# 4. Mean-field Dynamics for Bosons

## 4.1 Hartree Theory

We consider the Hamiltonian $H_N = \sum_{i=1}^{N} (-\Delta_j) + \overbrace{\frac{1}{N-1}}^{\text{coupling constant}} \sum_{\substack{i,j=1 \\ i<j}}^{N} v(x_i - x_j)$ and the associated many-body Schrödinger equation $i \frac{d}{dt} \psi_N(t) = H_N \psi_N(t)$, with $\psi_N(t) \in L^2(\mathbb{R}^{3N})$ and $\psi_N^t(x_1, \dots, x_N) = \psi_N^t(x_{\sigma(1)}, \dots, x_{\sigma(N)})$ $\forall \sigma \in S_N$ ($S_N$ = symmetric group = all permutations of $1, \dots, N$).

$\psi_N$ symmetric (bosons)

The choice of $\frac{1}{N-1}$ as coupling constant is called mean-field limit. It describes weak interaction, and is a simple model of a Bose-Einstein-condensate (BEC).

Well-posedness:

With Kato-Rellich and HW 11, we find that $H_N$ is self-adjoint on $\mathcal{D}(H_N) = H^2(\mathbb{R}^{3N})$ if $v: \mathbb{R}^3 \to \mathbb{R}$ even, and $v = v_1 + v_2$ with $v_1 \in L^2(\mathbb{R}^3)$, $v_2 \in L^\infty(\mathbb{R}^3)$ (we write $v \in L^2 + L^\infty$).

In this section, we aim at studying the dynamics of initial data $\underbrace{\psi_N^{t=0}(x_1, \dots, x_N) = \prod_{i=1}^{N} \varphi^{t=0}(x_i)}_{\text{most simple bosonic state}}$, for some $\varphi^{t=0} \in L^2(\mathbb{R}^3)$.

Such initial data mean that all particles are iid distributed.

We hope to prove that also $\psi_N^t(x_1, \dots, x_N) \approx \prod_{i=1}^{N} \varphi^t(x_i)$ for some $\varphi(t) \in L^2(\mathbb{R}^3)$ in the limit $N \to \infty$.

What equation should hold for $\varphi(t)$?

- Idea: Let $X_i$ be an iid random variable with distribution $|\varphi^t(x)|^2$.

  Then $\frac{1}{N-1}\sum_{i=1}^{N} v(X_i-y)$ should converge to $\int dx\, v(x-y)\,|\varphi^t(x)|^2 = (v * |\varphi^t|^2)(y)$ as $N\to\infty$ according to the law of large numbers.

- Thus we guess: $$i\frac{\partial}{\partial t}\varphi(t,x) = -\Delta\varphi(t,x) + (v*|\varphi(t)|^2)(x)\,\varphi(t,x)$$ $$=: h^{\varphi(t)}\varphi(t,x)$$

  This is called Hartree equation. It is a non-linear PDE, and one example of a non-linear SE (NLS). Thus, our previous well-posedness results for the linear SE do not apply. We come back to the question of well-posedness later.

- But note that formally:

$$\frac{d}{dt}\|\varphi(t)\|_{L^2}^2 = \frac{d}{dt}\langle\varphi(t),\varphi(t)\rangle = \langle\tfrac{d}{dt}\varphi(t),\varphi(t)\rangle + \langle\varphi(t),\tfrac{d}{dt}\varphi(t)\rangle$$

$$= i\langle\left(-\Delta\varphi(t) + (v*|\varphi(t)|^2)\varphi(t)\right),\varphi(t)\rangle - i\langle\varphi(t),\left(-\Delta\varphi(t)+(v*|\varphi(t)|^2)\varphi(t)\right)\rangle$$

assuming $\varphi(t)\in H^2$ and $(v*|\varphi(t)|^2)\varphi(t)\in L^2$

$$= 0 \quad \text{(integration by parts and } v*|\varphi(t)|^2\in\mathbb{R}\text{)},$$

so $\|\varphi(t)\|_{L^2} = \|\varphi(0)\|_{L^2}$ as for the linear SE

Next, let us look at expressions of the type $\langle \Psi_N, A_1 \Psi_N \rangle$ more closely, where $A \in \mathcal{L}_\infty(L^2(\mathbb{R}^3))$, and $A_1$ denotes the action of $A$ on variable $x_1$ only. We call $A_1$ a one-body operator. We want to ask the question: Can we approximate $\langle \Psi_N(t), A_1 \Psi_N(t) \rangle$ by its BEC mean value $\langle \varphi(t), A \varphi(t) \rangle$? E.g., for $A = 1\!\!1_\Lambda$ $(\Lambda \subset \mathbb{R}^3)$, $\langle \Psi_N(t), A_1 \Psi_N(t) \rangle$ is the probability for finding particle one (or any one of the particles by symmetry) in the region $\Lambda \subset \mathbb{R}^3$.

