Spectral asymptotics of the one-particle density matrix for the Coulombic multi-particle systems

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Multi-particle system

Begin with the Schrödinger operator

$$H = \sum_{k=1}^{N} \Big(-\Delta_k - \frac{Z}{|x_k|} \Big) + \sum_{1\le j<k\le N} \frac{1}{|x_j - x_k|}.$$

Here $X = (x_1, x_2, \dots, x_N)$,
$x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, N$, are coordinates of "electrons",
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$Z > 0$ is the "nuclear" charge.
The underlying space is $\mathsf{L}^2(\mathbb{R}^{3N})$,
H is self-adjoint on $\mathsf{H}^2(\mathbb{R}^{3N})$.
Let $\psi \in \mathsf{L}^2(\mathbb{R}^{3N})$ be an eigenfunction of H:

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

with some $E \in \mathbb{R}$.

Density matrix

Define *the one-particle density matrix:*

$$\gamma(x,y) = \int \overline{\psi(\hat{X},x)}\,\psi(\hat{X},y)\,d\hat{X},$$

and *the one-particle kinetic energy density matrix:*

$$\tau(x,y) = \int_{\mathbb{R}^{3N-3}} \overline{\nabla_x\psi(\hat{X},x)}\cdot\nabla_y\psi(\hat{X},y)\,d\hat{X}.$$

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Let Γ, T be the operators with kernel $\gamma(x, y)$.
Represent: $\Gamma = \Psi^* \Psi$, where $\Psi : \mathsf{L}^2(\mathbb{R}^3) \mapsto \mathsf{L}^2(\mathbb{R}^{3N-3})$ is given by

$$(\Psi u)(\hat{X}) = \int_{\mathbb{R}^3} \psi(\hat{X}, x) u(x) dx,$$

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$$(\Psi u)(\hat{X}) = \int_{\mathbb{R}^3} \psi(\hat{X}, x) u(x) dx,$$

and $\mathsf{T} = \mathsf{V}^*\mathsf{V}$, where $\mathsf{V} : \mathsf{L}^2(\mathbb{R}^3) \mapsto \mathsf{L}^2(\mathbb{R}^{3\mathrm{N}-3}, \mathbb{C}^3)$ is given by

$$(\mathsf{V}u)(\hat{X}) = \int_{\mathbb{R}^3} \nabla_x \psi(\hat{X}, x) u(x) dx.$$

Since $\psi, \nabla_x \psi \in \mathsf{L}^2(\mathbb{R}^{3N})$, the operators Ψ, V are Hilbert-Schmidt, and hence Γ and T are trace class: $\|\Gamma\|_1 = \|\Psi\|_2^2$, $\|\mathsf{T}\|_1 = \|\mathsf{V}\|_2^2$.

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Plan:

1. Spectral estimates for the operator Γ
2. Spectral asymptotics for Γ.

Asymptotics

Suppose that $|\psi(X)| \lesssim e^{-\varkappa|X|}$, $\varkappa > 0$, $X \in \mathbb{R}^{3N}$: Agmon(1982), Froese-Herbst(1982) and many others.

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Let $\tilde{X}_j = (x_1, x_2, \dots, x_{j-1}, x_{j+1}, \dots, x_{N-1})$, $j = 1, 2, \dots, N-1$, so $\hat{X} = (\tilde{X}_j, x_j)$, $X = (\tilde{X}_j, x_j, x)$.

Theorem. Let $H(x) = \frac{1}{4}\psi(x, x)$, for $N = 2$, and

$$H(x) = \frac{1}{4}\bigg[\sum_{j=1}^{N-1}\int_{\mathbb{R}^{3N-6}} \big|\psi(\tilde{X}_j, x, x)\big|^2 \, d\tilde{X}_j\bigg]^{\frac{1}{2}}, \quad \text{for} \quad N \ge 3.$$

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Define

$$A = \frac{1}{3}\left(\frac{2}{\pi}\right)^{5/4} \int_{\mathbb{R}^3} |H(x)|^{\frac{3}{4}}\, dx, \quad B = \frac{4}{3\pi}\int_{\mathbb{R}^3} H(x)\, dx.$$

Then

$$\lim_{k\to\infty} k^{8/3}\lambda_k(\Gamma) = A^{8/3}, \quad \lim_{k\to\infty} k^2 \lambda_k(\mathrm{T}) = \mathrm{B}^2.$$

Remark

If ψ is antisymmetric (i.e. for spinless fermions), then $A = 0$.

