Recent analytic and spectral results for the multi-particle Schrödinger operator
Lecture 1: background and results

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Multi-particle system

Begin with the Schrödinger operator

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

Here $x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, N$, are coordinates of "electrons",
$\mathbf{x} = (x_1, x_2, \dots, x_N) = (\hat{\mathbf{x}}, x), \hat{\mathbf{x}} = (x_1, x_3, \dots, x_{N-1})$,
Similar notation $\mathbf{x} = (\hat{\mathbf{x}}_j, x_j)$, where $\hat{\mathbf{x}}_j = (x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_N)$
$Z > 0$ is the "nuclear" charge.
The underlying space is $\mathsf{L}^2(\mathbb{R}^{3N})$.

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$Z > 0$ is the "nuclear" charge.
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For the Fermions: space of L^2-functions u such that $u \to -u$ under the interchange $x_j \leftrightarrow x_k$,
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 $E \in \mathbb{R}$.

One-particle density matrix

Define *the one-particle density matrix:*

$$\tilde{\gamma}(x, y) = \sum_{j=1}^{N} \int_{\mathbb{R}^{3N-3}} \overline{\psi(\hat{\mathbf{x}}_j, x)} \psi(\hat{\mathbf{x}}_j, y) d\hat{\mathbf{x}}_j.$$

For the Fermions:

$$\tilde{\gamma}(x, y) = N \int_{\mathbb{R}^{3N-3}} \overline{\psi(\hat{\mathbf{x}}, x)} \psi(\hat{\mathbf{x}}, y) d\hat{\mathbf{x}}.$$

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For our purposes we adopt the definition

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

The one-particle density:

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

Advantage: dramatic reduction in the number of variables!

Elementary fact.
Let Γ be the operator on $\mathsf{L}^2(\mathbb{R}^3)$ with kernel $\gamma(x, y)$,
and let $\Psi : \mathsf{L}^2(\mathbb{R}^3) \to \mathsf{L}^2(\mathbb{R}^{3N-3})$ be the operator with kernel $\psi(\hat{\mathbf{x}}, x)$:

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

Then $\Gamma = \Psi^* \Psi$.

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Lemma. The operator Γ is trace class and

$$\operatorname{tr} \Gamma = \|\Gamma\|_1 = \|\Psi\|_2^2 = \|\psi\|_{\mathsf{L}^2}^2.$$

Questions

1. Smoothness and decay of the eigenfunctions,
2. Smoothness and decay of the one-particle density and of the one-particle density matrix,
3. How fast do the eigenvalues $\lambda_k(\Gamma)$ decay as $k \to \infty$? In other words, how well do finite rank operators approximate Γ?

Fall-off at infinity and smoothness of the eigenfunction

Classical result:

$$|\psi(\mathbf{x})| \lesssim e^{-\varkappa_0|\mathbf{x}|}, \ \varkappa_0 > 0, \mathbf{x} \in \mathbb{R}^{3N}.$$

J-M.Combes-L.Thomas (1973), Sh. Agmon(1982), R. Froese-I.Herbst(1982) and many others.

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Denote $x_0 = 0$ and let

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

- Since $|x|^{-1}$ is real analytic away from $x = 0$, the function ψ is real analytic on the set
$$\mathrm{U} = \bigcap_{0 \le l < s \le N} \mathrm{S}_{ls}.$$
Follows from the classical elliptic theory.
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- S. Fournais, T. and M. Hoffmann-Ostenhof, T. Ø. Sørensen: FHOS2005, FHOS2009, FS2018.
Detailed analytic structure of the eigenfunctions near the coalescence points.

Pair coalescence points

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:

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

Observe that the sets $\mathsf{U}_j, \mathsf{U}_j^{(\mathrm{d})}$ are of full measure in $\mathbb{R}^{3N}$ and $\mathbb{R}^{3N-3}$ respectively,

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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:

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

Effective bounds

The previous proposition provides no information is available on ξ_j and η_j near the points $x_k = x_l$, $k, l \neq N$.
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*

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

with some $\varkappa_m > 0$.

Note: $|m| \geq 1$.

Spectral estimates

G. Friesecke (2003): Γ has infinite rank.
Suppose that

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

Theorem (Main Theorem 1: Estimates, Sob2020)

Assume (1). *Then Then* $\lambda_k(\Gamma) \lesssim k^{-8/3}$.

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Assume (1)*. Then Then* $\lambda_k(\Gamma) \lesssim k^{-8/3}$*.*

Theorem (Main Theorem 2: Asymptotics)

Assume (1)*. Then*

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

with an explicit constant $A \geq 0$*.*

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Theorem (Main Theorem 2: Asymptotics)

Assume (1). *Then*

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

with an explicit constant $A \geq 0$.

Since $\Gamma = \Psi^*\Psi$, we have $\lambda_k(\Gamma) = s_k(\Psi)^2$, where $s_k(\Psi)$ are singular values (or s-values) of Ψ. Thus:

$$s_k(\Psi) \lesssim k^{-4/3}, \qquad \lim_{k\to\infty} k^{4/3} s_k(\Psi) = A^{1/2}.$$

Recall:

$$\psi(\hat{\mathbf{x}}, x) = \xi_j(\hat{\mathbf{x}}, x) + |x_j - x|\eta_j(\hat{\mathbf{x}}, x), j = 1, 2, \dots, N.$$

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

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

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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

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

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

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

Smoothness of $\gamma(x, y)$

One-particle density: $\rho(x) = \gamma(x, x), x \in \mathbb{R}^3$.

- FHOS2002: $\rho \in C^\infty(\mathbb{R}^3 \setminus \{0\})$, $|\partial_x^m \rho(x)| \lesssim e^{-c|x|}, \ |x| \geq 1$.
- FHOS2004: ρ is real analytic on $\mathbb{R}^3 \setminus \{0\}$.
- FS2018: $|\partial_x^m \rho(x)| \lesssim |x|^{1-|m|} e^{-\varkappa_m |x|}, x \neq 0$.

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Theorem (Main Theorem 3, HS2020)

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

Remark

$\gamma(x, y)$ is analytic in the variable $x + y$ in the neighbourhood of $\{|x||y| \ne 0, x = y\}$. This implies the analyticity of $\rho(x)$.
However, $\gamma(x, y)$ is not smooth in the variable $x - y$.

Plan

- Lecture 2: Classes of compact operators
- Lecture 3: Spectral estimates and spectral asymptotics: proof of Theorems 1 and 2.
- Lecture 4: Real analyticity of the one-particle density matrix: proof of Theorem 3.

Exponential decay:

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Smoothness of solutions

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