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REGULAR ARTICLE

A re-statement of the Hohenberg–Kohn theorem and its extension to finite subspaces

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Abstract Bearing in mind the insight into the Hohenberg–Kohn theorem for Coulomb systems provided recently by Kryachko (Int J Quantum Chem 103:818, 2005), we present a re-statement of this theorem through an elaboration on Lieb's proof as well as an extension of this theorem to finite subspaces.

Keywords Hohenberg–Kohn theorem · DFT · Finite subspaces

1 Introduction

Density functional theory, DFT [1–12] has become a basic tool in contemporary quantum chemistry [13–15] but, as shown some decades ago by Lieb [16] and more recently by several authors [17–23] due to its subtleties, this theory cannot be considered as yet to be entirely elaborated.

The Hohenberg–Kohn theorem [24,25] has played a fundamental role in the development of DFT. In a recent work, however, Kryachko [26] has pointed out that the usual *reductio ad absurdum* proof of this theorem is unsatisfactory since the would-be-refuted assumptions on the one-electron density and the assumption on the external potential evince incompatibilities with the Kato cusp condition. Nevertheless, as shown by Kryachko [26], application of the Kato cusp conditions actually leads to a satisfactory proof of this theorem.

In the present work, within the context of Kryachko's analysis, we advance an alternative proof of the Hohenberg–Kohn theorem, which is based on the rigorous examination of the original formulation of this theorem made by Lieb [16], a number of years ago. In Lieb's proof, it is required that the N-particle wavefunction Ψ not vanish in a set of positive measure. This condition, however, cannot be easily fulfilled. In order to avoid this difficulty we present below an essentially algebraic proof of the Hohenberg–Kohn theorem which dispenses with the latter condition.

In addition, we propose an extension of the present reformulation of the Hohenberg–Kohn theorem to the case of finite subspaces. This finite subspace problem has been treated in a restricted sense by Epstein and Rosenthal [27] and by Katriel et al. [28,29] and in a general sense by Harriman [30]. More recently, Görling and Ernzerhof have reexamined this problem in relation to the linear response method to determine Kohn–Sham orbitals (and, purportedly, Kohn–Sham wavefunctions; strictly speaking, it is not possible to attach a rigorous meaning to Kohn–Sham wavefunctions as through the application of the variational principle there only result Kohn–Sham single-particle equations and their corresponding single-particle orbitals) from electron densities [31].

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In order to set the proper background for our discussion, we review in Sect. 1 both the original proof given by Hohenberg and Kohn, in the context of Kryachko's work, as well as Lieb's reformulation. In Sect. 2 we discuss the modifications introduced in our present proof. In Sect. 3, we consider the conditions that must be fulfilled in order that this theorem be extended to finite subspaces.

2 The original Hohenberg–Kohn proof and Lieb's reformulation

Let us consider a system formed by N-electrons interacting with a positive background through an "external" potential

$$V(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_{i=1}^{N} v(\mathbf{r}_i). \tag{1}$$

The many-electron Hamiltonian for such a system is

$$\widehat{H}_v = \widehat{H}_o + \widehat{V} \tag{2}$$

where $\widehat{H}_o$ is defined by

$$\widehat{H}_o = -\frac{1}{2}\sum \nabla^2_{\mathbf{r}_i} + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{3}$$

It is assumed that the selected class $\{v(\mathbf{r})\}$ of single-particle external potentials is such that it possesses a ground-state wavefunction $\{\Psi_o^v\}$. The one-electron density $\rho_o^v(\mathbf{r})$ associated with Ψ_o^v is defined by

$$\rho_o^v(\mathbf{r}_1) = N \int d^3\mathbf{r}_2 \cdots \int d^3\mathbf{r}_N |\Psi_o^v(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2. \tag{4}$$

For such systems, the Hohenberg–Kohn theorem states that there exists a one to one correspondence between an external potential $v(\mathbf{r})$ and the exact ground-state density $\rho_o^v(\mathbf{r})$. The original proof of this theorem [24] is carried out by *reductio ad absurdum*. Consider two potentials $v(\mathbf{r})$ and $v'(\mathbf{r})$ differing by more than a constant. The exact ground-state wavefunctions for the corresponding Hamiltonians $\widehat{H}_v$ (or $\widehat{H}_{v'}$) are *assumed* to be different (actually, these assumptions immediately evoke the Kato theorem and show the way to a proof that dispenses with the *reductio ad absurdum* argument) and for this reason the following strict variational inequalities hold:

$$\langle \Psi_o^{v'} | \widehat{H}_v | \Psi_o^{v'} \rangle > \langle \Psi_o^v | \widehat{H}_v | \Psi_o^v \rangle \equiv E_o^v \tag{5}$$

and

$$\langle \Psi_o^v | \widehat{H}_{v'} | \Psi_o^v \rangle > \langle \Psi_o^{v'} | \widehat{H}_{v'} | \Psi_o^{v'} \rangle \equiv E_o^{v'}. \tag{6}$$

