# Unique continuation for the Hohenberg-Kohn theorem

Louis Garrigue

Banff, January 28, 2019

# Hohenberg-Kohn theorem

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

**Theorem (Hohenberg-Kohn)**

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

$$v_1 = v_2 + \frac{E_1 - E_2}{N}.$$

- (1983) Lieb conjectured ? $= L^{\frac{3}{2}}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.
- Works for bosons and fermions, in any dimension $d$.
- Relies on **strong unique continuation property** (SUCP).

# Proof

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 $\Psi_2$ 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 $\Psi_2$ 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 $v_1 = v_2 + (E_1 - E_2)/N$.

# Strong UCP

**Theorem (Strong UCP for many-body Schrödinger operators)**

*Assume that the potentials satisfy*

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

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

- In $3D$, we can take **?** $= L^{p>2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Covers 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*, Math. Phys. Anal. Geom., 21 (2018), p. 27.
- L. Garrigue, *Unique continuation for many-body Schrödinger operators and the Hohenberg-Kohn theorem. II. The Pauli Hamiltonian*, (2019), arXiv:1901.03207.

# History

- Carleman (1939), bounded potentials for $N = 1$
- Hörmander (1963), singular potentials for $N = 1$
- Georgescu (1980) and Schechter-Simon (1980) weak UCP for any $N$
- Jerison-Kenig (1985), Koch-Tataru (2001) strong UCP, singular potentials, $N = 1$
- Zhou (2012, 2017)
- Laestadius-Benedicks-Penz (2017), strong UCP for $N$-body magnetic Schrödinger, with extra assumptions
- Lammert (2018)

# Carleman-type inequality

- de Figueiredo-Gossez (1992) : if $|\{\Psi(X) = 0\}| > 0$, then

$\int \frac{|\Psi|^2}{|X - X_0|^\tau}$ is finite for all $\tau$.

**Theorem (Carleman-type inequality)**

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

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

- We use $|V_{\text{many-body}}|^2 \leqslant \epsilon(-\Delta)^{\frac{3}{2}-\epsilon} + c$
- With Hardy's inequality $|X|^{-2s} \leqslant (-\Delta)^s$, gives the strong UCP.

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# 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*

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

*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).

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

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 $(\Psi_1, a_1)$ and $(\Psi_2, a_2)$. If $\rho_{\Psi_1} = \rho_{\Psi_2}$ and $j_{(\Psi_1,a_1)} = j_{(\Psi_2,a_2)}$, then $A_1 = A_2$ and $v_1 = v_2 + (E_1 - E_2)/N$.*