**Definition 4.7.:** For $\Psi_N \in L^2(\mathbb{R}^{3N})$, we define the reduced one-particle density matrix

$$\gamma_{\Psi_N}(x,y) := \int dx_2 \ldots dx_N \, \overline{\Psi_N(y, x_2, \ldots, x_N)} \, \Psi_N(x, x_2, \ldots, x_N).$$

E.g., $\gamma_{\prod_{i=1}^{N} \varphi}(x,y) = \int dx_2 \ldots dx_N \, \overline{\varphi(y)\varphi(x_2)\ldots\varphi(x_N)} \, \varphi(x)\varphi(x_2)\ldots\varphi(x_N) = \overline{\varphi(y)}\,\varphi(x)$.

**Definition 4.8:** For any $K \in \mathcal{S}'(\mathbb{R}^6)$, we define the integral operator

$A: \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}'(\mathbb{R}^3)$, $f(x) \mapsto (Af)(x) := \int dy \, K(x,y) f(y)$. We call $K$ the integral kernel of $A$.

E.g., the identity has integral kernel $K_{1\!\!1}(x,y) = \delta(x-y)$ (since $\int dy \, \delta(x-y) f(y) = f(x)$).

Thus, we can define $\gamma_{\Psi_N}$ as the operator with integral kernel $\gamma_{\Psi_N}(x,y)$.

**Lemma 4.9:** $\gamma_{\Psi_N}$ has the following properties:

(i) $\gamma_{\Psi_N} \in \mathcal{L}_\infty(L^2(\mathbb{R}^3))$, $\|\gamma_{\Psi_N}\|_\infty \leq 1$, $\gamma_{\Psi_N}^* = \gamma_{\Psi_N}$

(ii) $\gamma_{\Psi_N}$ is non-negative, i.e., $\langle \chi, \gamma_{\Psi_N} \chi \rangle \geq 0 \ \forall \chi \in L^2(\mathbb{R}^3)$

Proof of lemma 4.9:

(i) $\left| \int dy\, \gamma_{\psi_N}(x,y)\, \chi(y) \right| = \left| \int dx_2 \dots dx_N \int dy\, \chi(y)\, \overline{\psi_N(y,x_2,\dots,x_N)}\, \psi_N(x,x_2,\dots,x_N) \right|$

$$\leq \int dx_2 \dots dx_N\, dy\, |\psi_N(y,x_2,\dots,x_N)|\, |\chi(y)|\, |\psi_N(x,x_2,\dots,x_N)|$$

Cauchy-Schwarz

$$\leq \left( \int dy\, dx_2 \dots dx_N\, |\psi_N(y,x_2,\dots,x_N)|^2 \right)^{\frac{1}{2}} \left( \int dy\, dx_2 \dots dx_N\, |\chi(y)|^2 |\psi_N(x,x_2,\dots,x_N)|^2 \right)^{\frac{1}{2}}$$

$$= \|\psi_N\|\, \|\chi\| \underbrace{\left( \int dx_2 \dots dx_N\, |\psi_N(x,x_2,\dots,x_N)|^2 \right)^{\frac{1}{2}}}_{\in L^2(\mathbb{R}^3)}$$

$\Rightarrow \|\gamma_{\psi_N} \chi\|_{L^2} \leq \|\chi\|$ $(\|\psi_N\| = 1)$, so $\|\gamma_{\psi_N}\|_{op} \leq 1$.

$\gamma_{\psi_N}^* = \gamma_{\psi_N}$ clear from def.

(ii) $\langle \chi, \gamma_{\psi_N} \chi \rangle = \int dy\, \overline{\psi_N(y,x_2,\dots,x_N)}\, \chi(y) \int dx\, \overline{\chi(x)}\, \psi_N(x,x_2,\dots,x_N) = \langle \psi_N, p_1^{\chi} \psi_N \rangle$

$$= \|p_1^{\chi} \psi_N\|^2 \geq 0 .$$

$\square$

Goal: prove that $\gamma_{\psi_N(t)} \xrightarrow[N\to\infty]{} \gamma_{\Pi\varphi(t)}$.

Note: $\gamma_{\Pi\varphi}(x,y) = \int dx_2 \dots dx_N\, \overline{\varphi(y)\varphi(x_2)\cdots\varphi(x_N)}\, \varphi(x)\varphi(x_2)\cdots\varphi(x_N)$
$= \overline{\varphi(y)}\, \varphi(x)$

But technically it is easier to control a different quantity. We will def. $\alpha(\psi,\varphi)$ s.t. $\alpha \to 0$ implies $\gamma_\psi \to \gamma_{\Pi\varphi}$. The main work will then be to prove that indeed $\alpha \to 0$.

