Hohenberg-Kohn, revisited

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Abstract. The Hohenberg-Kohn theorem is a cornerstone of electronic density functional theory, yet completing its proof in the traditional way requires the assumption that ground state wavefunctions never vanish on sets of nonzero Lebesgue measure. This is an unsatisfactory situation, since DFT is supposed to obviate knowledge of many-body wavefunctions. We approach the issue from a more density-centric direction, allowing mild hypotheses on the density which can be regarded as checkable in a DFT context. By ordinary Hilbert space analysis, the following is proved: If the density $\rho$ is continuous and everywhere nonzero, then there can be at most one potential (modulo constants) expressible as a sum of a square-integrable and a bounded function (i.e., Kato-Rellich) with $\rho$ as a ground state density. In case $\rho$ is not nonzero everywhere, the theorem allows an independent constant on each connected component of the set where the density is positive, a weakening which can be reversed by requiring locally weak-$L^3$ potentials and calling on a unique continuation result of Schechter and Simon.

1. Introduction

The Hohenberg-Kohn (HK) Theorem is perhaps the most basic principle of density functional theory (DFT). It states that, for a system of identical interacting particles, a given one-body density $\rho(x)$ is realized as a ground state density for a unique (modulo constants) one-body potential, if any. This is considered a cornerstone of DFT since it implies that the ground state density of a system indirectly determines all its properties. Alas, there remains to this day a gap which is frequently glossed over, particularly in more “pragmatic” discussions. The direct way to close the gap would be to show that ground-state wavefunctions cannot vanish on a set of nonzero Lebesgue measure, but that turns out to be a very difficult task without severe restrictions on potentials. Here we approach the underlying issue from a different direction. In DFT, densities have priority, rather than wavefunctions. Mild restrictions on both potentials and densities are appropriate and acceptable. We prove that if $\rho$ is continuous and nowhere zero, then $\rho$ is a ground-state density of at most one potential (mod constants) which can be expressed as the sum of a square-integrable function and a bounded function. Note...
that this class of potentials (three-dimensional Kato-Rellich potentials) contains in particular the Coulomb potential of a finite number of point charges. The method of proof follows a simple intuition: If $\rho$ is a ground-state density for $v$, then it is stable in the sense that any deformation of $\rho$ will raise the total energy. Changing the potential by more than a constant ought to destabilize $\rho$, so that some small deformation lowers the total energy. Using smooth “velocity” fields to deform $\rho$ as though it were a classical compressible fluid, we show the existence of a velocity field which witnesses the instability. The requirement that $\rho(x) > 0$ everywhere can be lifted, at the cost of a more complicated and less satisfactory conclusion. In that case, uniqueness holds only up to a constant on each connected component of $\{x \mid \rho(x) > 0\}$ (hereafter abbreviated to $\{\rho > 0\}$) and no restriction at all where $\rho = 0$. With the aid of a weak unique continuation property and imposing a stronger condition (local weak $L^3$) on potentials, all but one of the constants can be eliminated.

Section 2 prepares the ground for the main result, Thm. 1. Section 2.1 establishes notations and gives some relevant technical background. No previous knowledge of DFT is assumed of the reader. Section 2.2 explains where the usual “proof” of the HK theorem gets into a sticky situation and discusses a way out by very strong conditions on potentials. The main results are finally stated and a sketch given of the proof methods, in Section 2.3. Finally, Section 3 presents the actual proof of Thm. 1 in a discursive style. Section 3.1 describes a versatile method of deforming densities and wavefunctions using smooth velocity fields. That technology is then combined with some simple abstract functional analytic considerations in Section 3.2 to finish the proof.

