Foundations of Mathematical Physics, Constructor University Bremen — Session 27

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Last time we proved:

Let $\alpha(\Psi_N(t),\varphi(t)) := \langle \Psi_N(t), q_1^{\varphi(t)} \Psi_N(t)\rangle$, with $i\frac{d}{dt}\Psi_N(t) = H_N \Psi_N(t)$, $i\frac{d}{dt}\varphi(t) = h^{\varphi(t)}\varphi(t)$,

where $H_N = -\sum_{j=1}^{N}(-\Delta_j) + \frac{1}{N-1}\sum_{i<j} v(x_i - x_j)$, $h^{\varphi(t)} = -\Delta + v * |\varphi(t)|^2$, $q^{\varphi(t)} := 1 - p^{\varphi(t)}$, $p^{\varphi(t)} = |\varphi(t)\rangle\langle\varphi(t)|$.

Let $\Psi_N(0) \in H^2(\mathbb{R}^{3N})$, $\varphi(t) \in H^2(\mathbb{R}^3)$. Then

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

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

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

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

where $W_{12} := v_{12} - \left(v * |\varphi(t)|^2\right)_1$ $\qquad \overbrace{\left(v_{12} - (v*|\varphi(t)|^2)_1\right)}$

Now note that

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

$$\langle\varphi(t)_2| v_{12} |\varphi(t)\rangle_2 = (v*|\varphi(t)|^2)_1$$

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

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

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

Similar to HW3

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

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

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

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

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

Using Gronwall's lemma, 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 $\Psi_N(0) \in H^2(\mathbb{R}^{3N})$, $\|\Psi_N(0)\| = 1$. Assume the Hartree equation has a unique solution $\varphi(t)$ given initial data $\varphi(0) \in L^2(\mathbb{R}^3)$, $\|\varphi(0)\| = 1$.
We assume $\varphi(t) \in H^2(\mathbb{R}^3)$. Then

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

Note: The assumption that $\varphi(t) \in H^2(\mathbb{R}^3)$ exists holds for any $\varphi(0) \in H^2(\mathbb{R}^3)$. This can be proven with a Gronwall argument as well, but we skip that here.

Note: We can relax the condition $v \in L^\infty$. Let us consider $v(x) = |x|^{-1}$. Then:

- H_N is still self-adjoint by Kato-Rellich.
- Term (I) = 0 still.
- $$|\text{term (III)}| \leq 2 \underbrace{\|q_2^{\varphi(t)}\psi_N(t)\|}_{\leq\sqrt{\alpha(t)}} \|p_1^{\varphi(t)} W_{12}\|_{\mathcal{L}} \underbrace{\|q_1^{\varphi(t)}\|_{\mathcal{L}}}_{\leq 1} \underbrace{\|q_2^{\varphi(t)}\psi_N(t)\|}_{\leq\sqrt{\alpha(t)}},$$

  and $\|p_1^{\varphi(t)} W_{12}\|_{\mathcal{L}} = \|W_{12} p_1^{\varphi(t)}\|_{\mathcal{L}} \leq \|v_{12} p_1^{\varphi(t)}\|_{\mathcal{L}} + \|v * |\varphi(t)|^2\|_{\mathcal{L}} \|p_1^{\varphi(t)}\|_{\mathcal{L}}$.

  Now: $$\|v_{12} p_1^{\varphi(t)}\|_{\mathcal{L}}^2 \leq \|\underbrace{p_1^{\varphi(t)} v_{12}^2 p_1^{\varphi(t)}}_{=(v^2 * |\varphi(t)|^2)_2 p_1^{\varphi(t)}}\|_{\mathcal{L}} \leq \|v^2 * |\varphi(t)|^2\|_{\mathcal{L}} = \sup_{y\in\mathbb{R}^3} \int dx\, v(x)\, |\varphi(t,y-x)|^2$$

  $$= \sup_{y\in\mathbb{R}^3} \underbrace{\langle \varphi_y(t), \tfrac{1}{|x|^2}\varphi_y(t)\rangle}, \text{ with } \varphi_y(t,x) = \varphi(t,y-x)$$

  $$\leq 4\langle\varphi_y(t), (-\Delta)\varphi_y(t)\rangle \text{ by Hardy's inequality (HW5 Problem 6)}$$

  $$= 4\int dx\, \varphi(t,y-x)\,(-\Delta_x)\,\varphi(t,y-x)$$

  $$= 4\int dx\, \varphi(t,x)(-\Delta_x)\,\varphi(t,x)$$

  $$= 4\,\|\nabla\varphi(t)\|^2$$

  Also: $\|v * |\varphi(t)|^2\|_{\mathcal{L}} \leq \|v^2 * |\varphi(t)|^2\|_{\mathcal{L}} \leq 4\|\nabla\varphi(t)\|^2$

  $$\Rightarrow \|p_1^{\varphi(t)} W_{12}\|_{\mathcal{L}} \leq 8\,\|\nabla\varphi(t)\|^2$$

- $|\text{term (II)}| \leq C\,\|\nabla\varphi(t)\|^2 \left(\alpha(t) + \frac{1}{N}\right)$ can be shown as well.

- Now recall energy conservation from HW12 Problem 2:

  For $E(\varphi(t)) := \|\nabla\varphi(t)\|^2 + \frac{1}{2}\int (v * |\varphi(t)|^2)(x)\,|\varphi(t,x)|^2\,dx$, we have $E(\varphi(t)) = E(\varphi(0))$.

  $$\Rightarrow \|\nabla\varphi(t)\|^2 = \underbrace{E(\varphi(t))}_{=E(\varphi(0))} - \frac{1}{2}\int (v * |\varphi(t)|^2)(x)\,|\varphi(t,x)|^2\,dx \leq E(\varphi(0)).$$

Conclusion: Derivation of Hartree equation still works if $v(x) = \frac{1}{|x|}$ (or, in fact, $v = v^{(1)} + v^{(2)}$ with $v^{(1)} \in L^\infty$ and $|v^{(2)}(x)| \leq \frac{C}{|x-R|}$).