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Hohenberg-Kohn and Percus-Levy-Lieb proofs of density-functional theory

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The premise of density-functional theory is that knowledge of the ground-state density uniquely determines the Hamiltonian, and thereby, via solution of the corresponding time-independent Schrödinger equation, all the properties of the system. The density therefore constitutes a basic variable of quantum mechanics. There are at present two paths from the density to the Hamiltonian: the Hohenberg and Kohn proof of the bijectivity between the external potential and the basic variable, and the Percus, Levy, and Lieb constrained-search proof. We argue the Hohenberg- and Kohn-type proof to be the more fundamental, and that this is the case in general when both external electrostatic and magnetostatic fields are present, and the basic variables are the ground-state density and physical current density.

Density-functional theory (DFT) is an extensively employed theory of the electronic structure of matter. In the context of DFT, matter is defined as a system of N electrons in the presence of an external field $\mathcal{F}^{\text{ext}}(\mathbf{r}) = -\boldsymbol{\nabla} v(\mathbf{r})$, with $v(\mathbf{r})$ a scalar potential. The premise of DFT is that knowledge of the ground-state density $\rho(\mathbf{r})$ of a system *uniquely* determines the Hamiltonian $\hat{H}$ to within a constant, and thereby via the solution Ψ of the corresponding time-independent Schrödinger equation, *all* the properties of that system. The density $\rho(\mathbf{r})$, a gauge-invariant property, is thus considered a basic variable of quantum mechanics. There are two proofs of the path from the ground-state density $\rho(\mathbf{r})$ of a system to its Hamiltonian $\hat{H}$. There is the original path derived for a nondegenerate ground state due to Hohenberg and Kohn (HK) [1] based on the proof of bijectivity between $\rho(\mathbf{r})$ and the external potential $v(\mathbf{r})$. Then there is the constrained-search proof of Percus, Levy, and Lieb (PLL) [2]. The two proofs are independent, and as such are considered at present to be at par with each other. We argue that the HK proof is more fundamental, and that this is the case in general when the electrons are also subject to other external fields such as a magnetostatic field. The principal reason for this is that it is solely via the proof of bijectivity between the external potentials and certain gauge-invariant properties of the system that determines what constitutes the basic variables of quantum mechanics. Consequently, the PLL proof, which requires the *a priori* knowledge of what the basic variables are, is dependent on the conclusions of an HK-type proof of bijectivity and is therefore less fundamental. More significantly, the choice of what constitutes a basic variable is *not arbitrary* but governed by the one-to-one relationships of HK. The use of PLL-type proofs for arbitrarily chosen properties, or those properties assumed to be basic variables on the basis of proofs that ignore the presence of the external potentials, is thus no longer justified.

In order to explain our reasoning, we begin with a brief review of the two paths from the ground-state density $\rho(\mathbf{r})$ to

the Hamiltonian $\hat{H}$. The Hamiltonian in atomic units ($e = \hbar = m = 1$) is $\hat{H} = \hat{T} + \hat{U} + \hat{V}$, where the respective operators are the kinetic $\hat{T} = \frac{1}{2}\sum_k p_k^2, \hat{\mathbf{p}}_k = -i\boldsymbol{\nabla}_{\mathbf{r}_k}$, electron interaction $\hat{U} = \frac{1}{2}\sum'_{k,\ell} 1/|\mathbf{r}_k - \mathbf{r}_\ell|$, and external potential $\hat{V} = \sum_k v(\mathbf{r}_k)$. The Schrödinger equation is $\hat{H}(\mathbf{R})\Psi(\mathbf{X}) = E\Psi(\mathbf{X})$, where $\{\Psi(\mathbf{X}),E\}$ are the eigenfunctions and eigenenergies, with $\mathbf{R} = \mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{X} = \mathbf{x}_1, \ldots, \mathbf{x}_N; \mathbf{x} = \mathbf{r}\sigma, \{\mathbf{r}\sigma\}$ being the spatial and spin coordinates of the electron. The energy E is the expectation value of the Hamiltonian $\hat{H}$: $E = \langle\Psi(\mathbf{X})|\hat{H}|\Psi(\mathbf{X})\rangle = T + E_{ee} + \int \rho(\mathbf{r})v(\mathbf{r})d\mathbf{r}$, where T and E_{ee} are the kinetic and electron-interaction energies being the expectation values of the corresponding operators, and where the ground-state density $\rho(\mathbf{r})$ is the expectation value $\rho(\mathbf{r}) = \langle\Psi(\mathbf{X})|\hat{\rho}(\mathbf{r})|\Psi(\mathbf{X})\rangle$ with the density operator $\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r})$.