If spin is present, consider $N = 2$. There are two possible pair configurations: *singlet* and *triplet*.
Singlet: ψ is symmetric, thus $A \neq 0$.
Triplet: ψ is antisymmetric and then $A = 0$. In this case $\lambda_k \lesssim k^{-\frac{10}{3}}$.

Asymptotics

Since $\Gamma = \Psi^*\Psi, \mathrm{T} = \mathrm{V}^*\mathrm{V}$, we have $\lambda_k(\Gamma) = s_k(\Psi)^2$, $\lambda_k(\mathrm{T}) = s_k(\mathrm{V})^2$ where $s_k(G) = \sqrt{\lambda_k(G^*G)}$ are singular values (or s-values) of G. Thus:

$$\lim_{k\to\infty} k^{4/3}\, s_k(\Psi) = A^{4/3}, \quad \lim_{k\to\infty} k\, s_k(\mathrm{V}) = B.$$

The key fact: the decay rate of s_k depends on the smoothness of ψ.
We focus on the operator Ψ only.

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We focus on the operator Ψ only.
For simplicity: $N = 2$. Then if x, t are away from 0, then

$$\psi(t,x) \sim \tilde{\phi}(t,x) + |x-t|\phi(t,x), \quad \text{with smooth} \quad \phi, \tilde{\phi}.$$

Proposition (M.Birman-M.Solomyak 1970-1977)

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

$$\lim_{k\to\infty} \big(k^{1/p} s_k(T)\big)^p = \mu_{\alpha,d} \int\limits_{X\cap Y} |\rho_1(x)\phi(x, x)\rho_2(x)|^p \, dx,$$

with

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

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

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

Remark: for $\alpha = 1, d = 3$, we have $1/p = 4/3$, as required: $\lim_{k\to\infty} k^{4/3} s_k(\Psi) = A^{4/3}$.

Intuition

Consider the operator T on $\mathsf{L}^2(\mathbb{T})$, $\mathbb{T} = \mathbb{R}^d/(2\pi\mathbb{Z})^d$, with the kernel $\mathcal{T}(\mathbf{x}-\mathbf{y})$, where $\mathcal{T}$ is $(2\pi\mathbb{Z})^d$-periodic. Then the equation $Tu = \lambda u$ transforms into $\hat{\mathcal{T}}_{\mathbf{n}}\hat{u}_{\mathbf{n}} = \lambda\hat{u}_{\mathbf{n}}$, $\mathbf{n}\in\mathbb{Z}^d$. If $\mathcal{T}(\mathbf{x}) = |\mathbf{x}|^\alpha\phi(\mathbf{x}),\ \mathbf{x}\in[0,2\pi)^d$, then $\hat{\mathcal{T}}_{\mathbf{n}}\sim|\mathbf{n}|^{-\alpha-d}$, so $\lambda_k\sim k^{-1-\alpha d^{-1}}$.

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Pathway to the estimates:

- Study regularity of ψ.
- Estimates for s-values of integral operators via regularity of their kernels.

Regularity of the eigenfunctions

- Since $|x|^{-1}$ is real analytic away from $x = 0$, the function ψ is real analytic away from the coalescence points.
- T. Kato (1957): ψ is Lipschitz.
- Fournais, T. and M. Hoffmann-Ostenhof, Sørensen: 2006–2020.

Regularity

Represent the solution ψ of the equation $-\Delta\psi + (V - E)\psi = 0$: $\psi(X) = e^{F_0(X)}\phi(X)$, where

$$F_0(X) = -\frac{Z}{2}\sum_{j=1}^{N}|x_j| + \frac{1}{4}\sum_{1\le j<k\le N}|x_j - x_k|,$$

The function e^{F_0} is called the Jastrow factor. Important: $V = \Delta F_0$ and $\nabla F_0 \in \mathsf{L}^\infty(\mathbb{R}^{3N})$:

$$-\Delta\phi - 2\nabla F_0\cdot\nabla\phi - (|\nabla F_0|^2 + E)\phi = 0.$$

Then ϕ is "smoother" than ψ.

