Let us summarize the results from last time (+ HW 11):

<u>Theorem 4.12</u>: Derivation of the Hartree equation

Assume v is even and $v \in L^\infty$. Let $\Psi_N(t)$ be the solution to the Schrödinger equation $(*)$ with symmetric initial data $\Psi_N(0) \in H^2(\mathbb{R}^{3N})$. Assume the Hartree equation $(**)$ has a unique solution $\varphi(t)$ given initial data $\varphi(0) \in L^2(\mathbb{R}^3)$. We assume $\varphi(t) \in H^2(\mathbb{R}^3)$, and $\|\Psi_N(0)\| = \|\varphi(0)\| = 1$. Then

$$\alpha(\Psi_N(t), \varphi(t)) \leq e^{Ct} \alpha(\Psi_N(0), \varphi(0)) + (e^{Ct} - 1)\frac{1}{N} \qquad \text{for } C = 10\|v\|_\infty .$$

Note: The assumptions on $\varphi(t)$ can be proven with a Gronwall argument as well, but we skip that here.

4.2 Bogoliubov Theory

Next, we aim at proving a stronger kind of convergence by controlling also fluctuations around the average.

Recall that we decomposed $\Psi_N = \sum_{k=0}^{N} P_{N,k}^{\varphi} \Psi_N$, where $P_{N,k}^{\varphi}\Psi_N$ has projections p_j^{φ} in exactly k variables.

Thus, e.g., • $P^\varphi_{N,0}\Psi_N = p_1^\varphi \cdots p_N^\varphi \Psi_N = \prod_{i=1}^N \varphi(x_i) \underbrace{\langle \prod_{j=1}^N \varphi(x_j), \Psi_N\rangle}_{=: \chi^{(0)} \in \mathbb{C}}$

meaning we integrate over all $x_1, \dots, x_N$ except x_m.

$$\bullet\ P^\varphi_{N,1}\Psi_N = \sum_{m=1}^N \prod_{\substack{j=1\\ j\neq m}}^N p_j^\varphi q_m^\varphi \Psi_N = \sum_{m=1}^N \prod_{\substack{i=1\\ i\neq m}}^N \varphi(x_i) \langle \prod_{\substack{j=1\\ j\neq m}}^N \varphi(x_j), q_m^\varphi \Psi_N\rangle_{\substack{1\dots N\\ \neq m}}$$

$$= \frac{1}{\sqrt{N}} \sum_{m=1}^N \prod_{\substack{i=1\\ i\neq m}}^N \varphi(x_i) \underbrace{\sqrt{N} \langle \prod_{\substack{j=1\\ j\neq m}}^N \varphi(x_j), q_m^\varphi \Psi_N\rangle_{\substack{1\dots N\\ \neq m}}}_{=: \chi^{(1)}(x_m) \in L^2(\mathbb{R}^3)}$$

Here $\langle \varphi, \chi^{(1)}\rangle = 0$, since $\langle \prod_{j=1}^N \varphi(x_j), q_m^\varphi \Psi_N\rangle = 0$ $\quad (q^\varphi \varphi = 0)$.

Thus $\chi^{(1)} \in \{\varphi\}^\perp$.

We have chosen the $\sqrt{N}$ factor such that

$$\|P_{N,1}\Psi_N\|^2 = \frac{1}{N} \langle \sum_{m=1}^N \prod_{\substack{i=1\\ i\neq m}}^N \varphi(x_i) \chi^{(1)}(x_m), \sum_{n=1}^N \prod_{\substack{j=1\\ j\neq n}}^N \varphi(x_j) \chi^{(1)}(x_n)\rangle$$

$$= \frac{1}{N} \sum_{m=1}^N \langle \prod_{\substack{i=1\\ i\neq m}}^N \varphi(x_i) \chi^{(1)}(x_m), \prod_{\substack{j=1\\ j\neq m}}^N \varphi(x_j) \chi^{(1)}(x_m)\rangle$$

$$= \frac{1}{N} \sum_{m=1}^N \langle \chi^{(1)}, \chi^{(1)}\rangle = \|\chi^{(1)}\|^2$$

In general, we find:

symmetric

<u>Lemma 4.13:</u> For any $\Psi_N \in L^2(\mathbb{R}^{3N})$ and $\varphi \in L^2(\mathbb{R}^3)$, there is a unique decomposition

$$\Psi_N(x_1, \dots, x_N) = \sum_{k=0}^N \sum_{\substack{m_1, \dots, m_k = 1\\ m_i < m_{i+1}\ \forall i = 1, \dots, k-1}}^N \prod_{\substack{i=1\\ i\neq m_1, \dots, i\neq m_k}}^N \varphi(x_i)\ \chi^{(k)}(x_{m_1}, \dots, x_{m_k})$$

with $\chi^{(k)}(x_{m_1}, \dots, x_{m_k}) := \binom{N}{k}^{\frac{1}{2}} \langle \prod_{\substack{j=1\\ j\neq m_1, \dots, j\neq m_k}}^N \varphi(x_j), q_{m_1}^\varphi \cdots q_{m_k}^\varphi \Psi_N\rangle_{\substack{1\dots N\\ \neq m_1, \dots, m_k}}$.

We have that $\chi^{(k)} \in L^2(\mathbb{R}^{3k})$, $p_j^\varphi \chi^{(k)} = 0$ $\forall j = 1, \dots, k$, and $\|\Psi_N\|^2_{L^2(\mathbb{R}^{3N})} = \sum_{k=0}^N \|\chi^{(k)}\|^2_{L^2(\mathbb{R}^{3k})}$.

All $\chi^{(k)}$ for $k=0,\ldots,N$ describe the particles not in the product state.