Adding these inequalities and carrying out the integration over all coordinates but one, one obtains

$$\int d^3\mathbf{r}(v'(\mathbf{r}) - v(\mathbf{r}))(\rho_0^{v'}(\mathbf{r}) - \rho_0^v(\mathbf{r})) < 0\,. \tag{7}$$

Because Eq. (7) is a strict inequality, a contradiction ensues ($0 < 0$) when it is assumed that different potentials yield the same one-particle density. Thus, it follows that there is a one to one correspondence between the exact ground-state one-particle densities and their corresponding external potentials.

In the present notation, Lieb's statement of this theorem (Theorem 3.2 of Ref. [16]) is the following: suppose Ψ_o^v (respectively, $\Psi_o^{v'}$) is a ground state for v (respectively, v') and $v \neq v' + constant$. Then $\rho_0^v(\mathbf{r}) \neq \rho_0^{v'}(\mathbf{r})$. Lieb's proof starts from the suppositions that $\rho_0^v(\mathbf{r}) = \rho_0^{v'}(\mathbf{r}) = \rho_0$ and $\Psi_o^v \neq \Psi_o^{v'}$ because they satisfy different Schrödinger equations, and proceeds as in the original proof showing that this leads to a contradiction. As it was mentioned above, the argument for writing the strict inequalities [Eqs. (5) and (6)] in Hohenberg–Kohn's paper [24] is based on the *assumption* that Ψ_o^v and $\Psi_o^{v'}$ satisfy different Schrödinger equations, namely, that $\Psi_o^v \neq \Psi_o^{v'}$.

The fact that the space of single particle potentials is not specified in the original Hohenberg–Kohn proof was remedied in Lieb's proof [16] by selecting this space as $Y = L^{3/2}(\mathcal{R}^3) + L^{\infty}(\mathcal{R}^3)$ (where $f(x) \in L^m$ if $\int dx\, |f(x)|^m < \infty$. $f \in L^m_{loc}$ if $f \in L^m$ and it is integrable in any bounded set; $f \in H^1$ if $f, \nabla f \in L^2$) and by demanding that $v(\mathbf{r}) \in Y$. This choice—which follows from the requirement that $\rho^{1/2} \in H^1(\mathcal{R}^3)$—guarantees that the integral $\int d^3\mathbf{r}\rho(\mathbf{r})v(\mathbf{r})$ (in fact, the essentially self-adjoint character of the Hamiltonian [32]) is well defined.

An important difference arises, however, from the fact that Lieb notes that in order to prove the statement that Ψ_o^v and $\Psi_o^{v'}$ satisfy different Schrödinger equations it is necessary to show that the equivalence

$$V(\mathbf{r}_1, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = V'(\mathbf{r}_1, \ldots, \mathbf{r}_N)\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

implies that $v(\mathbf{r}) = v'(\mathbf{r})$. Fulfillment of this condition requires that the Ψ_o^v corresponding to the external potential $v \in Y$ not vanish on a set of positive measure. As has been indicated by Lieb [16] (p. 255), the unique continuation theorem may be invoked to guarantee that Ψ_o^v does not vanish in an open set. However, this theorem strictly holds only for $v \in L^3_{\text{loc}}$ although it is believed to hold also for $v \in Y$. But let us mention that there are subtle problems related to the space to which a single particle potential belongs and to its relation to the wavefunction. Thus, for example, as shown by Englisch and Englisch [33], for a one particle case there exists a non-vanishing density ρ (or equivalently, a non-vanishing wavefunction given as $\Psi = \rho^{1/2}$) which does not arise from any v, in the sense that for a $v = \rho^{-1/2}\nabla^2\rho^{1/2}$, $-\nabla^2 + v$ cannot be defined as a semibounded operator. Precisely in order to avoid these difficulties, we advance an algebraic proof of the Hohenberg–Kohn theorem where these issues are avoided.