2. Preparations

2.1. Background and Notation. We deal with a system of $N$ identical non-relativistic spin-$\frac{1}{2}$ fermions in three dimensions, with a Hilbert space of states, $\mathcal{H}_N$, comprising antisymmetric elements of $L^2(\{\uparrow, \downarrow\} \times \mathbb{R}^3)^N; \mathbb{C})$, or if we prefer to think in spin components, elements of $\{\uparrow, \downarrow\}^N \rightarrow L^2(\mathbb{R}^3^N; \mathbb{C})$ anti-equivariant with respect to the action of the particle permutation group. Actually, neither spin nor statistics plays any significant role; other cases can be handled by trivial modifications. As usual, the Hamiltonian of this system consists of kinetic energy $T$, the energy

$$V_{\text{int}} = \sum_{1 \leq i < j \leq N} v_{\text{int}}(x_i - x_j)$$

(1)

of interaction among the particles, and a variable one-body “external” potential

$$V_{\text{ext}} = (\oplus^N v)(x_1, \ldots, x_N) := \sum_{i=1}^N v(x_i).$$

(2)

We write $H_0 = T + V_{\text{int}}$ for the part of the Hamiltonian that we think of as fixed. Usually, $v_{\text{int}}$ is a Coulomb interaction, but we take as standing assumption only that $v_{\text{int}}$ and the external potential $v$ are in the class of three-dimensional Kato-Rellich potentials $^{16}$

$$K_{R3} := L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3),$$

(3)
which are each a sum of a square-integrable and a bounded function. Associated to state vector \( \psi \in \mathcal{H}_N \) is the one-body density

\[
\text{dens } \psi(y) = \mathcal{N} \sum_n |\psi_n(y, x_2, \ldots, x_N)|^2 \, dx_2 \cdots dx_N.
\]  

(4)

And, its total energy in presence of the one-body potential is

\[
\mathcal{E}_v(\psi) = \langle \psi | H_0 + \otimes^N v | \psi \rangle = \langle \psi | H_0 | \psi \rangle + \int v(x) \text{dens } \psi(x) \, dx
= \mathcal{E}_0(\psi) + \langle v, \text{dens } \psi \rangle.
\]  

(5)

Alternate notations have been implicitly introduced here, but we need to say something about the interpretation of the matrix elements. Since spin and statistics are not significant in these considerations, we consider a single spin component \( L^2(\mathbb{R}^{3N}; \mathbb{C}) \). With \( F \) denoting the normalized (unitary) Fourier transformation, and adopting natural units with \( h = 2m = 1 \), the kinetic energy operator is \( T = F^{-1} |\rho|^2 F \). Thus, the operator domain of \( T \), \( \text{Dom} \, T \), is the Sobolev space \( H^2(\mathbb{R}^{3N}; \mathbb{C}) \). This is a standard notation: \( H^m(\mathbb{R}^3; \mathbb{C}) \) denotes the subspace of \( \psi \in L^2(\mathbb{R}^3; \mathbb{C}) \) with \( |k|^m \, F \psi \in L^2(\mathbb{R}^3; \mathbb{C}) \), turned into a Hilbert space by the inner product

\[
\langle \psi | \phi \rangle_m = \int F \psi(k)^* F \phi(k) \left[ 1 + |k|^{2m} \right] \frac{dk}{(2\pi)^{3N}}.
\]

However, \( \langle \psi | T | \phi \rangle \) makes sense on a bigger domain than just \( \text{Dom} \, T \). If we interpret \( T \) as a sesquilinear form \( \mathcal{S} \) according to

\[
\langle \psi | T | \phi \rangle = \int F \psi(k)^* F \phi(k) \frac{|k|^2 \, dk}{(2\pi)^{3N}},
\]  

(6)

then it has finite matrix elements over a space bigger than \( \text{Dom} \, T \), called the form domain of \( T \), and denoted Quad \( T \). We see that Quad \( T = H^1(\mathbb{R}^{3N}; \mathbb{C}) \). Putting spin back in, a wavefunction is in the operator or form domain of \( T \) just in case each spin component is. The significance of the restriction to Kato-Rellich potentials \( [3] \) is that it makes the operator and form domains of the full Hamiltonian the same as those of the kinetic energy \( [8, 31, 25, 16] \).