We proceed in several steps:

## Step 1: Type of convergence

**Definition 4.1:**

For $\varphi \in L^2, \|\varphi\|_{L^2}=1$, we define the operator $p^\varphi : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$, $\chi \mapsto \langle \varphi, \chi \rangle \varphi$, and $q^\varphi := \mathbb{1} - p^\varphi$. For any $j = 1, \dots, N$, we define $p_j^\varphi : L^2(\mathbb{R}^{3N}) \to L^2(\mathbb{R}^{3N})$ by
↳ identity on $L^2(\mathbb{R}^3)$

$$(p_j^\varphi \Psi_N)(x_1, \dots, x_N) = \varphi(x_j) \int \overline{\varphi(y)}\, \Psi_N(x_1, \dots, x_{j-1}, y, x_{j+1}, \dots, x_N)\, dy, \text{ and } q_j^\varphi := \mathbb{1} - p_j^\varphi.$$
↳ identity on $L^2(\mathbb{R}^{3N})$

The following properties hold:

**Lemma 4.2:**

For any $\varphi \in L^2$ with $\|\varphi\|_2 = 1$, $j = 1, \dots, N$ we have:

(i) $p_j^\varphi, q_j^\varphi \in \mathcal{L}(L^2(\mathbb{R}^{3N}))$ with $\|p_j^\varphi\|_{\mathcal{L}} = 1 = \|q_j^\varphi\|_{\mathcal{L}}$,

(ii) $p_j^\varphi, q_j^\varphi$ are orthogonal projectors ($P: \mathcal{H} \to \mathcal{H}$ is an orthogonal projector if $P^2 = P = P^*$),

(iii) $p_j^\varphi q_j^\varphi = 0$, $[r_j^\varphi, s_k^\varphi] = 0$ for all $j, k$ and $r, s \in \{p, q\}$.

Proof:

(ii)
$$\begin{aligned}
\langle \chi, p_j^\varphi \Psi \rangle &= \int dx_1 \dots dx_N\, \overline{\chi(x_1, \dots, x_N)}\, \varphi(x_j) \int dy\, \overline{\varphi(y)}\, \Psi(x_1, \dots, y, \dots, x_N) \\
&= \int dx_1 \dots dx_N dy\, \overline{\varphi(y)\, \overline{\varphi(x_j)}\, \chi(x_1, \dots, x_N)}\, \Psi(x_1, \dots, y, \dots, x_N) \\
&= \int dx_1 \dots dy \dots dx_N\, \overline{\varphi(y) \int dx_j\, \overline{\varphi(x_j)}\, \chi(x_1, \dots, x_N)}\, \Psi(x_1, \dots, y, \dots, x_N) \\
&= \langle p_j^\varphi \chi, \Psi \rangle, \quad \text{so} \quad p_j^\varphi = (p_j^\varphi)^*
\end{aligned}$$

and $(p_j^\varphi p_j^\varphi \Psi)(x_1,\dots,x_N) = \varphi(x_j)\int dy\, \overline{\varphi(y)}\, (p_j^\varphi \Psi)(x_1,\dots,y,\dots,x_N)$

$$= \varphi(x_j)\underbrace{\int dy\, \overline{\varphi(y)}\, \varphi(y)}_{=\|\varphi\|_{L^2}^2=1}\int dz\, \overline{\varphi(z)}\, \Psi(x_1,\dots,z,\dots,x_N)$$

$$= (p_j^\varphi \Psi)(x_1,\dots,x_N).$$

Also, $q_j^{\varphi *} = \mathbb{1} - p_j^{\varphi *} = \mathbb{1} - p_j^\varphi = q_j^\varphi$ and $q_j^{\varphi^2} = (\mathbb{1}-p_j^\varphi)(\mathbb{1}-p_j^\varphi) = \mathbb{1} - 2p_j^\varphi + p_j^{\varphi^2} = \mathbb{1} - p_j^\varphi = q_j^\varphi$.

(i) $\|p_j^\varphi \Psi\|_{L^2}^2 = \langle p_j^\varphi \Psi, p_j^\varphi \Psi\rangle = \langle \Psi, p_j^{\varphi^2}\Psi\rangle = \langle \Psi, p_j^\varphi \Psi\rangle \le \|\Psi\|\, \|p_j^\varphi \Psi\|$

$\Rightarrow \|p_j^\varphi \Psi\|_{L^2} \le \|\Psi\|$ , i.e., $\|p_j^\varphi\|_{op} \le 1$

Also: $p_j^\varphi \prod_{i=1}^N \varphi(x_i) = \varphi(x_j)\int dy\, \overline{\varphi(y)}\, \varphi(x_1)\dots\varphi(y)\dots\varphi(x_N) = \prod_{i=1}^N \varphi(x_i)$,

so $\|p_j^\varphi\|_{op} := \sup_{\Psi, \|\Psi\|=1} \|p_j^\varphi \Psi\| \ge \|p_j^\varphi \prod_{i=1}^N \varphi(x_i)\| = \|\prod_{i=1}^N \varphi(x_i)\| = 1.$

Same argument holds for $q_j^\varphi$, with $\varphi$ replaced by any $\varphi^\perp \in \{\varphi\}^\perp$.

(iii) $p_j^\varphi q_j^\varphi = p_j^\varphi(\mathbb{1}-p_j^\varphi) = p_j^\varphi - p_j^{\varphi^2} = p_j^\varphi - p_j^\varphi = 0$, and $r_j s_k = s_k r_j$ clear by def. $\square$

Note: • $p_j^\varphi \Psi_N$ tells us "how much" of the j-th particle is in the state $\varphi$

• $p_j^\varphi \prod_{i=1}^N \varphi(x_i) = \prod_{i=1}^N \varphi(x_i)$, and $q_j^\varphi \prod_{i=1}^N \varphi(x_i) = 0$