Let

$$F(X) = -\frac{Z}{2}\sum_{j=1}^{N} |x_j|\zeta(x_j) + \frac{1}{4}\sum_{1\le j<k\le N} |x_j - x_k|\zeta(x_j - x_k),$$

and $\zeta \in \mathsf{C}_0^\infty(\mathbb{R}^3)$, $\zeta(t) = 1, |t| \le 1$. Then

$$-\Delta\phi - 2\nabla F\cdot\nabla\phi + (V - \Delta F - |\nabla F|^2 - E)\phi = 0.$$

Observe: $\nabla^k(V - \Delta F) \in \mathsf{L}^\infty(\mathbb{R}^{3N})$, $k = 0, 1, \dots,$ and $F, \nabla F \in \mathsf{L}^\infty(\mathbb{R}^{3N})$.
Thus for any $R > 0$:

$$|\psi(X)| + |\nabla\psi(X)| \lesssim |\phi(X)| + |\nabla\phi(X)| \lesssim \|\phi\|_{\mathsf{L}^2(B(X,R))} \lesssim \|\psi\|_{\mathsf{L}^2(B(X,R))}.$$

Fournais, T. and M. Hoffmann-Ostenhof, Sørensen.

The coalescence set:

$$\Sigma = \left\{ X = (\hat{X}, x) \in \mathbb{R}^{3N} : |x| \prod_{k=1}^{N-1} |x - x_k| = 0 \right\}.$$

The distance to Σ:

$$d(\hat{X}, x) := \min \left\{ |x|, \frac{1}{\sqrt{2}} |x - x_j|, \ j = 1, 2, \dots, N-1 \right\},$$

$$\delta(\hat{X}, x) := d(\hat{X}, x) \wedge 1.$$

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Theorem. (Fournais–Sørensen 2018) For all $X \in \mathbb{R}^{3N} \setminus \Sigma$ and any $R > 0$:

$$|\partial_x^m \phi(\hat{X}, x)| \lesssim \delta(\hat{X}, x)^{1-|m|} \|\psi\|_{\mathsf{L}^2(B(X,R))}, \quad |m| \geq 1,$$

and hence,

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Need more smoothness!

Indeeed, assume again $N = 2$ and represent

$$\psi(t,x) = e^{-Z/2(|t|+|x|)\zeta(t)\zeta(x)}\left(\phi(t,x) + \frac{1}{4}|t-x|\phi(t,x) + \dots\right).$$

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Recall from general theory: $\phi \in \mathrm{W}^{2,p}$, where $p < \infty$ is arbitrary.

Represent $\phi = e^{F_3}\tilde{\phi}$ where

$$F_3(X) = Z\frac{2-\pi}{12\pi}\sum_{1\le j<k\le N}(x_j \cdot x_k)\ln\left(|x_j|^2 + |x_k|^2\right)\zeta(x_k)\zeta(x_j).$$

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Proposition. [FHOS2005] $\tilde{\phi} \in \mathrm{W}^{2,\infty}(\mathbb{R}^{3N})$ and for any $R > 0$ and $r \in (0, R)$:

$$\|\tilde{\phi}\|_{\mathrm{W}^{2,\infty}(B(X,r))} \lesssim \|\psi\|_{\mathrm{L}^2(B(X,R))}.$$

Observing that $|\partial_x^m F_3(\hat{X}, x)| \lesssim 1$ for $|m| \le 2$, we conclude that

$$|\partial_x^m \phi(\hat{X}, x)| \lesssim \|\psi\|_{\mathsf{L}^2(B(X,R))}, \quad |m| = 2.$$

Theorem. For all $X \in \mathbb{R}^{3N} \setminus \Sigma$ and any $R > 0$:

$$|\partial_x^m \phi(\hat{X}, x)| \lesssim \delta(\hat{X}, x)^{2-|m|} \|\psi\|_{\mathsf{L}^2(B(X,R))}, \quad |m| \ge 2.$$

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Having obtained bounds for the derivatives of ψ and ϕ can now proceed to estimating singular values of the corresponding integral operators.

The Besov and Nikol'skii spaces

For a function $u = u(x)$, $x \in \mathbb{R}^d$, and arbitrary $l = 0, 1, 2, \dots,$ define the finite difference

$$\Delta_h^{(l)} u(x) = \sum_{j=0}^{l} (-1)^{j+l} \binom{l}{j} u(x + jh),$$

and the L^q*-modulus of smoothness of order* l:

$$\omega_q^{(l)}(u; t) = \sup_{|h| \le t} \|\Delta_h^{(l)} u\|_{\mathsf{L}^q}, \quad t > 0.$$

We say that u belongs to the Besov space $\mathsf{B}^s_{q,\infty}(\mathbb{R}^d)$, $s > 0$, $q \in [1, \infty]$, if for some $l > s$ we have

$$\|u\|_{\mathsf{B}^s_{q,\infty}} := \|u\|_{\mathsf{L}^q} + \sup_{t>0} t^{-s} \omega_q^{(l)}(u; t) < \infty.$$

Notation $\mathsf{N}^s_q(\mathbb{R}^d) = \mathsf{B}^s_{q,\infty}(\mathbb{R}^d)$, the Nikol'skii space.
Scale of spaces: $\mathsf{B}^s_{q,r}(\mathbb{R}^d)$, $0 < r \le \infty$.