E.g., $\alpha(\Psi_N,\varphi)=\sum_{k=0}^{N}\frac{k}{N}\underbrace{\|P_{N,k}^{\varphi}\Psi_N\|^2}_{=\|\chi^{(k)}\|^2 \text{ as above}} = \sum_{k=0}^{N}\frac{k}{N}\|\chi^{(k)}\|^2$.

We call $(\chi^{(k)})_{k=0,\ldots,N}$ the fluctuation vector.

Note that $\|\Psi_N\|^2 = \|\underbrace{\sum_{k=0}^{N}P_{N,k}^{\varphi}}_{=\mathbb{1}}\Psi_N\|^2 = \sum_{k=0}^{N}\langle\Psi_N, P_{N,k}^{\varphi}\Psi_N\rangle = \sum_{k=0}^{N}\|P_{N,k}^{\varphi}\Psi_N\|^2 = \sum_{k=0}^{N}\|\chi^{(k)}\|^2$.

$P_{N,k}P_{N,\ell}=P_{N,k}\delta_{k\ell}$ $\qquad$ $P_{N,k}^2=P_{N,k}$

Let us next define the appropriate Hilbert spaces for $(\chi^{(k)})_{k=0,\ldots,N}$.

First:

Definition 4.14: Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. Then their direct sum is $\mathcal{H}_1\oplus\mathcal{H}_2 := \mathcal{H}_1\times\mathcal{H}_2$ with scalar product $\langle\Psi,\tilde{\Psi}\rangle_{\mathcal{H}_1\oplus\mathcal{H}_2} := \langle\Psi_1,\tilde{\Psi}_1\rangle_{\mathcal{H}_1}+\langle\Psi_2,\tilde{\Psi}_2\rangle_{\mathcal{H}_2}$ (i.e., $\Psi=(\Psi_1,\Psi_2)$, $\tilde{\Psi}=(\tilde{\Psi}_1,\tilde{\Psi}_2)$).

Note: $\mathcal{H}_1\oplus\mathcal{H}_2$ is again a Hilbert space.

Definition 4.15:

We define $\left(L_s^2(\mathbb{R}^{3k}) := \{\Psi\in L^2(\mathbb{R}^{3k}) : \Psi(x_1,\ldots,x_k)=\Psi(x_{\sigma(1)},\ldots,x_{\sigma(k)})\ \forall\sigma\in S_N\}\right)$:

- The truncated Fock space
$$\mathcal{F}^{\le N} := \mathbb{C}\oplus L^2(\mathbb{R}^3)\oplus L_s^2(\mathbb{R}^6)\oplus\cdots\oplus L_s^2(\mathbb{R}^{3N}) = \bigoplus_{k=0}^{N} L_s^2(\mathbb{R}^{3k}) \text{ with scalar product}$$
$$\langle\chi,\tilde{\chi}\rangle_{\mathcal{F}^{\le N}} := \sum_{k=0}^{N}\langle\chi^{(k)},\tilde{\chi}^{(k)}\rangle_{L^2(\mathbb{R}^{3k})}.$$

- Fock space $\mathcal{F} := \bigoplus_{k=0}^{\infty} L_s^2(\mathbb{R}^{3k})$ with scalar product $\langle\chi,\tilde{\chi}\rangle_{\mathcal{F}} := \sum_{k=0}^{\infty}\langle\chi^{(k)},\tilde{\chi}^{(k)}\rangle_{L^2(\mathbb{R}^{3k})}$.

- The truncated excitation Fock space w.r.t. $\varphi\in L^2(\mathbb{R}^3)$.

$$\mathcal{F}_\varphi^{\leq N} := \{ \psi \in \mathcal{F}^{\leq N} : p_j^\varphi \psi^{(k)} = 0 \ \forall j = 1,\dots,k, k = 1,\dots,N \}.$$

- The excitation Fock space w.r.t. $\varphi \in L^2(\mathbb{R}^3)$

$$\mathcal{F}_\varphi := \{ \psi \in \mathcal{F} : p_j^\varphi \psi^{(k)} = 0 \ \forall j = 1,\dots,k, \ k \in \mathbb{N}_0 \}.$$

In general, if $\chi \in \mathcal{F}_{(\varphi)}^{(\leq N)}$, we call $\chi^{(k)}$ the k-particle sector.

Thus, the vector χ from Lemma 4.13 is an element of $\mathcal{F}_\varphi^{\leq N} \subset \mathcal{F}^{\leq N}$.

By the trivial extension $(\chi^{(0)}, \chi^{(1)}, \dots, \chi^{(N)}, 0, \dots)$ it is also an element of $\mathcal{F}_\varphi \subset \mathcal{F}$.

We note:

<u>Lemma 4.16:</u> For $\varphi \in L^2(\mathbb{R}^3)$, the map

$U_{N,\varphi} : L^2(\mathbb{R}^{3N}) \to \mathcal{F}_\varphi^{\leq N}, \ \psi_N \mapsto (\chi^{(k)})_{k=0,\dots,N}$ from Lemma 4.13 is unitary.

Proof: $U_{N,\varphi}$ and $U_{N,\varphi}^{-1}$ are explicitly given in Lemma 4.13. Also, $U_{N,\varphi}$ is isometric: above: $\langle U_{N,\varphi}\psi, U_{N,\varphi}\psi\rangle = \langle \psi, \psi \rangle \ (= \langle \chi, \chi \rangle)$, so $U_{N,\varphi}^* U_{N,\varphi} = \mathbb{1}$, i.e., $U_{N,\varphi}^* = U_{N,\varphi}^{-1}$. $\square$

Next: We would like to approximate the fluctuation dynamics $U_{N,\varphi(t)} \psi_N(t)$, where $\varphi(t)$ solves the Hartree eq., and $i\frac{d}{dt}\psi_N(t) = H_N \psi_N(t)$.