Recent analytic and spectral results for the multi-particle Schrödinger operator
Lecture 4: Real analyticity of the density matrix

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Multi-particle system

Begin with the Schrödinger operator

$$H = -\Delta + V \quad \text{on} \quad \mathsf{L}^2(\mathbb{R}^{3N}),$$

with

$$\Delta = \sum_{k=1}^{N} \Delta_k, \quad V(\mathbf{x}) = -\sum_{k=1}^{N} \frac{Z}{|x_k|} + \sum_{1\le j<k\le N} \frac{1}{|x_j - x_k|}.$$

Notation: $\mathbf{x} = (x_1, x_2, \dots, x_{N-1}, x_N) = (\hat{\mathbf{x}}, x_N)$.
Let $\psi \in \mathsf{L}^2(\mathbb{R}^{3N})$ be an eigenfunction of H:

$$H\psi = E\psi,$$

with some $E \in \mathbb{R}$.
The one-particle density matrix:

$$\gamma(x, y) = \int \overline{\psi(\hat{\mathbf{x}}, x)}\psi(\hat{\mathbf{x}}, y) d\hat{\mathbf{x}}, \quad (x, y) \in \mathbb{R}^3 \times \mathbb{R}^3.$$

The one-particle density:

$$\rho(x) = \gamma(x, x).$$

Smoothness of $\gamma(x, y)$

Theorem (Main Theorem 3, HS2020)

$\gamma(x, y)$ *is real analytic on* $\{(x, y) \in \mathbb{R}^3 \times \mathbb{R}^3 : |x||y||x - y| \neq 0\}$.

Definition. The function f is real analytic in $\Omega \subset \mathbb{R}^d$ (i.e. $f \in C^\omega(\Omega)$) if for every point $\mathbf{x}_0 \in \Omega$ there is a neighbourhood $U \ni \mathbf{x}_0$ such that the function f can be represented as a series

$$f(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{N}_0^d} a_{\mathbf{m}} (\mathbf{x} - \mathbf{x}_0)^{\mathbf{m}}$$

convergent in U.

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Theorem. The function f is $C^\omega(\Omega)$ if and only if for each $\mathbf{x}_0 \in \Omega$ there is a neighbourhood $U \ni \mathbf{x}_0$ and positive constants C and A such that

$$|\partial_{\mathbf{x}}^{\mathbf{m}} f(\mathbf{x})| \le C A^{|\mathbf{m}|} \mathbf{m}!, \ \mathbf{m}! = m_1! m_2! \cdots m_d!,$$

for all $\mathbf{x} \in U$.

Corollary. If for all $\mathbf{x} \in \Omega$,

$$|\partial_{\mathbf{x}}^{\mathbf{m}} f(\mathbf{x})| \le CA^{|\mathbf{m}|}(1+|\mathbf{m}|)^{|\mathbf{m}|}, \mathbf{m} \in \mathbb{N}_0^d,$$

then f is real analytic in Ω.

Proof. From Stirling's formula it follows that $(p+1)^p \le Ce^p p!$, $p = 0, 1, \dots$. The multinomial formula

$$d^p = \left(\sum_{l=1}^{d} 1\right)^p = \sum_{|k|=p} \frac{|k|!}{k!},$$

implies that

$$|\mathbf{m}|! \le d^{|\mathbf{m}|}\mathbf{m}!, \quad \forall \mathbf{m} \in \mathbb{N}_0^d.$$

Thus

$$(|\mathbf{m}|+1)^{|\mathbf{m}|} \le Ce^{|\mathbf{m}|}|\mathbf{m}|! \le Ce^{|\mathbf{m}|}d^{|\mathbf{m}|}\mathbf{m}!$$

□

Corollary. If for all $\mathbf{x} \in \Omega$,

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Proof. From Stirling's formula it follows that $(p+1)^p \le C e^p p!$, $p = 0, 1, \dots$.
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$$(|\mathbf{m}|+1)^{|\mathbf{m}|} \le C e^{|\mathbf{m}|}|\mathbf{m}|! \le C e^{|\mathbf{m}|} d^{|\mathbf{m}|}\mathbf{m}!$$

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Corollary-L^1**.** If

$$\int_\Omega |\partial_{\mathbf{x}}^{\mathbf{m}} f(\mathbf{x})| d\mathbf{x} \le C A^{|\mathbf{m}|}(1+|\mathbf{m}|)^{|\mathbf{m}|}, \mathbf{m} \in \mathbb{N}_0^d,$$

then f is real analytic in Ω.

