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Recall: We consider • $i\frac{d}{dt}\Psi_N(t) = H_N\Psi_N(t)$, with $H_N = \sum_{j=1}^{N}(-\Delta_j) + \frac{1}{N-1}\sum_{\substack{i,j=1\\ i<j}}^{N} v(x_i - x_j)$ (*)

• $i\frac{d}{dt}\varphi(t) = h^{\varphi(t)}\varphi(t)$, with $h^{\varphi(t)} = -\Delta + v * |\varphi(t)|^2$. (**)

We defined $\alpha(\Psi_N(t),\varphi(t)) = \langle \Psi_N(t), q_1^{\varphi(t)}\Psi_N(t)\rangle$ as a good indicator of convergence.

We aim at proving a Gronwall estimate, i.e., $\dot\alpha(\Psi_N(t),\varphi(t)) \le C\left(\alpha(\Psi_N(t),\varphi(t)) + \varepsilon_N\right)$ with some $\varepsilon_N \xrightarrow{N\to\infty} 0$. This would imply $\alpha(\Psi_N(t),\varphi(t)) \le e^{Ct}\alpha(\Psi_N(0),\varphi(0)) + (e^{Ct}-1)\varepsilon$.

Last time we proved:

$$\frac{d}{dt}\alpha(\Psi_N(t),\varphi(t)) = i\langle \Psi_N(t), \underbrace{[H_N - h_1^{\varphi(t)}, q_1^{\varphi(t)}]}\Psi_N(t)\rangle.$$ Let us continue the computation.

$$= \Big[\sum_{j=1}^{N}(-\Delta_j) + \frac{1}{N-1}\sum_{i<j}\underbrace{v_{ij}}_{:=v(x_i-x_j)} - (-\Delta_1) - (v*|\varphi(t)|^2)_1, q_1^{\varphi(t)}\Big]$$

$[-\Delta_j, q_1^{\varphi(t)}] = 0$ for $j>1$

$$= \Big[\frac{1}{N-1}\sum_{j=2}^{N} v_{1j} - (v*|\varphi(t)|^2)_1, q_1^{\varphi(t)}\Big]$$

$$\Rightarrow \frac{d}{dt}\alpha(\Psi_N(t),\varphi(t)) = i\langle\Psi_N(t), \Big[\frac{1}{N-1}\sum_{j=2}^{N} v_{1j} - (v*|\varphi(t)|^2)_1, q_1^{\varphi(t)}\Big]\Psi_N(t)\rangle$$

$\Psi_N(t)$ symmetric

$$= i\langle\Psi_N(t), [v_{12} - (v*|\varphi(t)|^2)_1, q_1^{\varphi(t)}]\Psi_N(t)\rangle$$

For A, B symmetric:
$\langle\Psi, [A,B]\Psi\rangle$
$= \langle A\Psi, B\Psi\rangle - \langle B\Psi, A\Psi\rangle$
$= \langle A\Psi, B\Psi\rangle - \overline{\langle A\Psi, B\Psi\rangle}$
$= 2i\,\mathrm{Im}\langle A\Psi, B\Psi\rangle$

$$= -2\,\mathrm{Im}\langle\Psi_N(t), \left(v_{12} - (v*|\varphi(t)|^2)_1\right) q_1^{\varphi(t)}\Psi_N(t)\rangle$$

$$= -2\,\mathrm{Im}\langle\Psi_N(t), p_1^{\varphi(t)}\overbrace{\left(v_{12} - (v*|\varphi(t)|^2)_1\right)}^{=:W_{12}} q_1^{\varphi(t)}\Psi_N(t)\rangle$$

term with $q_1^{\varphi(t)}$ here vanishes since then the scalar product is real

Inserting also $\mathbb{1} = p_2^{\varphi(t)} + q_2^{\varphi(t)}$ leads to

$$\frac{d}{dt}\alpha(\Psi_N(t),\varphi(t)) = -2\,\mathrm{Im}\langle\Psi_N(t),\, p_1^{\varphi(t)} p_2^{\varphi(t)} W_{12}\, q_1^{\varphi(t)} p_2^{\varphi(t)} \Psi_N(t)\rangle \quad \Big\}\text{ term (I)}$$

