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Hohenberg–Kohn-like theorems for current densities

Banff workshop 2019

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What happens if we try to generalize the Hohenberg–Kohn (HK) theorem to include current densities?

Outline

The HK theorem deconstructed

Current-density-functional theory

- Paramagnetic current-density-functional theory
- Physical current-density-functional theory

The HK theorem deconstructed

Current-density-functional theory

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HK argument deconstructed

$$\hat{H}(v) = \hat{H}_0 + \sum_{k=1}^{N} v(x_k) = \hat{H}_0 + \hat{V},$$

$$E(v) = \int_{\mathbb{R}^3} v\rho_0 \, \mathrm{d}x + \min_{\psi \mapsto \rho_0} \langle \psi, \hat{H}_0 \psi \rangle.$$

HK1.
-Assume two systems share ground-state density ρ_0.
-Then the two systems share all ground-states ψ that fulfill $\psi \mapsto \rho_0$.

HK2.
-Assume two systems share an eigenstate ψ.
-Then $v_1 = v_2$ + const.

Remarks.
(i) The equation that determines ψ, i.e.,

$$(\hat{H}_0 + \hat{V} - E(v))\psi = 0,$$

needs to have measure UCP.[1]
(ii) No strict inequality in the variational principle is needed.

[1] P.E. Lammert J. Math. Phys. 59 (2018), L. Garrigue, Math. Phys. Anal. Geom. 21 (2018)

All proofs of HK theorems follow the HK1 + HK2 argument.
This breaks down with current densities.

The HK theorem deconstructed

Current-density-functional theory

- Paramagnetic current-density-functional theory
- Physical current-density-functional theory

Current-density-functional theory

$$-i\nabla_k \to -i\nabla_k + A(x_k),$$

$$\hat{H}(v,A) = \hat{H}_0 + \sum_{k=1}^{N} \Big[\{-i\nabla_k, A(x_k)\} + v(x_k) + A(x_k)^2 \Big],$$

$$j_\psi^{\mathrm{p}} = N \,\mathrm{Im} \int_{\mathbb{R}^{3(N-1)}} \overline{\psi} \nabla_1 \psi \, \mathrm{d}x_2 \cdots \mathrm{d}x_N, \quad j_{\psi;A} = j_\psi^{\mathrm{p}} + \rho_\psi A.$$

Energy:

$E(v,A) = \inf_\psi \langle \psi, H(v,A)\psi\rangle$ obtained from (suppose $\nabla \cdot A = 0$)

$$\langle \psi, \hat{H}(v,A)\psi\rangle = \langle \psi, \hat{H}_0 \psi\rangle + 2\int_{\mathbb{R}^3} A \cdot j_\psi^{\mathrm{p}} \, \mathrm{d}x + \int_{\mathbb{R}^3} (v + |A|^2)\rho_\psi \, \mathrm{d}x,$$

or

$$\langle \psi, \hat{H}(v,A)\psi\rangle = \langle \psi, \hat{H}_0 \psi\rangle + 2\int_{\mathbb{R}^3} A \cdot j_{\psi;A} \, \mathrm{d}x + \int_{\mathbb{R}^3} (v - |A|^2)\rho_\psi \, \mathrm{d}x.$$

To obtain a current-density-functional theory we need to replace $\langle \psi, \hat{H}_0 \psi\rangle$.

Paramagnetic current-density-functional theory

Vignale and Rasolt:[2]

$$F(\rho, j^{\mathrm{p}}) = \inf_{\psi \mapsto (\rho, j^{\mathrm{p}})} \langle \psi, \hat{H}_0 \psi \rangle,$$

$$E(v, A) = 2 \int_{\mathbb{R}^3} A \cdot j_0^{\mathrm{p}} \, \mathrm{d}x + \int_{\mathbb{R}^3} (v + |A|^2) \rho_0 \, \mathrm{d}x + \min_{\psi \mapsto (\rho_0, j_0^{\mathrm{p}})} \langle \psi, \hat{H}_0 \psi \rangle.$$

HK1: $(\rho_0, j_0^{\mathrm{p}})$ determines at most one non-degenerate ground state ψ_0.[3]

HK2 does *not* hold! Solution ψ to $\hat{H}\psi = E\psi$ does not uniquely determine (v, A).

Choose v s.t. $H(v, 0) = -\Delta + v$ has a unique ground state ψ_0.

Set $A = u \times \nabla \psi_0$ s.t. $\nabla \cdot A = 0$. Then

$$H(v - A^2, A)\psi_0 = -\Delta \psi_0 + \left(v - A^2 + A^2\right)\psi_0 = E\psi_0.$$

ψ_0 is a ground state if u is sufficiently small.[4]

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[2] Phys. Rev. Lett. 59 (1987)

[3] Weak HK result and degeneracies, AL and E.I. Tellgren Phys. Rev. A 97 (2018)

[4] Idea by Lieb, AL and M. Benedicks Int. J. Quant. Chem. 114 (2014)

HK1 does *not* work

$$\inf_{\psi\mapsto(\rho,j)} \langle \psi, \hat{H}_0 \psi\rangle = \inf\{\langle \psi, \hat{H}_0\psi\rangle : \rho_\psi = \rho, j^{\mathrm{p}}_\psi + \rho A = j\}.$$

HK for total j is open.

Remarks.
(i) Measure UCP can be proven.[5]
(ii) HK hold for $N = 1$ by direct construction (m-UCP).[6]
(iii) QEDFT has HK theorem (current is an internal variable together with the vector potential A).[7]
(iv) Tellgren's MDFT[8] has a HK theorem. Can be structured HK1 + HK2.[9] Need the internal part that vanishes at $\mu = 0$.

[5] L. Garrigue arXiv:1901.03207, AL, M. Benedick and M. Penz arXiv:1710.01403v3
[6] Tellgren et al. Phys. Rev A 86 (2012), AL and M. Benedicks, Int. J. Quant. Chem. 114 (2014)
[7] M. Ruggenthaler arXiv:1509.01417
[8] Phys. Rev. A 97 (2018)
[9] L. Garrigue arXiv:1901.03207

Concluding remark

Generalized HK theorem for CDFT much more difficult than first thought.

Question:

Why do we need the Hohenberg–Kohn theorem for density-functional methods?

Relevance e.g. to the Kohn–Sham algorithm.

Not having the potentials determined can cause some spurious effects, e.g., undetermined degeneracy with the paramagnetic formulation.

Acknowledgment

- E.I. Tellgren, M. Penz, S. Kvaal, L. Garrigue, M. Ruggenthaler, P.E. Lammert, A.M. Teale, S. Sen, A. Borgoo.
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