Proof of Theorem 3. Simplifications: instead of $\gamma(x, y)$ look at $\rho(x) = \gamma(x, x)$.
Consider $N = 2$:

$$\rho(x_2) = \int |\psi(x_1, x_2)|^2 dx_1.$$

Aim: to establish the bound

$$\int_{|x_2|>2\varepsilon} |\partial_{x_2}^m \rho(x_2)| dx_2 \le A^{|m|+1}(|m|+1)^{|m|}, \ \ m \in \mathbb{N}_0^3, \tag{1}$$

with some $A = A(\varepsilon) > 0$.

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with some $A = A(\varepsilon) > 0$. A straightforward differentiation w.r.t. x_2 works if x_2 is separated from x_1, i.e. on the set

$$\mathrm{U}_2(\varepsilon) = \{(x_1, x_2) \in \mathbb{R}^6 : |x_2| > 2\varepsilon, |x_1 - x_2| > \varepsilon/4\}.$$

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Otherwise we use the *directional derivatives*. On the set

$$\mathrm{U}_{12}(\varepsilon) = \{(x_1, x_2) : |x_2| > 2\varepsilon, |x_1 - x_2| < \varepsilon/4\}$$

the potential $|x_1 - x_2|^{-1}$ is infinitely differentiable w.r.t. $\nabla_{12} = \nabla_1 + \nabla_2$. Indeed, $\nabla_{12}|x_1 - x_2|^{-1} = 0$. Thus ψ is also ∇_{12}-smooth on $\mathrm{U}_{12}(\varepsilon)$.

Lemma. For all $m, n \in \mathbb{N}_0^3$, $|m| + |n| \geq 1$, the function $\partial_{12}^m \partial_2^n V$ is C^∞ on

$$\|\partial_{12}^m \partial_2^n V\|_{\mathsf{L}^\infty(\mathsf{U}(\varepsilon))} \leq A_0^{1+|m|+|n|}(|m| + |n| + 1)^{|m|+|n|}, \quad A_0 = A_0(\varepsilon),$$

holds, where $\mathsf{U}(\varepsilon) = \mathsf{U}^{(m,n)}(\varepsilon)$ is
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$\mathsf{U}(\varepsilon) = \mathsf{U}_2(\varepsilon) \cap \mathsf{U}_{12}(\varepsilon)$ if $|m| \geq 1$ and $|n| \geq 1$.

Lemma. For all $m, n \in \mathbb{N}_0^3$, $|m| + |n| \geq 1$, the function $\partial_{12}^m \partial_2^n V$ is C^∞ on

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Let $u_{m,n} = \partial_{12}^m \partial_2^n \psi$. Then

$$\begin{aligned}(H - E)u_{m,n} &= [H - E, \partial_{12}^m \partial_2^n]\psi = [V, \partial_{12}^m \partial_2^n]\psi \\ &= -\sum_{\substack{0 \leq s \leq m \\ 0 \leq p \leq n \\ |s|+|p| \leq |m|+|n|-1}} \binom{m}{s}\binom{n}{p}(\partial_{12}^{m-s}\partial_2^{n-p} V)u_{s,p} = f_{m,n}.\end{aligned}$$

Lemma.

$$\int_{\mathrm{U}(\varepsilon)} |\partial_{12}^m \partial_2^n \psi(x_1, x_2)|^2 dx_1 dx_2 \le A_1^{|m|+|n|+1} (|m| + |n| + 1)^{|m|+|n|},$$
$$\int_{\mathrm{U}(\varepsilon)} \partial_{12}^m \partial_2^n |\psi(x_1, x_2)|^2 dx_1 dx_2 \le A_2^{|m|+|n|+1} (|m| + |n| + 1)^{|m|+|n|},$$

with some $A_1 = A_1(\varepsilon), A_2 = A_2(\varepsilon)$.

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with some $A_1 = A_1(\varepsilon), A_2 = A_2(\varepsilon)$.

Proof. Based on the elliptic estimate

$$\delta^s \|\nabla^s u_{m,n}\|_{L^2(U(\varepsilon+\delta))} \le C\big(\delta^2 \|f_{m,n}\|_{L^2(U(\varepsilon))} + \delta \|\nabla u_{m,n}\|_{L^2(U(\varepsilon))} + \|u_{m,n}\|_{L^2(U(\varepsilon))}\big),$$

for $s \le 2$ and any $\delta > 0$. $\square$

Lemma.