\( \mathcal{E}_0(\psi) = \langle \psi | H_0 | \psi \rangle \) is called the intrinsic energy of state \( \psi \). Both the energy (\( \mathcal{E}_0 \)) and the single-particle density function (\( \text{dens} \)) naturally extend linearly to mixed states \( \gamma = \sum \lambda_i |\psi_i\rangle \langle \psi_i| \) as \( \text{dens } \gamma = \sum \lambda_i \text{dens } \psi_i \), and \( \mathcal{E}_0(\gamma) = \sum \lambda_i \mathcal{E}_0(\psi_i) \). The intrinsic energy of a density \( \rho \) is \( F(\rho) := \inf \{ \mathcal{E}_0[\gamma] | \text{dens } \gamma = \rho \} \). The minimization is carried out over mixed states with the prescribed density. \( F(\rho) \) is finite if and only if \( \rho \) is \( L^1 \)-integrable and \( \sqrt{\rho} \in H^1(\mathbb{R}^3) \), which is the same as integrability of \( |\nabla \rho|^2/\rho \). If this condition fails, then \( \rho \) cannot be a ground-state density of a KR potential, so Thm. \( \ref{thm:ground_state} \) holds vacuously. Thus, we hereafter restrict attention to densities meeting this condition. Since by continuity \( \rho \) is bounded above on bounded sets, both \( \rho \) and \( \nabla \rho \) are locally (i.e., over any bounded set) square integrable. That is, \( \rho \in H^1_{\text{loc}}(\mathbb{R}^3) \). This property will be important in Section \( \ref{sec:3.1} \).

2.2. the problem. What Hohenberg and Kohn truly did prove in their paper \( [17] \) is that if two one-body potentials have a common ground state density, then they have a common ground state. Using the constrained-search \( [22] \) idea, which developed later, this is easy for us to see. The external potential enters the energy only via the integral \( \int \rho(x) v(x) \, dx \). So, if \( \rho \) is a ground-state density, then every state
which minimizes the intrinsic energy (among all with density \( \rho \)) must be a ground state. So far, so good. To finish the proof of the full HK theorem, therefore, we need to show that potentials which are not equal modulo constants cannot have a common ground state wavefunction. Hohenberg and Kohn simply made the bald assertion that it is so. We attempt to flesh that out a bit, following textbook treatments\cite{9, 12, 10}. With \( H_0 \) the sum of kinetic and interparticle interaction energy and \( V, V' \) two one-body potentials, suppose that \( \psi \) is a ground state for both:

\[
(H_0 + V)\psi = 0, \quad (H_0 + V')\psi = 0.
\] (7)

Without essential loss, we took the total energies to be zero by shifting the potentials, and these are a priori interpreted as distributional equations. Subtracting,

\[
(V - V')\psi = 0, \quad \text{in } L^1_{\text{loc}}(\mathbb{R}^3N).
\] (8)

We would like to conclude from this that \( V = V' \) almost everywhere. And, that seems to require a warrant that \( \{\psi = 0\} \) is Lebesgue-null. We can avoid that if we put severe enough restrictions on potentials to guarantee that \( V = V' \) either almost everywhere, or almost nowhere.

**Proposition 2.1.** Suppose \( f \) is real analytic on an open set \( \Omega \subset \mathbb{R}^n \). Then, \( f \) is equal to zero either everywhere or almost nowhere.

**Proof.** Since \( \Omega \) can be covered by a countable collection of overlapping \( n \)-cubes, the special case \( \Omega = (0,1)^n \) suffices. The latter is easily done by induction on \( n \), using the Fubini theorem and analyticity of the restriction of \( f \) to line segments. For \( n = 1 \), the result is clear since zeros of \( f \) must be isolated unless \( f \equiv 0 \).

