4. Mean-field Dynamics for Bosons

4.1 Hartree Theory

We consider the Hamiltonian $H_N = \sum_{i=1}^N (-\Delta_j) + \overbrace{\frac{1}{N}}^{\text{coupling constant}} \sum_{\substack{i,j=1 \\ i<j}}^N v(x_i - x_j)$ 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 $1,\dots,N$).

Ψ_N symmetric (bosons)

The choice of $\frac{1}{N}$ 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 10, 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 $\frac{1}{N}\sum_{i=1}^{N} v(X_i - y)$ 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:

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

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

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

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

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

In order to prove $\Psi_N^t(x_1,\dots,x_N) \approx \prod_{i=1}^N \varphi^t(x_i)$, we proceed in several steps.

Step 1: Type of convergence

Definition 4.1:

For $\varphi \in L^2$, $\|\varphi\|_2 = 1$, 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) $p_j^\varphi, q_j^\varphi \in \mathcal{B}(L^2(\mathbb{R}^{3N}))$ with $\|p_j^\varphi\|_{\mathcal{B}} = 1 = \|q_j^\varphi\|_{\mathcal{B}}$,

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

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

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

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

Same argument holds for q_j^φ, with φ 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 φ

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