Recent analytic and spectral results for the multi-particle Schrödinger operator: Lecture 3: spectrum of the one-particle 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:

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

Spectral estimates

Suppose that

$$|\psi(\mathbf{x})| \lesssim e^{-\varkappa_0|\mathbf{x}|}, \quad \mathbf{x} \in \mathbb{R}^{3N}. \tag{1}$$

Main Theorem 1: Estimates. Assume (1). Then $\lambda_k(\Gamma) \lesssim k^{-8/3}$, i.e. $\|\Gamma\|_{3/8,\infty} < \infty$.

Main Theorem 2: Asymptotics. Assume (1). Then

$$\lim_{k\to\infty} k^{8/3}\lambda_k(\Gamma) = A, \quad \mathrm{G}_{3/8}(\Gamma) = A^{3/8},$$

with an explicit constant $A \geq 0$.

Since $\Gamma = \Psi^*\Psi$,

Main Theorem 1Ψ: Estimates. Assume (1). Then $s_k(\Psi) \lesssim k^{-4/3}$, i.e. $\|\Psi\|_{3/4,\infty} < \infty$.

Main Theorem 2Ψ: Asymptotics. Assume (1). Then

$$\lim_{k\to\infty} k^{4/3}\lambda_k(\Psi) = A^{1/2}, \quad \mathrm{G}_{3/4}(\Psi) = \mathrm{g}_{3/4}(\Psi) = A^{3/8}.$$

Ingredients of the proof

Denote $x_0 = 0$ and let

$$\mathsf{S}_{ls} = \mathsf{S}_{sl} = \{\mathbf{x} \in \mathbb{R}^{3N} : x_l \neq x_s\}, \ l \neq s, \quad l, s = 0, 1, 2, \dots, N.$$

Define

$$\mathsf{U}_j = \bigcap_{0 \le l < s \le N-1} \mathsf{S}_{ls} \bigcap_{\substack{0 \le s \le N-1 \\ s \neq j}} \mathsf{S}_{sN}, \quad j = 0, 1, \dots, N-1.$$

In words, U_j includes the coalescence point $x_j = x_N$, but excludes all the others. The diagonal set:

$$\mathsf{U}_j^{(\mathrm{d})} = \{\mathbf{x} \in \mathsf{U}_j : x_j = x_N\}.$$

Proposition[FHOS2009]. For each index $j = 1, \dots, N-1$, there exists an open connected set $\Omega_j \subset \mathsf{U}_j$, such that $\mathsf{U}_j^{(d)} \subset \Omega_j$, and two functions ξ_j, η_j, real analytic on Ω_j, such that for all $\mathbf{x} \in \Omega_j$ the following representation holds:

$$\psi(\hat{\mathbf{x}}, x) = \xi_j(\hat{\mathbf{x}}, x) + |x_j - x|\eta_j(\hat{\mathbf{x}}, x).$$

Theorem (The value of A)

If $N = 2$, *then the function* $\eta_1(x, x)$ *belongs to* $\mathsf{L}^{\frac{3}{4}}(\mathbb{R}^3)$ *and*

$$A = 2^{\frac{10}{3}} 3^{-\frac{8}{3}} \pi^{-\frac{10}{3}} \left[\int_{\mathbb{R}^3} |\eta_1(x, x)|^{\frac{3}{4}} dx \right]^{\frac{8}{3}}.$$

If $N = 3$, *then* $\eta_1(x, \cdot\,, x), \eta_2(\,\cdot\,, x, x) \in \mathsf{L}^2(\mathbb{R}^3)$ *a.e.* $x \in \mathbb{R}^3$ *and*

$$H(x) = \left[\int_{\mathbb{R}^3} \left(\big|\eta_1(x, t, x)\big|^2 + |\eta_2(t, x, x)|^2 \right) dt \right]^{\frac{1}{2}},$$

belongs to $\mathsf{L}^{\frac{3}{4}}(\mathbb{R}^3)$ *and*

$$A = 2^{\frac{10}{3}} 3^{-\frac{8}{3}} \pi^{-\frac{10}{3}} \left[\int_{\mathbb{R}^3} |H(x)|^{\frac{3}{4}} dx \right]^{\frac{8}{3}}.$$

Effective bounds

Effective bounds by S. Fournais and T. Ø. Sørensen:

Proposition (FS2018)

Let $\mathrm{d}(\hat{\mathbf{x}}, x) = \min\{|x|, |x - x_j|, j = 2, \dots, N\}$. *Then*

$$|\partial_x^m \psi(\hat{\mathbf{x}}, x)| \lesssim \mathrm{d}(\hat{\mathbf{x}}, x)^{1-|m|} e^{-\varkappa_m |\mathbf{x}|}, |m| \ge 1,$$

with some $\varkappa_m > 0$.