Assuming the result for \( n < m \), let \( J \) be the set of \( y \in (0,1) \) such that \( f \equiv 0 \) on the slice \( \{(x,y) \mid x \in (0,1)^{m-1}\} \). Then, the measure of \( f^{-1}(0) \) equals the (one-dimensional) measure of \( J \), by Fubini and the induction hypothesis. But if \( J \) has non-zero measure, then \( f \equiv 0 \) on every vertical line of fixed \( x \), by the one-dimensional case. \( \square \)

All is well, then, if we consider only potentials which are analytic on the complement of a (variable) Lebesgue null closed set. Coulomb potentials due to a finite number of point charges ("molecular potentials") fall into this class. However, density functional theory puts densities first, and is committed, on grounds of both principle and computational pragmatics, to consideration of a broader class of densities than just ground state densities in molecular potentials. There is a considerable body of literature\cite{19, 21, 26, 3, 15, 14} on weak unique continuation properties (UCP), guaranteeing that an eigenfunction cannot vanish on an open set without vanishing everywhere, if the potential is in a certain class. Unfortunately, we need to rule out not just vanishing on an open set, but vanishing on a set of nonzero Lebesgue measure. The variational approach of Garofalo and Lin\cite{14, 15} gives that species of unique continuation, but at the cost of complicated and strong conditions on the potential.

We take a different approach, which focusses more on densities than wavefunctions and do not hesitate to impose physically reasonable hypotheses on the density. In the DFT context, it seems acceptable to impose the condition that densities be continuous. One notes that electronic densities of eigenstates in a molecular potential are not only continuous, but analytic away from the nuclei\cite{13, 18}. We do not place any restrictions on \( \{\rho = 0\} \), but note that the main result becomes
2.3. results. The main result is

**Theorem 1.** Let \( \rho \) be continuous, and \( v, v' \in KR_3 \) two external one-body potentials with \( \rho \) as a ground-state density. Then, \( v - v' \) is uniform over each connected component of \( \{ \rho > 0 \} \).

Of course, essentially nothing can be said about the behavior of \( v \) on \( \{ \rho = 0 \} \). The most pleasant special case occurs when \( \rho > 0 \) everywhere. In that case, the ambiguity in the potential reduces to the unavoidable global constant.

We will now sketch the ideas involved in proving this theorem. Suppose that \( \psi_0 \), with density \( \rho_0 = \text{dens} \psi_0 \in C(\mathbb{R}^3) \), is a ground state of \( H_0 + \oplus^N v_0 \) for \( v_0 \in KR_3 \).

The denotations of \( \psi'_0 \), \( \rho'_0 \) and \( v'_0 \) are now fixed, but in a moment the subscript \( 0 \) will become just a particular value of a real parameter. Imagine \( \psi_0 \) in presence of \( v_0 \) when, suddenly, the potential is switched to \( v' \in KR_3 \), differing from \( v_0 \) by more than a constant over some component of \( \{ \rho > 0 \} \). The object is to show that the changed potential landscape inevitably presents opportunities to lower total (not just potential) energy by shifting particle number slightly.

To implement the idea of “shifting particle number slightly”, we embed \( \psi_0 \) in a smoothly varying one-parameter family \( \mathbb{R} \ni s \mapsto \psi_s \in H_N \) of normalized wavefunctions with corresponding densities \( \rho_s = \text{dens} \psi_s \). Since total energy is minimized at \( s = 0 \), assuming differentiability,

\[
0 = \frac{d}{ds} \mathcal{E}_v(\psi_s) \big|_{s=0} = \frac{d}{ds} \mathcal{E}_0(\psi_s) \big|_{s=0} + \langle v, \frac{d\rho_s}{ds} \rangle \big|_{s=0}.
\]  

(9)

Then, in presence of the second potential \( v' \),

\[
\frac{d}{ds} \mathcal{E}_{v'}(\psi_s) \big|_{s=0} = \langle v' - v, \frac{d\rho_s}{ds} \rangle \big|_{s=0}.
\]  

(10)

If \( \psi_0 \) is a ground-state density also for \( v' \), then the left-hand side of (10) is zero. If we can show that the right-hand side is nonzero, it will follow that \( \psi_0 \) is not a ground state density for \( v' \). The strategy has two parts. First, we develop a parametrization of smooth deformation families so that \( d\rho_s/ds = -\text{div}(\rho_s \mathbf{u}) \), where \( \mathbf{u} \) is a smooth “velocity” field. Existence of the derivatives in (9,10) will follow from smoothness of \( \mathbf{u} \), as shown in Sec. 3.1. Then, in Sec. 3.2, we use an abstract functional analysis (denseness) argument to show that some such velocity field will make the right-hand side of (10) nonzero.