$$-2\,\mathrm{Im}\underbrace{\langle\Psi_N(t),\, p_1^{\varphi(t)} q_2^{\varphi(t)} W_{12}\, q_1^{\varphi(t)} p_2^{\varphi(t)} \Psi_N(t)\rangle}_{\in\mathbb{R}\ (\text{since } W_{12}=W_{21})} \quad \Big\} = 0$$

$$-2\,\mathrm{Im}\langle\Psi_N(t),\, p_1^{\varphi(t)} p_2^{\varphi(t)} W_{12}\, q_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\rangle \quad \Big\}\text{ term (II)}$$

$$-2\,\mathrm{Im}\langle\Psi_N(t),\, p_1^{\varphi(t)} q_2^{\varphi(t)} W_{12}\, q_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\rangle \quad \Big\}\text{ term (III)}$$

Now note that $p_2^{\varphi(t)} W_{12}\, p_2^{\varphi(t)} = \underbrace{p_2^{\varphi(t)} v_{12}\, p_2^{\varphi(t)}}_{\substack{= |\varphi(t)\rangle_2 \underbrace{\langle\varphi(t)|_2 v_{12} |\varphi(t)\rangle_2}_{=(v*|\varphi(t)|^2)_1} \langle\varphi(t)|_2 \\ = (v*|\varphi(t)|^2)_1\, p_2^{\varphi(t)}}} - (v*|\varphi(t)|^2)_1\, p_2^{\varphi(t)} = 0.$

Thus, term(I) $= 0$. This is the essential term where the interaction v_{12} is cancelled by its average $v*|\varphi|^2$.

Furthermore: $|\text{term (III)}| \le 2 \underbrace{\|p_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\|}_{\substack{\le \|q_2^{\varphi(t)}\Psi_N(t)\| \\ = \sqrt{\alpha(\Psi_N(t),\varphi(t))}}} \underbrace{\|W_{12}\|_{\infty}}_{\substack{\le \|v\|_{L^\infty} + \underbrace{\|v*|\varphi(t)|^2\|_{L^\infty}}_{\le \|v\|_{L^\infty} \underbrace{\||\varphi(t)|^2\|_{L^1}}_{=1}}}} \underbrace{\|q_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\|}_{\le\sqrt{\alpha(\Psi_N(t),\varphi(t))}}.$

Similar to HW3

$$\Rightarrow |\text{term (III)}| \le 4\|v\|_{L^\infty}\, \alpha(\Psi_N(t),\varphi(t)).$$

Finally: term (II) $= -2\,\mathrm{Im}\,\langle \Psi_N(t), p_1^{\varphi(t)} p_2^{\varphi(t)} \left(v_{12} - (v * |\varphi(t)|^2)_1\right) q_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\rangle$

$p_2^{\varphi(t)} (v*|\varphi(t)|^2)_1\, q_2^{\varphi(t)} = \underbrace{p_2^{\varphi(t)} q_2^{\varphi(t)}}_{=0} (v*|\varphi(t)|^2)_1$

$$= -2\,\mathrm{Im}\,\langle \Psi_N(t), p_1^{\varphi(t)} p_2^{\varphi(t)}\, v_{12}\, q_1^{\varphi(t)} q_2^{\varphi(t)} \Psi_N(t)\rangle$$

We prove in HW 11 that $|\text{term (II)}| \leq 6\,\|v\|_\infty \left(\alpha + \frac{1}{N}\right)$ (for all $N \geq 3$).

To summarize, we have proven:

Theorem 4.12: 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., • $P^{\varphi}_{N,0}\Psi_N = p^{\varphi}_1 \cdots p^{\varphi}_N \Psi_N = \prod_{i=1}^{N} \varphi(x_i) \underbrace{\langle \prod_{j=1}^{N} \varphi(x_j), \Psi_N \rangle}_{=: \chi^{(0)} \in \mathbb{C}}$

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

$$\bullet\ P^{\varphi}_{N,1}\Psi_N = \sum_{m=1}^{N} \prod_{\substack{j=1\\ j\neq m}}^{N} p^{\varphi}_j q^{\varphi}_m \Psi_N = \sum_{m=1}^{N} \prod_{\substack{i=1\\ i\neq m}}^{N} \varphi(x_i) \langle \prod_{\substack{j=1\\ j\neq m}}^{N} \varphi(x_j), q^{\varphi}_m \Psi_N \rangle_{\substack{1\dots N\\ \neq m}}$$

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

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

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:

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

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