3 A re-statement of the Hohenberg–Kohn theorem

The present proof is essentially based on Lieb's version of the HK theorem (Theorem 3.2 and Remark (ii) in p. 255 of Ref. [16]). But as mentioned above, in order to avoid some mathematical complications, we have, however, removed the assumption that $\Psi_o^v \neq \Psi_o^{v'}$, i.e., we consider the case where $v \neq v' + constant$ but $\Psi_o^v = \Psi_o^{v'}$ (Case **I** of Kryachko [26]) and have added the condition on the ground state wavefunction that it vanishes at most on a zero-measure set. Let $\widehat{H}_o$ be the Hamiltonian of an electronic Coulomb system without external potential [cf. Eq. (3)]. In fact, the form of $\widehat{H}_o$ is not very important, as the proof is essentially algebraic. Let us consider the many-electron Hamiltonian $\widehat{H}_v$ given by Eq. (2). We denote Y as in the above Section. We assume that ρ_o^v is the ground-state density of $\widehat{H}_v$ if there exists a ground-state wavefunction Ψ_o^v of $\widehat{H}_v$. We denote by E_o^v the corresponding eigenvalue.

Theorem 1 (Hohenberg–Kohn) *Let v, v' be in Y. Let ρ_o^v be a ground state density of $\widehat{H}_v$ and $\rho_o^{v'}$ a ground state density of $\widehat{H}_{v'}$. We assume that the ground state wavefunction Ψ_o^v of $\widehat{H}_v$ vanishes at most on a Lebesgue's zero-measure set of $\mathcal{R}^{3N}$. Suppose that $\rho_o^v = \rho_o^{v'}$. Then almost everywhere in the Lebesgue's measure sense (a.e.)*

$$v(\mathbf{r}) - v'(\mathbf{r}) = (E_o^v - E_o^{v'})/N. \tag{8}$$

Proof We essentially make explicit what was implicit in Lieb's proof [16]. Let us introduce the notation $\Delta E = E_o^{v'} - E_o^v$, $\Delta v = v' - v$ and $\Delta V = \sum_{i=1}^N \Delta v(\mathbf{r}_i)$. We have then $\widehat{H}_v = \widehat{H}_{v'} - \Delta V$ and

$$E_o^v = \langle \Psi_o^v | \widehat{H}_v | \Psi_o^v \rangle \leq \langle \Psi_o^{v'} | \widehat{H}_v | \Psi_o^{v'} \rangle = E_o^{v'} - \int \rho_o^{v'} \Delta v. \tag{9}$$

where the equal sign must be included *as we are not assuming* that for $v \neq v' + constant$ the condition $\Psi_o^v \neq \Psi_o^{v'}$ holds.

So we get $a \geq 0$ where $a = \Delta E - \int \rho_o \Delta v$, and $\rho_o = \rho_o^v = \rho_o^{v'}$. Reversing v and v' we get similarly $a \leq 0$. So $a = 0$ and this implies also that all the preceding inequalities are in fact equalities. In particular, we have $E_o^v = \langle \Psi_o^{v'} | \widehat{H}_v | \Psi_o^{v'} \rangle$ so $\Psi_o^{v'}$ is also a ground state of $\widehat{H}_v$: $\widehat{H}_v \Psi_o^{v'} = E_o^v \Psi_o^{v'}$. In the same way: $\widehat{H}_{v'} \Psi_o^v = E_o^{v'} \Psi_o^v$. Using also $\widehat{H}_v \Psi_o^v = E_o \Psi_o^v$ and $\widehat{H}_{v'} - \widehat{H}_v = \Delta V$, by subtraction we obtain

$$\Delta V \; \Psi_o^v = \Delta E \; \Psi_o^v. \tag{10}$$

or, equivalently,

$$(\Delta V - \Delta E) \Psi_o^v = 0. \tag{11}$$

Since we have by assumption that Ψ vanishes at most on a set of zero measure (we take it to be a nodeless ground state wavefunction) it follows from Eq. (11) that $\Delta V = \Delta E$ almost everywhere for $(\mathbf{r}_1, \ldots, \mathbf{r}_N) \in \mathcal{R}^{3N}$, except for a set of zero measure. Then setting $\mathbf{r}_1 = \cdots = \mathbf{r}_N = \mathbf{r}$ we obtain $N \, \Delta v(\mathbf{r}) = \Delta E$ (see also Harriman's comments in p. 641 and in the Appendix of Ref. [30]). The present argument is rigorous provided v is continuous; otherwise, the proof can be completed using Lemma 1 proved in the Appendix. □

4 The Hohenberg–Kohn theorem in finite subspaces

We first state a Hohenberg–Kohn theorem that holds in subspaces which are not necessarily finite-dimensional.

