the form $V_N^\beta(x) = N^{-1+3\beta} V(N^\beta x)$:

$$H = \sum_{j=1}^{N} -\Delta_j + \sum_{j \neq k} N^{-1+3\beta} V(N^\beta (x_j - x_k))$$

→ By heuristic arguments, one expect to arrive at the effective equation (Hartree equation) with some potential V_N s.t.

$$i \frac{d}{dt} \varphi_t = (-\Delta + V_N * |\varphi_t|^2) \varphi_t$$

→ the potential V_N converges to δ as $N \to \infty$. The effective equation can be approximated by

$$i \frac{d}{dt} \varphi_t = (-\Delta + a |\varphi_t|^2) \varphi_t$$

$a = \int_{\mathbb{R}^3} V(x)\, dx^3$ is a number. We call the above equation a Non-Linear Schrödinger equation.

→ For $\beta = 1$, the system develops correlations that cannot be neglected (Leading-order effects). Thus, the behavior of the gas is not given by the above NLS. But modifying the above a to take into account this correlation would lead to the right description.

→ today, we pick a range of β such that the use of counting measure still helps and the effective description still holds.

→ To close Grönwall argument: we assume that $\exists\ L^\infty$ solution φ_t of NLS on a finite interval $[0,T]$.

For attractive potential ($V < 0$): we might have Blow-up of the solutions. And thus the proof must also fail. When the NLS blows up, then there must be discrepancy between the microscopic and the effective description of the gas.

Instability of the NLS

One can show that the Ground state of the NLS is not bounded from below.
→ Not rigorous proof of existence of Blow-up solutions but a strong hint on it.

Corollary

Let V be attractive in the sense that $V(x) < -c$ for some $c > 0$ and for all x in $B(0,R)$ (ball of radius R and center 0):

(a) For the Hamiltonian:

$$H = \sum_{j=1}^{N} -\Delta_j + \sum_{j \neq k} N^{-1+3\beta} V(N^{\beta}(x_j - x_k))$$

the energy is not bounded from below by an N- independent constant, i.e. there exists some sequence Ψ_N s.t.

$$\lim_{N \to \infty} \langle \Psi_N, H \Psi_N \rangle = -\infty$$

(b) $a < 0$. The NLS - energy functional given by

$$\mathcal{E}(\varphi) = \|\nabla \varphi\|_2^2 + \frac{a}{2} \|\varphi\|_4^4$$

is not bounded from below, i.e. there is a sequence φ_k s.t.

$$\lim_{k \to \infty} \mathcal{E}(\varphi_k) = -\infty$$

Rk : The term $\frac{1}{2}$ in the energy functional can be explained using variational principle: Varying the φ^4-term one gets the factor 4 from the derivative instead of 2.

$$\mathcal{E}(\varphi) \equiv \mathcal{E}(\varphi, \bar{\varphi}) = \|\nabla \varphi\|_2^2 + \frac{a}{2} \|\varphi\|_4^4$$

$$i \frac{d}{dt} \varphi = \frac{\partial \mathcal{E}}{\partial \bar{\varphi}}$$

Compute the variation : $\varphi \longmapsto \varphi + \varepsilon h$

$$\mathcal{E}(\varphi + \varepsilon h) = \mathcal{E}(\varphi) + \varepsilon \,\partial \mathcal{E}(\varphi) h + O(\varepsilon^2)$$

$$\partial \mathcal{E}(\varphi) h = 4 \frac{a}{2} \int |\varphi|^2 \operatorname{Re}(\varphi \bar{h})\, dx$$

$$\frac{\partial \mathcal{E}(\varphi)}{\partial \bar{\varphi}} = a |\varphi|^2 \varphi .$$

Proof :

(a) We will construct a trial state Ψ_N which collapse more and more particles in a region of $N^{-\beta}$.

Let φ to be a nice function: it is supported on a Ball of size $\frac{R}{2}$ and it has a Bounded kinetic energy E^{kin}.

Define $\Psi_N = C_N \prod_{j=1}^{N} \varphi(N^\beta x_j)$, C_N is the normalization.

The kinetic energy per particle $= N^{2\beta} E^{kin}$

The total kinetic energy is $\sim N \cdot N^{2\beta} E^{kin} = N^{1+2\beta} E^{kin}$.

The potential energy is bounded above by $-c\, N^2 \cdot N^{-1+3\beta} = -c N^{1+3\beta}$

The total energy of the state is

$$\langle \Psi_N, H \Psi_N \rangle \leq N^{1+2\beta} E^{kin} - c N^{1+3\beta}$$

Thus $$\langle \Psi_N, H\Psi_N \rangle \xrightarrow[N \to +\infty]{} -\infty$$

(b) Let $\varphi_k(x) = c_k \varphi(kx)$ with c_k is the normalization.

