



HAL
open science

On a stronger form of the Hohenberg-Kohn theorem

Patrick Cassam-Chenaï

► **To cite this version:**

| Patrick Cassam-Chenaï. On a stronger form of the Hohenberg-Kohn theorem. 2017. hal-01592428

HAL Id: hal-01592428

<https://hal.science/hal-01592428>

Preprint submitted on 24 Sep 2017

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

On a stronger form of the Hohenberg-Kohn theorem

P. Cassam-Chenai

Université Côte d'Azur, LJAD, UMR 7351, 06100 Nice, France

Abstract

We prove a stronger form of the Hohenberg-Kohn theorem.

Keywords:

Hohenberg-Kohn theorem

Suggested running head:

strong HK-th

All correspondance to be send to P. Cassam-Chenai,

cassam@unice.fr,

tel.: +33 4 92 07 62 60,

fax: +33 4 93 51 79 74.

1 Introduction

We have dug out one of our note from the early 90's proposing and proving a Hohenberg-Kohn-like theorem. It is kind of an old, autocensored joke, but jokes may trigger interesting thoughts sometimes. So, it is our hope that this letter will stimulate new discussions.

2 Theorem

The number of elements in the periodic table being finite, we consider that the set of all possible molecules is a countable set. So, let us index molecules by non negative integers $i \in \mathbb{N}$. Then, there exists a function, f , of two variables $i \in \mathbb{N}$ and $x \in \mathbb{R}$ such that for a given i , $f(i, x)$ has an absolute minimum equal to the ground state energy of molecule i , E_i :

$$\forall i \in \mathbb{N} \quad \mathbf{Min}_x f(i, x) = E_i \quad (1)$$

Proof:

It suffices to take for f the function defined by

$$\forall i \in \mathbb{N} \quad f(i, x) = E_i + x^2 \quad (2)$$

which satisfies the property.

3 Discussion

This theorem is reminiscent of the Hohenberg-Kohn theorem, however, the one-electron density is not even needed, a simple real variable is sufficient. Furthermore, one can take for E_i the true energy of the molecule including all possible contributions such as nuclear motion energy, electron-nuclei couplings ...

Note that the fact that the number of molecules is considered infinite, whereas there are

only a finite number appearing in chemists' handbooks, is not a problem: one can admit the existence of hydrogen chains of an arbitrary large number of H and this is enough to obtain a countable infinite set.

Note also that the function f of the theorem is not unique.

It is dubious that this theorem will be of practical use in the same way as the Hohenberg-Kohn theorem has proved to be. The function f is not known explicitly, and, unlike in DFT, we have no clue on how to guess an approximate explicit form which could be useful for molecule i , when E_i is not known. Moreover, in DFT, one can retrieve the external potential from the minimizing electronic density. So, in turn the Hamiltonian can be retrieved, and from the Hamiltonian, the corresponding ground state wave function, at least in principle. None of this is possible in the present case.

However, this existence theorem may justify in a sense, pragmatical interpolation of molecular properties, by machine-learning technology for example, since energy can be replaced by any well-defined molecular property. Or, even better, the construction of the function f in the proof could be refined in such a way that the function presents several non-degenerate minima, each minimum corresponding to the value of a given property, the set of properties being ordered according the relative heights of the different minima.

Acknowledgements

References

- [1] Hohenberg, P. and Kohn, W. Phys. Rev. B136 (1964) 864.