Theorem 2 (Infinite-dimensional subspaces) *Let v, v' be in Y. Let F be some subspace of the antisymmetric N-particle Hilbert space (in the domains of $\widehat{H}_v$ and $\widehat{H}_{v'}$) such that F be stable under the action of $\widehat{H}_v$ and $\widehat{H}_{v'}$, i.e., ($\widehat{H}_v \, F \subset F$ and $\widehat{H}_{v'} \, F \subset F$). Take ρ_o^v a ground state density of the restriction $\widehat{H}_v|_F$ and $\rho_o^{v'}$ a ground state density of $\widehat{H}_{v'}|_F$. Again, assume that the ground state wavefunction vanishes at most on a set of zero measure. Suppose that $\rho_o^v = \rho_o^{v'}$. Then*

$$v(\mathbf{r}) - v'(\mathbf{r}) = (E_0^v - E_0^{v'})/N. \tag{12}$$

Proof It is carried out along the same steps as in Theorem 1, except for the fact that Ψ_o^v and $\Psi_o^{v'}$ must be in F in order to apply the variational principle and obtain $a = 0$, and, hence, $E_o^v = \langle \Psi_o^{v'} | \widehat{H}_v | \Psi_o^{v'} \rangle$ implying that $\Psi_o^{v'}$ is a ground state of $\widehat{H}_v|_F$. □

We see, therefore, that it is possible to extend the HK formulation of Density Functional Theory to a subspace F *as long as the conditions of stability of Theorem 2 are satisfied*.

However, as shown in Theorem 3 below, it is not possible, in general, to satisfy the assumptions of Theorem 2. First note that if $\widehat{H}_v(F) \subset F$ and $\widehat{H}_{v'}(F) \subset F$ then by taking the difference we obtain $\Delta V(F) \subset F$. We recall also that the operator $\widehat{V}$ associated to a scalar potential V is defined by $(\widehat{V}(\Psi))(x) := V(x)\Psi(x)$.

Theorem 3 (Finite-dimensional subspaces) *Let F be a finite-dimensional subspace of $L^2(\mathcal{R}^n)$ ($n \geq 1$). We suppose that $F = Vect(u_1(x), \ldots, u_M(x))$ where the $(u_i(x))$ is an orthonormal set (i.e., $\int u_i u_j^* = \delta_{ij}$) and such that $\sum_{i=1}^M |u_i(x)|^2 > 0$ a.e. for $x \in \mathcal{R}^n$. Let $V(x)$ be real-valued potential, and continuous. Then*

$$(\widehat{V}(F) \subset F) \Longrightarrow (V(x) = const \text{ on } \mathcal{R}^n).$$

We note that this theorem also holds with weaker assumptions, such as, for instance, $F \subset L^1_{\text{loc}}(\mathcal{R}^n)$ (the space of locally integrable functions on $\mathcal{R}^n$), and $V \in H^1_{\text{loc}}(\mathcal{R}^n)$ [i.e. $V, \nabla V \in L^2_{\text{loc}}(\mathcal{R}^n)$].

Proof We first remark that V behaves on F as an $M \times M$ matrix since it is a linear operator. So there exists $\mathbf{M} = (m_{ij})$ such that

$$V(x)u_i(x) = \sum_{j=1,\ldots,M} m_{ij}u_j(x). \quad (13)$$

Since u_j is orthonormal, we have

$$m_{ij} = \int_{\mathcal{R}^n} \mathrm{d}x u_i(x)^* V(x) u_j(x)$$

using (13). Since V is real we obtain $m_{ij} = m_{ji}^*$ and thus M is an hermitian matrix. So, we can diagonalize $\mathbf{M}$ in an orthonormal basis: there exists a unitary matrix P ($P^\dagger P = PP^\dagger = I_d$) and a diagonal matrix $D = \mathrm{diag}(\lambda_1, \ldots, \lambda_M)$ such that $\mathbf{M} = P^\dagger DP$.

