Analytic Structure of Coulombic Wave Functions

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Outline

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1. Introduction and Results
   - Model and Problem
   - Previous Results
   - New Results
2. Idea of Proofs
   - Kustaanheimo-Stiefel Transformation
   - One-Particle Case
   - Many-Particle Case

Non-Relativistic Atom With Fixed Nucleus of Charge Z

Hamiltonian:

$$H = \sum_{j=1}^{N} -\Delta_j - \frac{Z}{|x_j|} + \sum_{1\leq i<j\leq N} \frac{1}{|x_i - x_j|} \equiv -\Delta + V$$

x_j: Position of electron # j
$-\Delta_j$: Kinetic energy of electron # j
$-\Delta$: Total kinetic energy V: Total potential energy

- Results valid more generally for molecules and moving nuclei.

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Regularity of Wave Functions

Problem:

What can be said about the structure/regularity of solutions to

$$H\psi = E\psi \quad ?$$

Away from Singularities of Potential

From analytic elliptic theory:

Let

$$\Sigma := \left\{ \mathbf{x} \in \mathbb{R}^{3N} \,\middle|\, \prod_j |x_j| \prod_{i<j} |x_i - x_j| = 0 \right\} \subset \mathbb{R}^{3N}.$$

be the set of 'coalescence points' - the singularities of V. If $\Omega \subset \mathbb{R}^{3N} \setminus \Sigma$ and $(-\Delta + V)\psi = E\psi$ in Ω then, since $V \in C^{\omega}(\Omega)$,

$$\psi \in C^{\omega}(\Omega) \qquad \text{(real analytic)}.$$

- Then what about at Σ ??

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Case Study: Hydrogen $N = 1$

Let $h = -\Delta_x - \frac{Z}{|x|}$, $x \in \mathbb{R}^3$. Then $\psi_0(x) = e^{-\frac{Z}{2}|x|}$ satisfies

$$h\psi_0 = -\frac{Z^2}{4}\psi_0 \, .$$

Regularity ψ_0:

$$\nabla\psi_0(x) = -\frac{Z}{2}\frac{x}{|x|}e^{-\frac{Z}{2}|x|}$$

which is **not** continuous at $x = 0$ - but which **is** bounded (L^∞)

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Previous Results: Many-Body Case

Theorem (Kato, 1957; Simon, 1974)

If $H\psi = E\psi$ then $\psi \in C^{\alpha}(\mathbb{R}^{3N})$ for any $\alpha \in (0,1)$.

Theorem (Kato 1957):

Let $\Omega \subset \mathbb{R}^{3N}$ be a neighbourhood of a two-particle coalescence point, say, $|x_1| = 0$ and $|x_j| \neq 0, j \neq 1, |x_i - x_j| \neq 0$.

If $H\psi = E\psi$ in Ω then $\psi \in C^{0,1}(\Omega)$.

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If $H\psi = E\psi$ in Ω then $\psi \in C^{0,1}(\Omega)$.

Many-Particle Coalescence Points

Theorem (SF, HO^2, TØS, 2005)

If $H\psi = E\psi$ *in* $\Omega \subset \mathbb{R}^{3N}$ *then*

$$\psi = e^{F_2+F_3}\phi\,, \quad \phi \in C^{1,1}_{\mathrm{loc}}(\Omega)$$

with $F_2 \in C^{0,1}_{\mathrm{loc}}(\mathbb{R}^{3N})$, $F_3 \in C^{1,\alpha}_{\mathrm{loc}}(\mathbb{R}^{3N})$, $\alpha \in (0,1)$, *given by*

$$F_2(x_1,\ldots,x_N) = \sum_{j=1}^{N} -\frac{Z}{2}|x_j| + \sum_{1\le i<j\le N} \frac{1}{4}|x_i - x_j|\,,$$

$$F_3(x_1,\ldots,x_N) = \frac{2-\pi}{12\pi} \sum_{1\le i<j\le N} (x_i\cdot x_j)\log(x_i^2 + x_j^2)\,.$$

Outline

Main Result Many-Particle Case

Two-Particle Coalescence points

Theorem (SF, HO², TØS, 2007)

Let $\Omega \subset \mathbb{R}^{3N}$ *be a neighbourhood of a two-particle coalescence point, say,* $|x_1| = 0$ *and* $|x_j| \neq 0, j \neq 1, |x_i - x_j| \neq 0$.