Some densities do not correspond to pure ground states, but only to mixed ground states, and we certainly intend the theorem to apply to them. Fortunately, the required modifications are very simple: just apply the deformations discussed above to each component of the mixed state. Therefore, we continue to treat the special case of a pure ground state, leaving the generalization implicit.

2.4. extension. The partition \( \{ \mathcal{C}_i \} \) of \( \{ \rho > 0 \} \) into connected components induces a corresponding product partition in \( N \)-particle phase space of \( \{ \psi \neq 0 \} \). Knowledge of which cells of the partition are occupied with nonzero probability can imply constraints on the constants in the potential. In particular, if a diagonal component \( \mathcal{C}_i^N \) is occupied, then the constant corresponding to \( \mathcal{C}_i \) can be fixed by specifying the ground state energy. Since \( \mathcal{C}_i^N \) is open, this provides an opportunity to apply a weak UCP to conclude that all the diagonal cells are occupied. The weak UCP of Schechter and Simon [26], which requires the interaction potential and the external one-body potential to be in \( L^3_{\text{weak,loc}}(\mathbb{R}^3) \). (\( f \in L^3_{\text{weak,loc}}(\mathbb{R}^3) \) if there is \( C \geq 0 \) such...
that for all $s > 0$, the Lebesgue measure of $\{|f| > s\}$ is no greater than $C/s^3$. The Coulomb potential, in particular, is in $L^3_{weak,loc}(\mathbb{R}^3)$. Thus, we obtain the following corollary.

**Corollary 2.1.** In the context of Thm. 7, if the interaction potential and external potentials are in $L^3_{weak,loc}$, then $v$ and $v'$ differ by a constant, uniform over $\{|\rho| > 0\}$.

### 3. Proof of the Theorem

#### 3.1. Smooth deformations

We now show how to generate smoothly varying one-parameter families of densities and wavefunctions using velocity fields; similar techniques have been utilized by Bokanowski and Grebert [5, 6]. Suppose a time-independent velocity field $u$ with continuous derivatives of all orders and vanishing outside some bounded set [i.e., $u \in C^\infty(\mathbb{R}^3; \mathbb{R}^3)$], is imposed on a compressible fluid.

Integration yields the one-parameter diffeomorphism group $\mathbb{R} \ni s \mapsto \varphi_s$ mapping position $x$ to the position $\varphi_s(x)$ it is swept to after time $s$. This flow satisfies

$$\frac{\partial}{\partial s}(\varphi_s(x)) = u(\varphi_s(x)), \quad (11)$$

and induces in turn a group of transformations $\Phi^u_s$ of the density field given by

$$\rho_s(x) := (\Phi^u_s \rho_0)(x) = J_{-s}(x) \rho_0(\varphi_{-s}(x)), \quad (12)$$

where $J$ is the Jacobian

$$J_s(x) := \det \left[ \frac{\partial \varphi_s(x)}{\partial x^j} \right] \in C^\infty(\mathbb{R}^3).$$

