Unique continuation for the Hohenberg-Kohn theorem

Louis Garrigue

Banff, January 28, 2019

Hohenberg-Kohn theorem

$$H^N(v) := \sum_{i=1}^{N} -\Delta_i + \sum_{1\leqslant i<j\leqslant N} w(x_i - x_j) + \sum_{i=1}^{N} v(x_i)$$

$$\rho_\Psi(x) := N \int_{\mathbb{R}^{d(N-1)}} |\Psi|^2 (x, x_2, \dots, x_N)\mathrm{d}x_2 \cdots \mathrm{d}x_N$$

Theorem (Hohenberg-Kohn, 1964)

Let $w, v_1, v_2 \in ?$. If there are two ground states Ψ_1 and Ψ_2 of $H^N(v_1)$ and $H^N(v_2)$, such that $\rho_{\Psi_1} = \rho_{\Psi_2}$, then $v_1 = v_2 + \frac{E_1 - E_2}{N}$

- Works for bosons and fermions, in any dimension d
- (1983) Lieb remarked that it relied on a **strong unique continuation property** (SUCP). He conjectured that $? = L^{\frac{d}{2}}(\mathbb{R}^3) + L^\infty(\mathbb{R}^d)$
- We can take $? = L^{\frac{d\mathbf{N}}{2}}(\mathbb{R}^d) + L^\infty(\mathbb{R}^d)$ by Jerison-Kenig (1985), but this covers Coulomb singularities only for $N = 1$. **We need a power independent of N**

Proof of the HK theorem (1964)

1. $E_1 \leqslant \left\langle \Psi_2, H^N(v_1)\Psi_2 \right\rangle = E_2 + \int_{\mathbb{R}^d} \rho(v_1 - v_2)$.
2. Exchanging $1 \leftrightarrow 2$ gives $E_1 - E_2 = \int_{\mathbb{R}^d} \rho(v_1 - v_2)$.
3. The $\leqslant$ above is an $=$, hence Ψ_2 is a ground state for $H^N(v_1)$, so $H^N(v_1)\Psi_2 = E_1\Psi_2$.
4. Substracting the two eigenvalue equations for Ψ_2 gives

$$\left(E_1 - E_2 + \sum_{i=1}^{N} (v_2 - v_1)(x_i) \right) \Psi_2 = 0.$$

5. By strong unique continuation, $|\{\Psi_2(X) = 0\}| = 0$, so $E_1 - E_2 + \sum_{i=1}^{N}(v_2 - v_1)(x_i) = 0$ and integrating on $[0, L]^{d(N-1)}$, we obtain $v_1 = v_2 + c$.

Strong UCP

Theorem (Strong UCP for many-body Schrödinger operators)

Assume that the potentials satisfy

$$v, w \in L^p_{\mathrm{loc}}(\mathbb{R}^d) \qquad \text{with } p > \max\left(\frac{2d}{3}, 2\right).$$

If $\Psi \in H^2_{\mathrm{loc}}(\mathbb{R}^{dN})$ *is a non zero solution to* $H^N(v)\Psi = E\Psi$, *then* $|\{\Psi(X) = 0\}| = 0$.

- In $3D$, we can take **?** $= L^{p>2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ in the HK theorem. Covers the physical case, ie Coulomb-like singularities
- Works for excited states
- Already known that $\{\Psi(X) = 0\}$ is not an open set (Georgescu 1980)

- L. Garrigue, *Unique continuation for many-body Schrödinger operators and the Hohenberg-Kohn theorem. II. The Pauli Hamiltonian*, (2019), arXiv:1901.03207.

History

	Date	Weak or Strong	Number of particles	Hypothesis on v (loc)	Magnetic ?
Carleman	39	W	1 (and N)	L^∞	No
Hörmander	63	W	1	$L^{2d/3}$	No
Georgescu	80	W	N	$L^{2d/3}$	No
Schechter-Simon	80	W	N	L^d	No
Jerison-Kenig	85	S	1	$L^{d/2}$	No
Kurata	97	S	1	Many	Yes
Koch-Tataru	01	S	1	$L^{d/2}$	Yes
Laestadius-Benedicks-Penz	18	S	N	Many	Yes
Garrigue	19	S	N	$L^{p>2d/3}$	Yes

Other related works : Kinzebulatov-Shartser (2010), Zhou (2012,2019), Lammert (2018)

Carleman-type inequality

- If $|\{\Psi(X)=0\}|>0$, then $\int \frac{|\Delta\Psi|^2}{|X-X_0|^\tau}$ is finite for all τ for some X_0 (we take $X_0=0$)

Theorem (Carleman-type inequality)