If $H\psi = E\psi$ *in* Ω *then*

$$\psi(\mathbf{x}) = \psi_1(\mathbf{x}) + |x_1|\psi_2(\mathbf{x}) \,, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^{3N} \,,$$

with $\psi_1, \psi_2 \in C^{\omega}(\Omega)$ *(real analytic).*

- Similarly around $|x_1 - x_2| = 0$.

Main Result One-Body Case

Theorem (SF, HO^2, TØS, 2007)

Let $\Omega \subset \mathbb{R}^3$ be a neighbourhood of the origin, and assume that $H\varphi = F$ in Ω, where

$$H = -\Delta_x + \frac{V}{|x|} + W\,,$$

$$F(x) = F^{(1)}(x) + \frac{F^{(2)}(x)}{|x|}\,, \quad x \in \Omega \subset \mathbb{R}^3\,,$$

with $V, W, F^{(1)}, F^{(2)} \in C^{\omega}(\Omega)$ (real analytic).
Then

$$\varphi(x) = \varphi^{(1)}(x) + |x|\varphi^{(2)}(x)\,, \quad x \in \Omega \subset \mathbb{R}^3$$

with $\varphi_1, \varphi_2 \in C^{\omega}(\Omega)$ (real analytic).

Main Result One-Body Case

Corollary (Hill, 1984; SF, HO^2, TØS, 2007)

Let $\Omega \subset \mathbb{R}^3$ be a neighbourhood of the origin, and assume that $H\varphi = 0$ in Ω, where

$$H = -\Delta_x - \frac{Z}{|x|} + W\,,$$

$$W(x) = W^{(1)}(x) + |x| W^{(2)}(x)\,, \quad x \in \Omega \subset \mathbb{R}^3\,,$$

with $W^{(1)}, W^{(2)} \in C^{\omega}(\Omega)$ (real analytic).
Then

$$\varphi(x) = \varphi^{(1)}(x) + |x| \varphi^{(2)}(x)\,, \quad x \in \Omega \subset \mathbb{R}^3$$

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MAIN Idea of Proofs
Kustaanheimo-Stiefel Transformation

Let $K : \mathbb{R}^4 \to \mathbb{R}^3$ be defined by

$$K(y) = \begin{pmatrix} y_1^2 - y_2^2 - y_3^2 + y_4^2 \\ 2(y_1 y_2 - y_3 y_4) \\ 2(y_1 y_3 + y_2 y_4) \end{pmatrix}, \quad y = (y_1, y_2, y_3, y_4) \in \mathbb{R}^4 .$$

Used in Celestial Mechanics to regularize the Kepler Problem (Kustaanheimo, Stiefel, Scheifele, Moser, Knauf,...)

Previously used for Schrödinger operators with Coulomb potentials by Jost, Chantelau, Knauf, Helffer, Siedentop, Weikard, C. Gérard, Castella, Jecko,...

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Properties of the KS Transformation $K : \mathbb{R}^4 \to \mathbb{R}^3$

Satisfies $|K(y)| = |y|^2$ for all $y \in \mathbb{R}^4$.

The restriction $\hat{K} : \mathbb{S}^3 \to \mathbb{S}^2$ is called the *Hopf fibration*, with fiber $\mathbb{S}^1$ (first example of map with non-trivial homotopy).

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Better in double polar coordinates: $\mathbb{R}^4 = \mathbb{R}^2 \times \mathbb{R}^2$,
$(y_1, y_4) = r_1(\cos\theta_1, \sin\theta_1)\ , \quad (y_3, y_2) = r_2(\cos\theta_2, \sin\theta_2)$

$$K(y) = \begin{pmatrix} r_1^2 - r_2^2 \\ -2r_1 r_2 \sin(\theta_1 - \theta_2) \\ 2r_1 r_2 \cos(\theta_1 - \theta_2) \end{pmatrix}.$$

Lemma

For $f : \mathbb{R}^3 \to \mathbb{R}$, let $f_K := f \circ K$, and let $L = \frac{\partial}{\partial\theta_1} + \frac{\partial}{\partial\theta_2}$. Then

- $[\Delta, L] = 0$.
- $(\Delta_x f)(K(y)) = \frac{1}{4|y|^2}\Delta_y f_K(y)$.
- *For $g : \mathbb{R}^4 \to \mathbb{R}$: $\quad Lg = 0 \Leftrightarrow g = f_K$ for some $f : \mathbb{R}^3 \to \mathbb{R}$.*

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Transformed Equation:

Using $(\Delta_x f)(K(y)) = \frac{1}{4|y|^2}\Delta_y f_K(y)$ and $|K(y)| = |y|^2$:

If

$$\Big[-\Delta_x + \frac{V(x)}{|x|} + W(x)\Big]\varphi(x) = F^{(1)}(x) + \frac{F^{(2)}(x)}{|x|}\,,$$

then $\big[-\Delta_y + 4V_K(y) + 4|y|^2 W_K(y)\big]\varphi_K(y) = 4|y|^2 F_K(y)\,.$

Using $|K(y)| = |y|^2$ and that K is real analytic:

All coefficients real analytic!