In our quantum mechanical context, the density derives from a wavefunction via the map $\text{dens}$ [11], so we need to lift the action $\Phi^u_s$ to a unitary group $\mathbb{R} \ni s \mapsto \Phi^u_s \in \text{Aut}(\mathcal{H}_N)$ in Hilbert space such that $\text{dens} \circ \Phi^u_s = \Phi^u_s \circ \text{dens}$. (Regarding mixed states, see the final paragraph of Sec. 2.3.) Note that we are writing ‘$\Phi^u_s$’ for the actions on both densities and wavefunctions. Explicitly, with $\varphi^N$ denoting the $N$-fold replication of $\varphi$,

$$(\Phi^u_s \psi)(\mathbf{x}, \mathbf{z}) = \left[ \prod_{i=1}^N J_{-s}(x_i) \right]^{1/2} \psi(\mathbf{x}, \varphi^N \varphi_{-s}(\mathbf{z})). \quad (13)$$

With a method to generate smoothly varying deformations in hand, we proceed to verify that the derivatives of $\langle \psi_s | H_0 | \psi_s \rangle$ and $\int v \Phi^u_s \rho_0 \, dx$ at $s = 0$, appearing on the right-hand side of (9) exist, the second for arbitrary $v \in \text{KR}_3$. This requires differential versions of $\Phi^u$. Abstractly [11], with $\mathbb{R} \ni t \mapsto T(t)$ a strongly continuous operator semigroup on a Hilbert space, $x$ is in the domain of the generator $A$ of $T$ if and only if $(T(t)x - x)/t \to Ax$ as $t \to 0$. In that case, $\frac{d}{dt} \langle y | T(t)x \rangle|_{t=0} = \langle y | Ax \rangle$ and $\frac{d}{dt} \langle T(t)x | T(t)x \rangle|_{t=0} = 2 \Re \langle x | Ax \rangle$.

Consider first $\int v \Phi^u_s \rho_0 \, dx$. Since $v \in \text{KR}_3$, $\rho_0$ is continuous, and $\Phi^u_s$ changes nothing outside some ball $B$ containing the support of $u$, we can truncate everything smoothly outside $B$ and interpret the integral in $L^2(B)$. The generator of (12) is given by the familiar continuity equation

$$\frac{d\rho_s}{ds} = -\text{div}(\rho_s u) = \nabla \rho_s \cdot u - (\text{div} u)\rho_s. \quad (14)$$
As noted at the very end of Section 2.1, we may assume that $\nabla \rho_0 \in L^2_{\text{loc}}$. Thus, the right-hand side of (14) is in $L^2$, so $\langle v, d\rho_s/ds \rangle_{s=0}$ from (9) becomes the $L^2$ inner product $-\langle v | \text{div}(\rho_0 u) \rangle$.

Now, for $d\langle \psi_s | H_0 | \psi_s \rangle/ds$, the first term on the right-hand side of (9), the generator of the group action (13) is

$$A_u := \otimes N(u \cdot \nabla) + \frac{N}{2} \text{div} u,$$

which we interpret in the Hilbert space $H^1(\mathbb{R}^3\mathbb{N})$, where expectation-of-$H_0$ is continuous. Again, since $u$ is smooth, the only troublesome part is $u \cdot \nabla$, which reduces degree of differentiability by one, so that

$$A_u \text{dom } H_0 \subset \text{Quad } (H_0 + \otimes N) = H^1(\mathbb{R}^3\mathbb{N}).$$

(16)

Therefore, since $\psi \in \text{dom } H_0 = H^1(\mathbb{R}^3)$, we obtain

$$\frac{d}{ds} E_0(\Phi^u_s \psi) = 2 \Re \langle \psi_s | H_0 | A_u \psi_s \rangle.$$

(17)

Altogether, we obtain a rigorously justified version of (9):

$$\frac{d}{ds} E_v(\Phi^u_s \psi) = 2 \Re \langle \psi_s | H_0 | A_u \psi_s \rangle - \langle v | \text{div}(\rho_0 u) \rangle.$$

(18)

For clarity and simplicity, we have discussed only pure states. That was a matter of convenience. It is easy to verify that the preceding generalizes to mixed states: one merely needs to do the same thing to each component of the mixed state.