Singular values of integral operators

M. Birman - M.Solomyak (1977). Let $\mathcal{C} = (0,1)^d$

Proposition. Let $T_{ba} : \mathsf{L}^2(\mathcal{C}) \to \mathsf{L}^2(\mathbb{R}^n)$, be the integral operator of the form

$$(T_{ba}u)(t) = b(t) \int T(t,x)a(x)u(x)\,dx,$$

where $a \in \mathsf{L}^2(\mathcal{C})$, $b \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$, and the kernel $T(t,x)$, $t \in \mathbb{R}^n$, $x \in \mathcal{C}$, is such that $T(t,\ \cdot\ ) \in \mathsf{H}^l(\mathcal{C})$ with some $l = 1, 2, \dots$, $2l > d$, a.e. $t \in \mathbb{R}^n$, and the function $\|T(t,\cdot)\|_{\mathsf{H}^l}$ is in $\mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^n)$. Then

$$s_k(T_{ba}) \lesssim k^{-\frac{1}{2}-\frac{l}{d}} \left[\int \|T(t,\ \cdot\ )\|^2_{\mathsf{H}^l}\, |b(t)|^2\, dt\right]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C})},$$

$k = 1, 2, \dots$, with some implicit constant independent of the kernel T, weights a, b and the index k. In other words, $T_{ba} \in \mathbf{S}_{q,\infty}$ with

$$\frac{1}{q} = \frac{1}{2} + \frac{l}{d},$$

and

$$\|T_{ba}\|_{q,\infty} \lesssim \left[\int \|T(t,\ \cdot\ )\|^2_{\mathsf{H}^l}\, |b(t)|^2\, dt\right]^{\frac{1}{2}} \|a\|_{\mathsf{L}^2(\mathcal{C})}.$$

Aim to prove

Lemma. Let $\mathcal{C}_n = [0,1)^3 + n$, $n \in \mathbb{Z}^3$.
Then $s_k(\Psi \mathbb{1}_{\mathcal{C}_n}) \lesssim e^{-c|n|} k^{-4/3}$.

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Proof. Assume $N = 2$, so

$$|\partial_x^m \psi(x_1, x)| \lesssim e^{-\varkappa_m |\mathbf{x}|} \big(|x - x_1|^{1-|m|} + |x|^{1-|m|}\big), \ |m| \geq 1.$$

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The following domains are treated differently:

1. $|x_1| < 2\varepsilon$, $(\phi_1^{(\varepsilon)})$,
2. $|x_1| > 2\varepsilon$.
   - 2.1 $|x - x_1| < \varepsilon$, $|x| > \varepsilon$, $(\phi_{2,1}^{(\varepsilon)})$,
   - 2.2 $|x - x_1| > \varepsilon$, $|x| < \varepsilon$, $(\phi_{2,2}^{(\varepsilon)})$,
   - 2.3 $|x - x_1| > \varepsilon$, $|x| > \varepsilon$, $(\phi_{2,3}^{(\varepsilon)})$.

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   - 2.3 $|x - x_1| > \varepsilon$, $|x| > \varepsilon$, $\quad (\phi_{2,3}^{(\varepsilon)})$.

Let $\zeta \in C_0^\infty(\mathbb{R})$ be s.t. $\zeta(t) = 0, |t| \geq 1$, $\zeta(t) = 1, |t| \leq 1/2$, and let $\omega(t) = 1 - \zeta(t)$.

Step 1: $|x_1| < 2\varepsilon$. Look at

$$\phi_1^{(\varepsilon)}(x_1, x) = \psi(x_1, x)\zeta(|x_1|(4\varepsilon)^{-1}).$$

Then

$$|\partial_x^2 \phi_1^{(\varepsilon)}(x_1, x)| \lesssim e^{-\varkappa_2|\mathbf{x}|}\big(|x_1 - x|^{-1} + |x|^{-1}\big)\zeta(|x_1|(4\varepsilon)^{-1}),$$