Define $\phi(X):=(-\ln|X|)^{-1/2}$*. We have*

$$\tau^3\int_{B_{1/2}}\phi^5\left|\frac{e^{(\tau+2)\phi}\Psi}{|X|^{\tau+2}}\right|^2+\tau\int_{B_{1/2}}\phi^5\left|\nabla\left(\frac{e^{(\tau+1)\phi}\Psi}{|X|^{\tau+1}}\right)\right|^2 +\tau^{-1}\int_{B_{1/2}}\phi^5\left|\Delta\left(\frac{e^{\tau\phi}\Psi}{|X|^{\tau}}\right)\right|^2\leqslant c\int_{B_{1/2}}\left|\frac{e^{\tau\phi}\Delta\Psi}{|X|^{\tau}}\right|^2.$$

- Proved using techniques of Hörmander, Koch-Tataru, ...

Fractional Carleman-type inequality

- With Hardy's inequality $|X|^{-2s} \leqslant (-\Delta)^s$, transforms into a fractional Carleman inequality

Corollary (Fractional Carleman inequality)

For any $\delta > 0$, $s \in [0,1]$, $s' \in \left[0, \frac{1}{2}\right]$, $\tau \geqslant \tau_0$, $u \in C_c^\infty(B_1 \setminus \{0\})$,

$$\tau^{3-4s} \left\| (-\Delta)^{(1-\delta)s} \left(e^{\tau\phi} \frac{u}{|X|^\tau} \right) \right\|_{L^2}^2 + \tau^{1-4s'} \sum_{i=1}^{n} \left\| (-\Delta)^{(1-\delta)s'} \left(e^{\tau\phi} \frac{\partial_i u}{|X|^\tau} \right) \right\|_{L^2}^2 \leqslant \frac{\kappa_n}{\delta^{5/2}} \left\| e^{\tau\phi} \frac{\Delta u}{|X|^\tau} \right\|_{L^2}^2 .$$

- This Carleman inequality pairs very naturally with Sobolev multipliers assumptions $|V_{\text{many-body}}|^2 \leqslant \epsilon(-\Delta)^{\frac{3}{2}-\epsilon} + c$ in the proof of the SUCP

Magnetic case, the Pauli Hamiltonian

$$H^N(v,A) := \sum_{j=1}^{N} \Big((\sigma_j \cdot (-i\nabla_j + A(x_j)))^2 + v(x_j) \Big) + \sum_{1 \leqslant i < j \leqslant N} w(x_i - x_j)$$

Theorem (Strong UCP for the many-body Pauli operator)

Assume that the potentials satisfy $\operatorname{div} A = 0$ *and*

$$A \in L^q_{\mathrm{loc}}(\mathbb{R}^d) \qquad \text{with } q > 2d,$$
$$\operatorname{curl} A, v, w \in L^p_{\mathrm{loc}}(\mathbb{R}^d) \qquad \text{with } p > \max\left(\frac{2d}{3}, 2\right).$$

If $\Psi \in H^2_{\mathrm{loc}}(\mathbb{R}^{dN})$ *is a non zero solution to* $H^N(v,A)\Psi = E\Psi$, *then* $|\{\Psi(X) = 0\}| = 0$.

Hohenberg-Kohn for the Maxwell-Schrödinger model

Tellgren (2018), Ruggenthaler et al. (2014).

$$\begin{aligned}\mathcal{E}_{v,A}(\Psi, a) &:= \left\langle \Psi, H^N(v, a + A)\Psi \right\rangle + \frac{1}{8\pi\alpha^2}\int |\mathrm{curl}\, a|^2 \\ &= \left\langle \Psi, H_0^N \Psi \right\rangle + \int \rho_\Psi \left(v + |a + A|^2 \right) \\ &\qquad + 2\int (j_\Psi + \mathrm{curl}\, m_\Psi)\cdot(A + a) + \frac{1}{8\pi\alpha^2}\int |\mathrm{curl}\, a|^2\end{aligned}$$

Internal current $j_{(\Psi,a)} := j_\Psi + \mathrm{curl}\, m_\Psi + \rho_\Psi a$

Theorem (Hohenberg-Kohn for Maxwell DFT)

Let $p > 2$ and $q > 6$ and let $w, v_1, v_2 \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $A_1, A_2 \in \left(L^q_{\mathrm{loc}} \cap H^1\right)(\mathbb{R}^3)$ be such that $\mathcal{E}_{v_1,A_1}$ and $\mathcal{E}_{v_2,A_2}$ are bounded from below and admit ground states (Ψ_1, a_1) and (Ψ_2, a_2). If $\rho_{\Psi_1} = \rho_{\Psi_2}$ and $j_{(\Psi_1,a_1)} = j_{(\Psi_2,a_2)}$, then $A_1 = A_2$ and $v_1 = v_2 + (E_1 - E_2)/N$.