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$$\int_{\mathrm{U}(\varepsilon)} \partial_{12}^m \partial_2^n |\psi(x_1, x_2)|^2 dx_1 dx_2 \le A_2^{|m|+|n|+1}(|m|+|n|+1)^{|m|+|n|},$$

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$$\delta^s \|\nabla^s u_{m,n}\|_{\mathrm{L}^2(\mathrm{U}(\varepsilon+\delta))} \le C\big(\delta^2 \|f_{m,n}\|_{\mathrm{L}^2(\mathrm{U}(\varepsilon))} + \delta \|\nabla u_{m,n}\|_{\mathrm{L}^2(\mathrm{U}(\varepsilon))} + \|u_{m,n}\|_{\mathrm{L}^2(\mathrm{U}(\varepsilon))}\big),$$

for $s \le 2$ and any $\delta > 0$. □

PROOF OF (1). Let $\zeta \in \mathrm{C}_0^\infty(\mathbb{R}^3)$ be such that $0 \le \zeta \le 1$, and $\zeta(x) = 1, |x| < \varepsilon/8$, and $\zeta(x) = 0, |x| > \varepsilon/4$. Denote $\omega(x) = 1 - \zeta(x)$. Rewrite:

$$\rho(x_2) = \int |\psi(x_1, x_2)|^2 \zeta(x_2 - x_1) dx_1 + \int |\psi(x_1, x_2)|^2 \omega(x_2 - x_1) dx_1$$
$$= \rho_\zeta(x) + \rho_\omega(x).$$

To estimate ρ_ζ write:

$$\rho_\zeta(x_2) = \int |\psi(t + x_2, x_2)|^2 \zeta(t) dt,$$

so, for $|m| = 1$,

$$\begin{aligned} \partial_{x_2}^m \rho_\zeta(x_2) &= \int \left(\partial_1^m |\psi(t + x_2, x_2)|^2 + \partial_2^m |\psi(t + x_2, x_2)|^2\right) \zeta(t) dt \\ &= \int \partial_{12}^m |\psi(x_1, x_2)|^2 \zeta(x_2 - x_1) dx_1 \end{aligned}$$

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and hence

$$\begin{aligned} \int_{|x_2| > 2\varepsilon} |\partial_{x_2}^m \rho_\zeta(x_2)| dx_2 \le \int_{\mathrm{U}_{12}(\varepsilon)} \left|\partial_{12}^m |\psi(x_1, x_2)|^2\right| dx_1 dx_2 \\ \le A_2^2 (1 + 1)^1. \end{aligned}$$

The same formula for $|m| > 1$, so that

$$\int_{|x_2| > 2\varepsilon} |\partial_{x_2}^m \rho_\zeta(x_2)| dx_2 \le \int_{\mathrm{U}_{12}(\varepsilon)} \left|\partial_{12}^m |\psi(x_1, x_2)|^2\right| dx_1 dx_2 \le A_2^{|m|+1} (|m| + 1)^{|m|}.$$

Consider ρ_ω. First assume that $|m| = 1$:

$$\partial_{x_2}^m \rho_\omega(x_2) = \int \partial_2^m |\psi(x_1, x_2)|^2 \omega(x_2 - x_1) dx_1 + \int |\psi(x_1, x_2)|^2 \partial_2^m \omega(x_2 - x_1) dx_1,$$

and hence

$$\begin{aligned}\int_{|x_2|>\varepsilon} |\partial_{x_2}^m \rho_\omega(x_2)| dx_2 \leq & \int_{\mathrm{U}_1(\varepsilon)} \left|\partial_2^m |\psi(x_1, x_2)|^2\right| dx_1 dx_2 + C \int |\psi(x_1, x_2)|^2 dx_1 dx_2 \\ & \leq A_2^2 (1+1)^1 + C A_2^1 \leq A_2^2 (1 + C)(1+1)^1.\end{aligned}$$

In the second term $|x_1 - x_2| < \varepsilon/4$, so that for further derivatives one can use ∂_{12}.

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and hence

$$\begin{aligned}\int_{|x_2| > \varepsilon} |\partial_{x_2}^m \rho_\omega(x_2)| dx_2 \le & \int_{\mathrm{U}_1(\varepsilon)} \left|\partial_2^m |\psi(x_1, x_2)|^2\right| dx_1 dx_2 + C \int |\psi(x_1, x_2)|^2 dx_1 dx_2 \\ & \le A_2^2 (1+1)^1 + C A_2^1 \le A_2^2 (1 + C)(1+1)^1.\end{aligned}$$

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For general N we introduce appropriate cut-offs, associated with various clusters of particles. □