The Besov spaces

For a domain $\Omega \subset \mathbb{R}^d$ the space $\mathsf{N}^s_q(\Omega)$ is defined as the restriction of $\mathsf{N}^s_q(\mathbb{R}^d)$ to Ω. The corresponding norm of the function $u \in \mathsf{N}^s_q(\Omega)$ is defined as

$$\|u\|_{\mathsf{N}^s_q(\Omega)} = \inf \|g\|_{\mathsf{N}^s_q(\mathbb{R}^d)},$$

where the infimum is taken over all functions $g \in \mathsf{N}^s_q(\mathbb{R}^d)$ such that $u = g$ for a.e. $x \in \Omega$. In other words, a function u belongs to $\mathsf{N}^s_q(\Omega)$ if it has an extension $g \in \mathsf{N}^s_q(\mathbb{R}^d)$.

An example

Let $u(x) = |x|^\alpha$. If $\alpha > -d/q$, then $\omega_q^{(l)}(u; t) \lesssim t^s$, $s = \alpha + d/q$, see Birman-Solomyak(1977).

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Let $u \in \mathsf{C}^\infty(\mathbb{R}^d \setminus \Xi)$, where $\Xi = \{a_1, a_2, \dots, a_N\}$, $a_k \in \mathbb{R}^d$, $k = 1, 2, \dots, N$.
Denote

$$\delta(x) = \mathrm{dist}(x, \Xi) \wedge 1$$

and assume that for some $\alpha \in \mathbb{R}$ and some $A \ge 0$ we have

$$|\partial_x^j u(x)| \lesssim A\big(1 + \delta(x)^{\alpha - |j|}\big), \quad \text{for all} \quad x \notin \Xi \quad \text{and} \quad |j| = 0, 1, \dots .$$

Lemma

Suppose that $d \ge 2$. If $\alpha > -d/q$ with some $1 \le q \le d$, then for all $x_0 \in \mathbb{R}^d$ and $R > 0$ the function u belongs to $\mathsf{N}_q^s(B)$, $B = B(x_0, R)$, with $s = \alpha + d/q$. Moreover, $\|u\|_{\mathsf{N}_q^s(B)} \lesssim A$ where the implicit constant does not depend on x_0 and the set Ξ, but may depend on the radius R.

Bounds for singular values of integral operators

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

Proposition

Assume that the kernel $T(t,x), t \in \mathbb{R}^l$, $x \in X$, *is such that* $T(t,\,\cdot\,) \in \mathsf{N}_2^s(\mathcal{C})$ *with some* $s > 0$, *for a.e.* $t \in \mathbb{R}^l$. *Assume that* $b \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^l)$ *and that* $a \in \mathsf{L}^r(\mathcal{C})$, *where*

$$\begin{cases} r = 2, & \text{if} \quad 2s > d, \\ r > 2, & \text{if} \quad 2s = d, \\ r > ds^{-1}, & \text{if} \quad 2s < d. \end{cases}$$

Then the operator T_{ba} *with kernel* $b(t)T(t,x)a(x)$ *satisfies the bound*

$$s_k(T_{ba}) \lesssim k^{-\frac{1}{2}-\frac{s}{d}} \left[\int_{\mathbb{R}^l} \|T(t,\,\cdot\,)\|^2_{\mathsf{N}_2^s(\mathcal{C})} |b(t)|^2\, dt\right]^{\frac{1}{2}} \|a\|_{\mathsf{L}^r(\mathcal{C})},$$

under the assumption that the right-hand side is finite.

Estimate for singular values of Ψ

Study the singular values of $b\Psi a$, where $a = a(x), b = b(\hat{X})$, $x \in \mathbb{R}^3, \hat{X} \in \mathbb{R}^{3N-3}$. Let $\mathcal{C}_n = [0,1)^3 + n, n \in \mathbb{Z}^3$. Assume

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

Assume that $b \in \mathsf{L}^2_{\mathrm{loc}}(\mathbb{R}^{3N-3})$, so that

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

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Theorem.

$$s_k(b\Psi a) \lesssim k^{-4/3} M(b) S(a), \; k = 1, 2, \dots .$$