3.2. Instability. The final task is to show that, if $v' \neq v_0$ by more than a constant on some connected component of $\{\rho_0 > 0\}$, then some velocity field $u \in C^\infty_c(\mathbb{R}^3; \mathbb{R}^3)$ makes the right-hand side of (18) nonzero. The problem is conveniently localized as follows. Since $\rho_0$ is continuous, for any point $x \in \{\rho_0 > 0\}$, there is a bounded open ball (“patch”) $\Omega \subset \{\rho_0 > 0\}$ centered at $x$, such that $\rho_0$ is upper-and-lower bounded over $\Omega$. That is, $0 < m < \rho_0 < M$ over $\Omega$ for some $m$ and $M$. We need a lemma.

**Lemma.** For an open ball $\Omega$, if $\rho_0 \in C(\Omega)$ is upper-and-lower bounded, and $w \in L^2(\Omega)$ is not constant, then there is $u \in C^\infty_c(\Omega; \mathbb{R}^3)$ such that

$$\langle w | \text{div}(\rho_0 u) \rangle \neq 0.$$

(19)

The theorem follows almost immediately from this since if $v' - v_0$ is non-constant on some component of $\{\rho_0 > 0\}$, then there is a patch $\Omega \subset \{\rho_0 > 0\}$ over which it is non-constant. And, when the latter holds, the lemma together with (18) provides a witness $u$ to the instability of $\rho_0$ in the potential $v'$.

Now to the proof of the lemma. Consider the chain of Hilbert spaces and bounded (to be verified) linear maps

$$H^1_0(\Omega; \mathbb{R}^3) \xrightarrow{\text{div}} L^2(\Omega) \xrightarrow{-\nabla} H^1_0(\Omega; \mathbb{R}^3).$$

(20)
Here, $H^1_0(\Omega; \mathbb{R}^3)$ is the completion of the space $C_c^\infty(\Omega; \mathbb{R}^3)$ of smooth vector fields with support contained in $\Omega$ with respect to the Sobolev inner product (using summation convention)

$$(u|w)_{+1} = \int_\Omega \{u_i w^i + (\partial_i u_j)(\partial^i w^j)\} \, dx,$$  \quad (21)$$

and $H^1_0(\Omega; \mathbb{R}^3)'$ is the dual space (hence the prime) of continuous linear functionals $H^1_0(\Omega; \mathbb{R}^3) \to \mathbb{R}$. Since $C_c^\infty(\Omega; \mathbb{R}^3)$ is dense in $H^1_0(\Omega; \mathbb{R}^3)$, we think of $H^1_0(\Omega; \mathbb{R}^3)'$ as being the (vector-valued) distributions on $\Omega$ which happen to be continuous with respect to the $H^1$ norm \([21]. The reflex to identify the Hilbert space $H^1_0(\Omega; \mathbb{R}^3)$ with its dual is being suppressed, but the corresponding isometry $H^1_0(\Omega; \mathbb{R}^3) \cong H^1_0(\Omega; \mathbb{R}^3)'$ is used to equip $H^1_0(\Omega; \mathbb{R}^3)'$ with a Hilbert space structure. Claim: ran div, the range of div, is dense in $L^2(\Omega)$. That div in (20) is a bounded linear map with norm less than 1 is evident from \([21]. Thus, its transpose $\text{div}' : L^2(\Omega) \to H^1_0(\Omega; \mathbb{R}^3)'$ is also bounded. $\text{div}'$ is identifiable as $-\nabla$ by testing its image against $C_c^\infty(\Omega; \mathbb{R}^3)$, and using integration by parts, orthogonality of constants to ran div, and denseness of $C_c^\infty(\Omega; \mathbb{R}^3)$ in $H^1_0(\Omega; \mathbb{R}^3)$. Thus, $(\text{ran div})^\perp = \text{ker } \text{div}' = \text{ker } (-\nabla)$. But, if the distributional gradient of a function is zero then that function is constant \([24, 29\].) Since $\text{div}$ is bounded, that holds if $\rho \in H^1_0(\Omega; \mathbb{R}^3)$ is lower-bounded, this shows that $\text{div} [H^1_0(\Omega; \mathbb{R}^3)]$ is dense in $L^2(\Omega)$. (Equal to it, even \([23, 24\]).) Since $C_c^\infty(\Omega; \mathbb{R}^3)$ is dense in $H^1_0(\Omega; \mathbb{R}^3)$, and div is bounded, $\text{div} [C_c^\infty(\Omega; \mathbb{R}^3)]$ is also dense in $L^2(\Omega)$.

