Foundations of Mathematical Physics, Jacobs University, Fall 2021 — Session 24

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Last time we introduced the reduced one-particle density matrix $\gamma_{\Psi_N}: L^2 \to L^2$ via its kernel

$$\gamma_{\Psi_N}(x,y) := \int dx_2 \dots dx_N \, \overline{\Psi_N(y, x_2, \dots, x_N)} \, \Psi_N(x, x_2, \dots, x_N).$$

We had also defined the expected number of particles not in the product state $\Pi\varphi$ as

$$\alpha(\Psi_N, \varphi) = \sum_{k=0}^{N} \frac{k}{N} \langle \Psi_N, P_{N,k}^{\varphi} \Psi_N \rangle = \langle \Psi_N, q_1^{\varphi} \Psi_N \rangle.$$

Their relation is: $\alpha(\Psi_N, \varphi) \leq \| \gamma_{\Psi_N} - p^{\varphi} \|_{\mathfrak{S}_1} \leq 4 \sqrt{\alpha(\Psi_N, \varphi)}$.

Furthermore, as in the proof of Lemma 4.10, we have for any $A \in \mathfrak{S}_\infty(L^2(\mathbb{R}^3))$:

$$\langle \Psi_N, A_1 \Psi_N \rangle - \langle \varphi, A\varphi \rangle$$

$$= \langle \Psi_N, \underbrace{(p_1^{\varphi} + q_1^{\varphi})}_{=\mathbb{1}} A_1 (p_1^{\varphi} + q_1^{\varphi}) \Psi_N \rangle - \langle \varphi, A\varphi \rangle$$

$$= \underbrace{\langle \Psi_N, \underbrace{p_1^{\varphi} A_1 p_1^{\varphi}}_{\substack{= |\varphi\rangle\langle\varphi| A |\varphi\rangle\langle\varphi| \\ = \langle \varphi, A\varphi \rangle p_1^{\varphi}}} \Psi_N \rangle - \langle \varphi, A\varphi \rangle}_{\substack{= \langle \varphi, A\varphi \rangle (\langle \Psi_N, p_1^{\varphi} \Psi_N \rangle - 1) \\ = -\langle \varphi, A\varphi \rangle \alpha_N(\Psi_N, \varphi)}} + \underbrace{\langle \Psi_N, p_1^{\varphi} A_1 q_1^{\varphi} \Psi_N \rangle}_{\substack{\leq \|A\| \, \|p_1^{\varphi}\Psi_N\| \, \|q_1^{\varphi}\Psi_N\| \\ \leq \|A\| \sqrt{\alpha(\Psi_N, \varphi)}}} + \langle \Psi_N, q_1^{\varphi} A_1 p_1^{\varphi} \Psi_N \rangle + \underbrace{\langle \Psi_N, q_1^{\varphi} A_1 q_1^{\varphi} \Psi_N \rangle}_{\leq \|A\| \alpha(\Psi_N, \varphi)}$$

Cauchy-Schwarz

$$\Rightarrow \left| \langle \Psi_N, A_1 \Psi_N \rangle - \langle \varphi, A\varphi \rangle \right| \leq \|A\| \, 4 \sqrt{\alpha(\Psi_N, \varphi)}$$

Conclusion: If we can show that $\alpha(\Psi_N(t), \varphi(t)) \xrightarrow{N \to \infty} 0$, then also $\gamma_{\Psi_N} \xrightarrow{N \to \infty} p^{\varphi}$ and $\langle \Psi_N, A_1 \Psi_N \rangle \xrightarrow{N \to \infty} \langle \varphi, A\varphi \rangle \; \forall \, A \in \mathfrak{S}_\infty$.

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 $\frac{d}{dt} f(t) \leq C f(t)$.

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

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

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

Note: Let us use $H_N = \sum_{i=1}^{N}(-\Delta_j) + \frac{1}{N-1}\sum_{\substack{i,j=1 \\ i<j}}^{N} v(x_i - x_j)$.

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

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

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

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

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

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

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

We continue this computation next time.