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so

$$\|\phi_1^{(\varepsilon)}(x_1, \ \cdot\ )\|_{\mathsf{H}^2}^2 \lesssim \mathbb{1}_{\{|x_1|<2\varepsilon\}}, \quad \mathsf{H}^2 = \mathsf{H}^2(\mathcal{C}_n),$$

and hence

$$\int_{\mathbb{R}^3} \|\phi_1^{(\varepsilon)}(x_1, \ \cdot\ )\|_{\mathsf{H}^2}^2 dx_1 \lesssim e^{-c|n|}\varepsilon^3.$$

Thus

$$s_k(\phi_1^{(\varepsilon)}) \lesssim k^{-1/2-2/3} e^{-c|n|}\varepsilon^{3/2} = k^{-7/6} e^{-c|n|}\varepsilon^{3/2}.$$

Step 2.1: $|x_1| > 2\varepsilon$, $|x - x_1| < \varepsilon$, $|x| > \varepsilon$. Look at

$$\phi_{2,1}^{(\varepsilon)}(x_1, x) = \psi(x_1, x)\zeta(|x - x_1|\varepsilon^{-1})\omega(|x_1|(4\varepsilon)^{-1}).$$

Then

$$|\partial_x^2 \phi_{2,1}^{(\varepsilon)}(x_1, x)| \lesssim e^{-\varkappa_2 |\mathbf{x}|}|x_1 - x|^{-1}\omega(|x_1|(4\varepsilon)^{-1})\mathbb{1}_{\{|x - x_1| < \varepsilon\}},$$

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so

$$\int_{\mathbb{R}^3} \|\phi_{2,1}^{(\varepsilon)}(x_1, \ \cdot\ )\|_{\mathrm{H}^2}^2 dx_1 \lesssim e^{-c|n|} \int e^{-c|x_1|} \bigg[\int_{|x-x_1|<\varepsilon} \frac{1}{|x - x_1|^2} dx \bigg] dx_1 \lesssim e^{-c|n|}\varepsilon.$$

Thus

$$s_k(\phi_{2,1}^{(\varepsilon)}) \lesssim k^{-1/2-2/3} e^{-c|n|}\varepsilon^{1/2} = e^{-c|n|}k^{-7/6}\varepsilon^{1/2}.$$

Step 2.2: $|x_1| > 2\varepsilon$, $|x - x_1| > \varepsilon$, $|x| < \varepsilon$. Look at

$$\phi_{2,2}^{(\varepsilon)}(x_1, x) = \psi(x_1, x)\zeta(|x|\varepsilon^{-1})\omega(|x_1|(4\varepsilon)^{-1}).$$

Then

$$|\partial_x^2 \phi_{2,2}^{(\varepsilon)}(x_1, x)| \lesssim e^{-\varkappa_2|\mathbf{x}|}|x|^{-1}\omega(|x_1|(4\varepsilon)^{-1})\mathbb{1}_{\{|x|<\varepsilon\}},$$

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so

$$\int_{\mathbb{R}^3} \|\phi_{2,2}^{(\varepsilon)}(x_1, \ \cdot\ )\|_{\mathsf{H}^2}^2 dx_1 \lesssim e^{-c|n|} \int\limits_{|x|<\varepsilon} \frac{1}{|x|^2} dx \lesssim e^{-c|n|}\varepsilon.$$

Thus

$$s_k(\phi_{2,2}^{(\varepsilon)}) \lesssim e^{-c|n|} k^{-7/6} \varepsilon^{1/2}.$$

Step 2.3: $|x_1| > 2\varepsilon$, $|x - x_1| > \varepsilon$, $|x| > \varepsilon$. Look at

$$\phi_{2,3}^{(\varepsilon)}(x_1, x) = \psi(x_1, x)\omega(|x|\varepsilon^{-1})\omega(|x - x_1|\varepsilon^{-1})\omega(|x_1|(4\varepsilon)^{-1}).$$

Then

$$|\partial_x^m \phi_{2,3}^{(\varepsilon)}(x_1, x)| \lesssim e^{-\varkappa_m|\mathbf{x}|}\big(\, |x|^{1-|m|} + |x - x_1|^{1-|m|}\big) \\ \times \omega(|x_1|(4\varepsilon)^{-1})\mathbb{1}_{\{|x|>\varepsilon\}}\mathbb{1}_{\{|x-x_1|>\varepsilon\}},$$

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so for all $l \geq 3$:

$$\int_{\mathbb{R}^3} \|\phi_{2,3}^{(\varepsilon)}(x_1, \,\cdot\,)\|_{\mathsf{H}^l}^2 dx_1 \\ \lesssim e^{-c|n|} \int e^{-c|x_1|}\Big[\int_{|x|>\varepsilon} |x|^{2-2l} dx + \int_{|x-x_1|>\varepsilon} |x - x_1|^{2-2l} dx\Big] dx_1 \\ \lesssim e^{-c|n|}\varepsilon^{5-2l}.$$

