Foundations of Mathematical Physics, Constructor University Bremen — Session 26

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Next we will prove that indeed $\alpha(\Psi_N(t),\varphi(t)) \xrightarrow{N\to\infty} 0 \quad \forall t\in\mathbb{R}$.

Step 2: Controlling $\alpha(\Psi_N(t),\varphi(t))$

A standard technique is based on (variations of) the following lemma:

Lemma 4.11: Gronwall Lemma

Let $\eta:\mathbb{R}\to\mathbb{R}$ be differentiable and satisfy $\frac{d}{dt}\eta(t)\leq C(\eta(t)+\varepsilon)$ for some $C,\varepsilon\geq 0$.
Then, for all $t>0$, we have

$$\eta(t)\leq e^{Ct}\eta(0)+(e^{Ct}-1)\varepsilon$$

Proof: First, consider differentiable $f:\mathbb{R}\to\mathbb{R}$ satisfying $\frac{d}{dt}f(t)\leq Cf(t)$.
Let $g(t):=e^{Ct}$ (i.e., $g(t)>0$). Then

$$\frac{d}{dt}\left(\frac{f(t)}{g(t)}\right)=\frac{\frac{df(t)}{dt}g(t)-f(t)\frac{dg(t)}{dt}}{g(t)^2}\leq\frac{Cf(t)g(t)-f(t)Cg(t)}{g(t)^2}=0.$$

$$\Rightarrow \frac{f(t)}{g(t)}\leq\frac{f(0)}{g(0)} \Rightarrow f(t)\leq \underbrace{g(t)}_{=e^{Ct}}f(0)\underbrace{\frac{1}{g(0)}}_{=1}=e^{Ct}f(t). \quad (*)$$

Next, define $h(t):=e^{Ct}\eta(0)+(e^{Ct}-1)\varepsilon$, s.t. $\frac{dh(t)}{dt}=Ce^{Ct}\eta(0)+Ce^{Ct}\varepsilon=C(h(t)+\varepsilon)$
and $h(0)=\eta(0)$.

Then $\frac{d}{dt}(\eta(t)-h(t))\leq C(\eta(t)+\varepsilon)-C(h(t)+\varepsilon)=C(\eta(t)-h(t))$, so $(*)$ implies

$$\eta(t)-h(t)\leq e^{Ct}(\eta(0)-h(0))=0, \text{ i.e., } \eta(t)\leq h(t). \qquad \square$$

We hope to apply the Gronwall lemma to $\alpha(\Psi_N(t),\varphi(t))$.

So let us compute:

$$\frac{d}{dt}\alpha(\Psi_N(t),\varphi(t)) = \frac{d}{dt}\langle \Psi_N(t), q_1^{\varphi(t)}\Psi_N(t)\rangle$$

$$= \langle \underbrace{\frac{d}{dt}\Psi_N(t)}_{=-iH_N\Psi_N(t) \text{ for } \Psi_N(0)\in H^2(\mathbb{R}^{3N})}, q_1^{\varphi(t)}\Psi_N(t)\rangle + \langle \Psi_N(t), q_1^{\varphi(t)}\frac{d}{dt}\Psi_N(t)\rangle + \langle \Psi_N(t), \underbrace{\left(\frac{d}{dt}q_1^{\varphi(t)}\right)}\Psi_N(t)\rangle$$

$$= -\frac{d}{dt}p_1^{\varphi(t)} = -\frac{d}{dt}|\varphi(t)\rangle\langle\varphi(t)|$$

If Hartree eq. holds in L^2 sense, which we assume here.

$$= -\left(|-ih^{\varphi(t)}\varphi(t)\rangle\langle\varphi(t)| + |\varphi(t)\rangle\langle -ih^{\varphi(t)}\varphi(t)|\right)$$

$$= -\left(-ih^{\varphi(t)}p^{\varphi(t)} + ip^{\varphi(t)}h^{\varphi(t)}\right)$$

$$= i\left[h^{\varphi(t)}, p^{\varphi(t)}\right]$$

$$= -i\left[h_1^{\varphi(t)}, q_1^{\varphi(t)}\right]$$

$$\Rightarrow \frac{d}{dt}\alpha(\Psi_N(t),\varphi(t)) = i\langle H_N\Psi_N(t), q_1^{\varphi(t)}\Psi_N(t)\rangle - i\langle\Psi_N(t), q_1^{\varphi(t)}H_N\Psi_N(t)\rangle - i\langle\Psi_N(t), [h_1^{\varphi(t)}, q_1^{\varphi(t)}]\Psi_N(t)\rangle$$

$$= i\langle \Psi_N(t), \underbrace{\left[H_N - h_1^{\varphi(t)}, q_1^{\varphi(t)}\right]}\Psi_N(t)\rangle$$

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

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

$[v_{ij}, q_1^{\varphi(t)}] = 0$ for $i\neq 1$ and $j\neq 1$

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

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

$\Psi_N(t)$ symmetric

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

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

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

$$= -2\,\mathrm{Im}\langle\Psi_N(t), \underbrace{p_1^{\varphi(t)}}_{\text{term with } q_1^{\varphi(t)} \text{ here vanishes since then the scalar product is real}}\overbrace{\left(v_{12} - (v*|\varphi(t)|^2)_1\right)}^{=:W_{12}}q_1^{\varphi(t)}\Psi_N(t)\rangle$$

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

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

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

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

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