Hohenberg-Kohn path. The HK theorem is proved for the case when the N-electron system is in a *nondegenerate* ground state. In the theorem, it is *first* proved (map C) that the relationship between the external *scalar* potential $v(\mathbf{r})$ and the wave function $\Psi(\mathbf{X})$ is bijective or one to one. *This fact is then employed* in the proof (map D) that the relationship between $\Psi(\mathbf{X})$ and $\rho(\mathbf{r})$ is bijective. Thus

$$v(\mathbf{r}) \overset{\text{Map C}}{\longleftrightarrow} \Psi(\mathbf{X}) \overset{\text{Map D}}{\longleftrightarrow} \rho(\mathbf{r}). \tag{1}$$

The proof is for v-representable densities, i.e., for densities obtained from wave functions that are solutions of Hamiltonians of the form given above. Knowledge of $\rho(\mathbf{r})$ then *uniquely* determines $v(\mathbf{r})$ to within a constant, and since the operators $\hat{T}$ and $\hat{U}$ are assumed known, and so is the Hamiltonian $\hat{H}(\mathbf{R})$. The solution $\Psi(\mathbf{X})$ of the Schrödinger equation then leads to all the properties of the system. The wave function $\Psi(\mathbf{X})$ is thus a functional of the density $\rho(\mathbf{r}) : \Psi(\mathbf{X}) = \Psi[\rho]$. Via a *density-preserving* unitary transformation [3,4] it has been shown that the wave function must also be a functional of a gauge function $\alpha(\mathbf{R})$. This ensures that the wave function when written as a functional is gauge variant. Thus, $\Psi(\mathbf{X}) = \Psi[\rho(\mathbf{r}),\alpha(\mathbf{R})]$. Furthermore, the HK proof is generalized [3,4] to be valid for each choice of gauge function $\alpha(\mathbf{R})$. The HK theorem thus defines [5,6] a basic variable of quantum mechanics

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as a gauge-invariant property, knowledge of which uniquely determines the external potential, hence the Hamiltonian, and thereby via the solution of the Schrödinger equation, all the properties of the system.

Percus-Levy-Lieb path. The PLL proof *assumes* knowledge of the fact that the basic variable is the density $\rho(\mathbf{r})$. The proof is valid for both *nondegenerate* and *degenerate* ground states and for N-representable densities. The proof involves a constrained search over all antisymmetric functions $\Psi_\rho(\mathbf{X})$ that generate the ground-state density $\rho(\mathbf{r})$. The true wave function $\Psi(\mathbf{X})$ is the one that yields the density $\rho(\mathbf{r})$ and minimizes the expectation value of $\hat{T} + \hat{U}$:

$$\min_{\Psi_\rho \to \rho} \langle \Psi_\rho(\mathbf{X}) | \hat{T} + \hat{U} | \Psi_\rho(\mathbf{X}) \rangle. \qquad (2)$$

This expectation value is *independent* of the external potential $v(\mathbf{r})$. [Implicit in this constrained-search procedure is that the functions $\Psi_\rho(\mathbf{X})$ lead to rigorous upper bounds to the ground-state energy, the true $\Psi(\mathbf{X})$ giving the exact value E.] Further, according to Levy [2], as $\Psi(\mathbf{X})$ cannot be an eigenfunction of more than one $\hat{H}$ with a multiplicative potential, it follows that $\rho(\mathbf{r})$ determines $\hat{H}$ *uniquely* within an additive constant, and hence via solution of the Schrödinger equation all the properties of the system. Thus, this path to the Hamiltonian is

$$\rho(\mathbf{r}) \longrightarrow \Psi(\mathbf{X}) \longrightarrow \hat{H}. \qquad (3)$$