The rest of the proof will be given in abbreviated form, using the shorthand \(x \simeq y [H]\) to mean \(\|x - y\|_H < \epsilon \) for some tolerance $\epsilon > 0$ (dependent on context). Standard $\epsilon$-$\delta$ forms can be reconstituted straightforwardly, if tediously. The previous paragraph shows that there is $u' \in C_c^\infty(\Omega; \mathbb{R}^3)$ satisfying $\text{div } u' \simeq w [L^2(\Omega)]$. What we need to finish the proof is $u \in C_c^\infty(\Omega; \mathbb{R}^3)$ satisfying $\text{div}(\rho_0 u) \simeq w [L^2(\Omega)]$. Since div is bounded, that holds if $\rho_0 u \simeq u' [H^1]$. That, in turn, is equivalent to

$$\rho_0 u \simeq u' [L^2] \quad (\ast) \quad \text{and} \quad \partial_i (\rho_0 u) \simeq \partial_i u' [L^2] \quad (\ast\ast).$$

Step one toward a smooth approximation of the merely continuous $u'/\rho_0$ is the formal computation

$$\partial_i (\rho_0^{-1} u') = \rho_0^{-1} \partial_i u' - \rho_0^{-2} (\partial_i \rho_0) u'. \quad (22)$$

Since $\rho_0 \in H^1(\Omega)$ is lower-bounded, this shows that $\rho_0^{-1} u'$ is in $H^1_0(\Omega; \mathbb{R}^3)$, and its support is a positive distance from the boundary of $\Omega$. Now, mollification (convolution with a $C_c^\infty$ function) produces $u$ which approximates $u'/\rho_0$ simultaneously in $H^1$ norm and in uniform (supremum over $\Omega$) norm:

$$u \simeq \rho_0^{-1} u' [H^1, \text{sup}]. \quad (23)$$

(\ast) now follows from \([23\) and continuity of $\rho_0$.

For (\ast\ast), we compute

$$\partial_i (\rho_0 u) = (\partial_i \rho_0) u + \rho_0 \partial_i u \simeq (\partial_i \rho_0) \frac{u'}{\rho_0} + \rho_0 \left( \frac{\partial u'}{\partial x^i} - \frac{\partial u}{\partial x^i} \right) [L^2].$$

In passing to the second line, the first term follows by $u \simeq \rho_0^{-1} u' [\text{sup}]$, and the second by $u \simeq \rho_0^{-1} u' [H^1]$ in conjunction with \([22\). Thus, $u$ satisfies (\ast\ast). The Lemma, and Theorem \([\) with it, is proven.
4. Conclusion

The aim of this work was to address the Hohenberg-Kohn problem from a density-centric, rather than wavefunction-centric, viewpoint, with modest technical complication. Physically reasonable restrictions on potentials and densities are acceptable. For potentials, there seems little reason to be unsatisfied with the Kato-Rellich class, except perhaps the fact that $L^{3/2} + L^\infty$ is a little more natural from an abstract general DFT perspective. As far as densities are concerned, the suggestion of a discontinuous ground state electronic density would probably be met with incredulity from most physicists; the requirement of continuity is not demanding. Indeed, it is known that eigenfunctions for a Kato class potential are continuous. This guarantees lower semicontinuity for the associated density, a little short of our needs. The hypothesis that $\rho > 0$ everywhere is less satisfactory, but the current approach is somewhat hobbled without it. One hopes that it might turn out to be provable; physical intuition certainly suggests that it is generic for ground states.

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