Let us write $\mathbf{u}(x) = (u_1(x), \ldots, u_M(x))$. Then (13) reads $V(x)\mathbf{u} = \mathbf{M}\mathbf{u}$. So, it follows that

$$V(x)P\mathbf{u} = PV(x)\mathbf{u} = P\mathbf{M}\mathbf{u} = PP^\dagger DP\mathbf{u} = DP\mathbf{u}.$$

Hence if we define $\boldsymbol{\psi}(x) = P\mathbf{u}$ and denote its components as $(\psi_0(x), \ldots, \psi_M(x))$, we obtain:

$$V(x)\psi_i(x) = \lambda_i\psi_i(x), \quad i = 1, \ldots, M. \quad (14)$$

We have simply diagonalized $V(x)$ in an orthonormal basis set. Then let us notice that $\sum_{i=1}^M |\psi_i(x)|^2 = ||\boldsymbol{\psi}||^2 = ||\mathbf{u}||^2 = \sum_{i=1}^M |u_i(x)|^2$ since P is unitary. Obviously this quantity is non-negative and thus we have a.e. $x \in R^n$ the existence of an $i \in \{1, \ldots, M\}$ such that $\psi_i(x) \neq 0$. From (14) we obtain $V(x) = \lambda_i$ for this x. This implies finally that the range of V is included in the finite set $\{\lambda_1, \ldots, \lambda_M\}$. For a regular $V(x)$ such as continuous or H^1_{loc} this means that V is a constant, which concludes the proof of Theorem 3. □

A consequence of Theorem 3 is that, in general, it is not possible to fulfill the stability conditions of Theorem 2 when F is finite dimensional, except if we suppose that $V(x)$ and $V'(x)$ are constants as then they would trivially satisfy the main conclusion of Theorem 2, namely, $\Delta V = \mathrm{const}$. Let us mention that this result is in agreement with the conclusion of Görling and Ernzerhof for local potentials in finite subspaces [see Eq. (A9) and the discussion below in Ref. [31]].

But in the infinite dimensional case Theorem 3 does not hold and thus Theorem 2 becomes interesting. As an example, let $F = L^2(\mathcal{R}^3)$ and $v(x) = 1/(1 + |x|^2)$. Then we have obviously $v(F) \subset F$ (since $v(x) \leq 1$) but $v(x)$ is not constant.

5 Conclusions

The main contribution of this article is to provide an algebraic proof for the Hohenberg–Kohn theorem that allows us to discuss in a very simple way the extensions of this theorem to both infinite-dimensional and finite-dimensional subspaces. In the former case, such an extension is possible as long as the subspace is stable under the action of $\widehat{H}_v$. In the latter case, when the external potentials V and V', or their one-particle components v and v' are constants.

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6 Appendix

Lemma 1 *Suppose that*

$$v(r_1) + \cdots + v(r_N) = 0, \ a.e.\ x = (r_1, \ldots, r_N) \in \mathcal{R}^{3N}. \quad (15)$$

Then $v(r_1) = 0$ *a.e.* $r_1 \in \mathcal{R}^3$.

Proof First note that we cannot (a priori) take $r_1 = r_2 = \cdots = r_N$ because $\{(r_1, \ldots, r_N) \in \mathcal{R}^{3N},\ r_1 = r_2 = \cdots = r_N\}$ is a set of zero measure in $\mathcal{R}^{3N}$. To bypass this difficulty, we consider a real-valued continuous function $\rho(r) > 0$, defined on $\mathcal{R}^3$, such that $\int \rho(r)\mathrm{d}r = 1$, and denote $\rho^\epsilon(x) = \frac{1}{\epsilon^3}\rho\left(\frac{x}{\epsilon}\right)$. We multiply Eq. (15) by $\rho^\epsilon(x_1 - r_1)\cdots\rho^\epsilon(x_N - r_N)$ and then integrate over $(r_1, \ldots, r_N) \in \mathcal{R}^{3N}$. We obtain

$$v^\epsilon(r_1) + \cdots + v^\epsilon(r_N) = 0, \ a.e., \quad (16)$$

where $v^\epsilon(x) = \int_{\mathcal{R}^3} v(y)\rho^\epsilon(x - y)\mathrm{d}y$ (convolution product). Then it is well known [34] that v^ϵ is a continuous function and thus Eq. (16) holds everywhere and not only almost everywhere. Then we can take $r_1 = \cdots = r_N = r$ and conclude that $v^\epsilon(r) = 0$ for all r. On the other hand it is also well known that, as $\epsilon \to 0^+$ $v^\epsilon(r) \to v(r)$ for a.e. $r \in \mathcal{R}^3$ (eventually for some subsequence v^{ϵ_n} extracted from v^ϵ, [34]). Hence we conclude that $v(r) = 0$ a.e. $r \in \mathcal{R}^3$. □

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