For Large k, this normalization c_k behaves like $c_k \sim k^{\frac{3}{2}}$

Then the kinetic energy $\|\nabla \varphi_k\|_2^2 \sim k^2$.

The potential energy

$$\frac{a}{2} \|\varphi_k\|_4^4 = \frac{a}{2} c_k^4 \int |\varphi(kx)|^4 d^3x = \frac{a}{2} c_k^2 \underbrace{c_k^2 \int |\varphi(kx)|^4 dx} = \frac{a}{2} c_k^2$$

This implies that the potential energy converges faster than the kinetic energy. And the potential energy is negative, this implies

$$\mathcal{E}(\varphi_k) \xrightarrow[|k| \to +\infty]{} -\infty \qquad \square$$

<u>RK</u> It can happen that V is negative at the origin ((a) occurs) but the integral is positive. So, it is possible that the effective description has an energy bounded from below, while the microscopic does not!

Derivation of the NLS:

<u>Thm</u> Assume that $V \in L^\infty \cap L^1$. let $\beta < \frac{1}{6}$, and assume that there is T such that the solution φ_t of the Hartree equation

$$i \frac{d\varphi}{dt} = (-\Delta + V_N * |\varphi_t|^2)\varphi_t$$

with $V_N = N^{3\beta} V(N^\beta x)$, has an L^∞ bound in the interval $[0,T]$

(so, $\exists\, 0 < C < +\infty$ such that $\|\varphi_t\|_\infty < C$ for all $t \in [0,T]$)

Then $\|\gamma_t^{\psi} - |\varphi_t\rangle\langle\varphi_t|\|_{tr} \xrightarrow[N\to+\infty]{} 0$

→ Instead of proving convergence in trace norm directly, we prove that the respective counting measure α goes to zero.

We will use the weight function to define our counting measure α

$$w(k) = \begin{cases} \frac{k}{N^\lambda} & \text{if } k \le N^\lambda \\ 1 & \text{otherwise} \end{cases}$$

λ will be chosen at the end to get good estimates.

The counting measure here $\alpha = \langle \psi_N, \hat{w}\, \psi_N \rangle$

$$\hat{w} = \sum_{k=0}^{N} w(k)\, P^{\varphi}_{N,k} \qquad P_{N,k} = (q^\varphi_1 \dots q^\varphi_k\, p^\varphi_{k+1} \dots p^\varphi_N)_{sym}, \qquad p^\varphi_i = |\varphi_t(x_i)\rangle\langle\varphi_t(x_i)|$$

↳ the weight operator

φ_t is a solution of Hartree equation

ψ_N^t is a solution of Many-body Schrödinger equation.

→ The fact that φ_t is approximated by solution of NLS will be considered later.

$$\frac{d\alpha}{dt} = \frac{d}{dt}\langle \psi_N, \hat{w}\, \psi_N \rangle \quad , \quad i\frac{d\hat{w}}{dt} = [H^H, \hat{w}], \quad H^H = \sum_{j=1}^{N} h_j$$

$$h_j = -\Delta_j + V_N * |\varphi_t|^2(x_j)$$

$$= i\langle \psi_N, [H - H^H, \hat{w}]\, \psi_N \rangle$$

$\frac{d\alpha}{dt}$ contains terms of three types

$$\mathrm{I} := N(N-1)\langle \psi, p_1 p_2\, O_{12}\, p_1 q_2\, (\hat{w}_1 - \hat{w})\, \psi \rangle$$

$$\mathrm{II} := N(N-1)\langle \psi, p_1 p_2\, O_{12}\, q_1 q_2\, (\hat{w}_2 - \hat{w})\, \psi \rangle$$

$$\mathrm{III} := N(N-1)\langle \psi, p_1 q_2\, O_{12}\, q_1 q_2\, (\hat{w}_1 - \hat{w})\, \psi \rangle$$

where $O_{12} = V_N(x_1 - x_2) - V_N * |\varphi_t|^2 (x_1) - V_N * |\varphi_t|^2 (x_2)$

$w_1(k) = w(k+1)$

$w_2(k) = w(k+2)$

The term $I \equiv 0$ because

$$P_1 P_2 O_{12} q_1 P_2 = 0 \quad \text{because} \quad P_2 V_N(x_1 - x_2) P_2 = V_N * |\varphi_t|^2 (x_1)$$

$$P_1 P_2 V_N * |\varphi_t|^2 (x_2) q_1 P_2 = 0$$

It remains to estimate the two terms II and III.