Elliptic regularity:

So φ_K is real analytic as a function of $y \in \mathbb{R}^4$!

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Proving $\varphi(x) = \varphi^{(1)} + |x|\varphi^{(2)}$, $\varphi^{(i)}$ analytic

Since φ_K is real analytic in $y \in \mathbb{R}^4$, and $K(\lambda y) = \lambda^2 K(y)$,

$$\varphi_K(y) = \sum_{\beta \in \mathbb{N}^4, |\beta|/2 \in \mathbb{N}} c_\beta y^\beta = \sum_{n=0}^{\infty} \sum_{|\beta|=2n} c_\beta y^\beta$$

For all $n \in \mathbb{N}$,

$$\sum_{|\beta|=2n} c_\beta y^\beta = \sum_{j=0}^{n} |y|^{2j} H_{2n-2j}^{(2n)}(y),$$

where the $H_{2n-2j}^{(2n)}$'s are homogeneous harmonic polynomials of degree $2n - 2j = 2(n - j)$.

Proving $\varphi(x) = \varphi^{(1)} + |x|\varphi^{(2)}$, $\varphi^{(j)}$ analytic

Lemma

There exist harmonic polynomials $Y_{n-j}^{(2n)}$, homogeneous of degree $n-j$, such that

$$H_{2n-2j}^{(2n)}(y) = Y_{n-j}^{(2n)}(K(y)) \ \text{for all } y \in \mathbb{R}^4 .$$

Then, since $|y|^2 = |K(y)|$,

$$\varphi_K(y) = \sum_{\beta\in\mathbb{N}^4, |\beta|/2\in\mathbb{N}} c_\beta y^\beta = \sum_{n=0}^{\infty} \sum_{j=0, j\,\text{even}}^{n} |K(y)|^j \, Y_{n-j}^{(2n)}(K(y))$$

$$+ |K(y)| \sum_{n=0}^{\infty} \sum_{j=1, j\ \text{odd}}^{n} |K(y)|^{j-1} \, Y_{n-j}^{(2n)}(K(y)) .$$

Outline

Many-Particle Case

Transformed Equation: Singular Elliptic Equation

Again using properties of K:

If $H\psi = E\psi$ then, with $(x_1, x') \in \mathbb{R}^3 \times \mathbb{R}^{3N-3}$,

$$Q(y, x', D_y, D_{x'})u = 0 \,,$$
$$Q(y, x', D_y, D_{x'}) := -\Delta_y - 4|y|^2\Delta_{x'} + 4|y|^2 W(y, x') - 4Z$$

where

$$u(y, x') := \psi(K(y), x') \,,$$
$$W(y, x') := V_E(K(y), x') \,,$$
$$V_E(x_1, x') = \sum_{j=2}^{N} -\frac{Z}{|x_j|} + \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} - E \,.$$

Analytic Hypoelliptic Operator

Grušin-Type Operator

The operator

$$P(y, x', D_y, D_{x'}) := -\Delta_y - 4|y|^2\Delta_{x'}$$

is a sum of squares of vectorfields (à la Hörmander), but vanishing at $y = 0$.

Theorem (Grušin, 1970):

If $(P + V)u = 0$ with $V \in C^\omega$ in a neighbourhood of $y = 0$, then $u \in C^\omega$ in a neighbourhood of $y = 0$.

Summary

Two-Particle Coalescence points

Theorem (SF, HO², TØS, 2007)

Let $\Omega \subset \mathbb{R}^{3N}$ be a neighbourhood of a two-particle coalescence point, say, $|x_1| = 0$ and $|x_j| \neq 0, j \neq 1, |x_i - x_j| \neq 0$.

If $H\psi = E\psi$ in Ω then

$$\psi(\mathbf{x}) = \psi_1(\mathbf{x}) + |x_1|\psi_2(\mathbf{x})\,, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^{3N}\,,$$

with $\psi_1, \psi_2 \in C^\omega(\Omega)$ (real analytic).