Step 2.3: $|x_1| > 2\varepsilon$, $|x - x_1| > \varepsilon$, $|x| > \varepsilon$. Look at

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$$\int_{\mathbb{R}^3} \|\phi_{2,3}^{(\varepsilon)}(x_1, \cdot\,)\|_{\mathsf{H}^l}^2 dx_1 \\ \lesssim e^{-c|n|}\int e^{-c|x_1|}\Big[\int_{|x|>\varepsilon} |x|^{2-2l}dx + \int_{|x-x_1|>\varepsilon} |x - x_1|^{2-2l}dx\Big]dx_1 \\ \lesssim e^{-c|n|}\varepsilon^{5-2l}.$$

Thus

$$s_k(\phi_{2,3}^{(\varepsilon)}) \lesssim e^{-c|n|}k^{-1/2-l/3}\varepsilon^{5/2-l}.$$

Use the inequality

$$s_{2k-1}(T_1 + T_2) \le s_k(T_1) + s_k(T_2)$$

three times:

$$\begin{aligned} s_{4k-3}(\Psi \mathbb{1}_{\mathcal{C}_n}) &\le s_k(\phi_1^{(\varepsilon)}) + s_k(\phi_{2,1}^{(\varepsilon)}) + s_k(\phi_{2,2}^{(\varepsilon)}) + s_k(\phi_{2,3}^{(\varepsilon)}) \\ &\lesssim e^{-c|n|}\big(k^{-7/6}\varepsilon^{3/2} + k^{-7/6}\varepsilon^{1/2} + k^{-1/2-l/3}\varepsilon^{5/2-l}\big) \\ &\lesssim e^{-c|n|} k^{-7/6}\varepsilon^{1/2}\big(1 + k^{(2-l)/3}\varepsilon^{2-l}\big). \end{aligned}$$

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Choice of ε:

$$k^{(2-l)/3}\varepsilon^{2-l} = 1, \quad \text{so} \quad \varepsilon = k^{-1/3},$$

and hence,

$$s_{4k-3}(\Psi \mathbb{1}_{\mathcal{C}_n}) \lesssim e^{-c|n|} k^{-4/3}.$$

□

Alternative formulation:

$$\|\Psi \mathbb{1}_{\mathcal{C}_n}\|_{3/4,\infty} = \sup_k k^{4/3} s_k(\Psi \mathbb{1}_{\mathcal{C}_n}) \lesssim e^{-c|n|}, \quad n \in \mathbb{Z}^3.$$

Recall: if $T \in \mathbf{S}_{p,\infty}, 0 < p < 1$, then

$$\| \sum_j T_j \|_{p,\infty}^p \le (1-p)^{-1} \sum_j \| T_j \|_{p,\infty}^p.$$

Therefore

$$\|\Psi\|_{3/4,\infty}^{3/4} \le 4 \sum_{n\in\mathbb{Z}^3} \|\Psi \mathbb{1}_{\mathcal{C}_n}\|_{3/4,\infty}^{3/4} \lesssim \sum_{n\in\mathbb{Z}^3} e^{-c|n|} < \infty,$$

as required.

Asymptotics

Proposition Asymptotics. Let $X, Y \subset \mathbb{R}^d$, $d \ge 1$, be bounded Borel sets. Let $T : \mathsf{L}^2(Y) \to \mathsf{L}^2(X)$ be the operator with the kernel

$$T(x, y) = \rho_1(x)|x - y|^\alpha \phi(x, y)\rho_2(y),$$

where $\alpha > -d$, $\rho_1 \in \mathsf{L}^\infty(X), \rho_2 \in \mathsf{L}^\infty(Y)$, and $\phi \in \mathsf{C}^\infty(\overline{X} \times \overline{Y})$. Then for $p^{-1} = 1 + \alpha d^{-1}$ we have

$$\mathsf{g}_p(T) = \mathsf{G}_p(T) = \mu_{\alpha,d} \int\limits_{X \cap Y} |\rho_1(x)\phi(x, x)\rho_2(x)|^p dx,$$

with

$$\mu_{\alpha,d} = \frac{1}{\Gamma\big(d/2 + 1\big)} \left[\frac{\Gamma\big((d + \alpha)/2\big)}{\pi^{\alpha/2}|\Gamma(-\alpha/2)|}\right]^p, \qquad \alpha \ne 0, 2, 4, \dots,$$

$$\mu_{\alpha,d} = 0, \quad \alpha = 0, 2, 4, \dots.$$

More precise bound

For some $\varkappa > 0$ assume

$$S(a) = \left[\sum_{n\in\mathbb{Z}^3} e^{-q\varkappa|n|}\|a\|^q_{\mathsf{L}^2(\mathcal{C}_n)}\right]^{\frac{1}{q}} < \infty, \quad q = \frac{3}{4}.$$

Assume that $b \in \mathsf{L}^\infty(\mathbb{R}^{3N-3})$, so that

$$M(b) = \left[\int_{\mathbb{R}^{3N-3}} |b(\hat{\mathbf{x}})|^2 e^{-2\varkappa|\hat{\mathbf{x}}|} d\hat{\mathbf{x}}\right]^{\frac{1}{2}} < \infty.$$

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Theorem. Assume (1). Then for some $\varkappa \in (0, \varkappa_0)$ we have

$$\mathsf{G}_{3/4}\big(b\Psi a\big) \lesssim \big[M(b)S(a)\big]^{3/4}.$$

Idea of the proof (for $N = 2$)

Use the representation

$$\psi(x_1, x) = \xi_1(x_1, x) + |x_1 - x|\eta_1(x_1, x). \tag{2}$$

Assume for simplicity that it holds everywhere except for $x = 0, x_1 = 0$.

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Assume for simplicity that it holds everywhere except for $x = 0, x_1 = 0$.
Let $\zeta \in \mathrm{C}_0^\infty(\mathbb{R})$ be s.t. $\zeta(t) = 0, |t| \ge 1$, $\zeta(t) = 1, |t| \le 1/2$, and let $\omega(t) = 1 - \zeta(t)$. Split:

$$\begin{aligned}\psi(x_1, x) = {} & \omega(x_1/\varepsilon)\zeta(x_1/R)\omega(x/\varepsilon)\zeta(x/R)\psi(x_1, x)\Big(= \psi_{\varepsilon,R}(x_1, x)\Big)\\ & + \Big[\zeta(x_1/\varepsilon) + \omega(x_1/\varepsilon)\zeta(x/\varepsilon) + \omega(x_1/\varepsilon)\omega(x/\varepsilon)\omega(x/R)\\ & + \omega(x_1/\varepsilon)\omega(x_1/R)\omega(x/\varepsilon)\zeta(x/R)\Big]\psi(x_1, x).\end{aligned}$$

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$$\psi(x_1, x) = \omega(x_1/\varepsilon)\zeta(x_1/R)\omega(x/\varepsilon)\zeta(x/R)\psi(x_1, x)\Big(= \psi_{\varepsilon,R}(x_1, x)\Big)$$

$$+ \Big[\zeta(x_1/\varepsilon) + \omega(x_1/\varepsilon)\zeta(x/\varepsilon) + \omega(x_1/\varepsilon)\omega(x/\varepsilon)\omega(x/R)$$

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Contribution from the last four terms $\to 0$ as $\varepsilon \to 0$ and $R \to \infty$. Therefore

$$G_{3/4}(\Psi) = \lim_{\varepsilon\to 0, R\to\infty} G_{3/4}(\Psi_{\varepsilon,R}),$$

$$g_{3/4}(\Psi) = \lim_{\varepsilon\to 0, R\to\infty} g_{3/4}(\Psi_{\varepsilon,R}).$$

Apply Proposition Asymptotics to the kernel

$$\omega(x_1/\varepsilon)\zeta(x_1/R)|x - x_1|\eta_1(x_1, x)\omega(x/\varepsilon)\zeta(x/R).$$

Then $\alpha = 1$, $1/p = 1 + 1/3 = 4/3$, and

$$\mathsf{G}_{3/4}(\Psi_{\varepsilon,R}) = \mathsf{g}_{3/4}(\Psi_{\varepsilon,R}) = \mu_{1,3} \int |\omega(x/\varepsilon)|^{3/2}\zeta(x/R)^{3/2}|\eta_1(x,x)|^{3/4}dx.$$

Both $\mathsf{G}_{3/4}(\Psi_{\varepsilon,R})$ and $\mathsf{g}_{3/4}(\Psi_{\varepsilon,R})$ have limits, so they are bounded. By the Monotone Convergence Theorem (Beppo-Levi), $\eta_1 \in \mathsf{L}^{3/4}(\mathbb{R})$.