If more than one $\Psi(\mathbf{X})$ satisfies Eq. (2), then these functions all give the same ground-state energy. Thus, when degeneracies exist, Eq. (3) once again follows (see Levy [2]). As the operators $\hat{T}$ and $\hat{U}$ are known, the path from $\Psi(\mathbf{X})$ to $\hat{H}$ in Eq. (3) requires knowledge of the external potential $v(\mathbf{r})$. The potential $v(\mathbf{r})$ may be determined explicitly, either by inversion [7] of the Schrödinger equation, or by a more physical description via the "quantal Newtonian" first law [3,7,8], according to which the sum of the external $\mathcal{F}^{\text{ext}}(\mathbf{r})$ and internal $\mathcal{F}^{\text{int}}(\mathbf{r})$ fields on an electron vanish. Thus, $v(\mathbf{r})$ is the work done to bring an electron from a reference point at infinity to its position at $\mathbf{r}$ in the force of the internal field:

$$v(\mathbf{r}) = \int_\infty^\mathbf{r} \mathcal{F}^{\text{int}}(\mathbf{r}') \cdot d\boldsymbol{\ell}', \qquad (4)$$

where $\mathcal{F}^{\text{int}}(\mathbf{r}) = \mathcal{E}_{\text{ee}}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{Z}(\mathbf{r})$. Here the component fields are [3,7] the electron interaction $\mathcal{E}_{\text{ee}}(\mathbf{r})$, differential density $\mathcal{D}(\mathbf{r})$, and kinetic $\mathcal{Z}(\mathbf{r})$. The sources of these fields are quantal in that they are expectation values of Hermitian operators taken with respect to the wave function $\Psi(\mathbf{X})$, which is known as a result of the constrained search. For the definitions of the quantal sources and fields, we refer the reader to [3,7]. To complete the PLL prescription, we note that it is possible to construct [9] antisymmetric functions $\Psi_\rho(\mathbf{X})$ that generate the density $\rho(\mathbf{r})$. It is also possible to construct [10] antisymmetric functions $\Psi_\rho(\mathbf{X})$ that are functionals of functions χ, i.e., $\Psi_\rho(\mathbf{X}) = \Psi_\rho[\chi](\mathbf{X})$ that also reproduce a given density $\rho(\mathbf{r})$.

Note that the constrained-search proof does not determine what property constitutes a basic variable. Had it not been known that the ground-state density $\rho(\mathbf{r})$ is a basic variable, the PLL proof would not be possible. This becomes more evident in the case of the added presence of a magnetostatic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, with $\mathbf{A}(\mathbf{r})$ the

vector potential. In this case in atomic units such that $e = \hbar = m = 1$, the Hamiltonian $\hat{H} = \hat{T} + \hat{U} + \hat{V}_A$, where the external potential operator $\hat{V}_A = \hat{V} + \frac{1}{c} \int \hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} - \frac{1}{2c^2} \int \hat{\rho}(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r}$ with the physical current-density operator $\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r})$, the paramagnetic current-density operator $\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2i} \sum_k [\nabla_{\mathbf{r}_k} \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \nabla_{\mathbf{r}_k}]$, and the diamagnetic current-density operator $\hat{\mathbf{j}}_d(\mathbf{r}) = \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r})/c$. The energy expectation value is $E = T + E_{ee} + \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} + \frac{1}{c} \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} - \frac{1}{2c^2} \int \rho(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r}$, with $\mathbf{j}(\mathbf{r})$ the physical current density. Once again, via a density-preserving unitary transformation, the wave function is a functional of a gauge function $\alpha(\mathbf{R}) : \Psi(\mathbf{X}) = \Psi[\alpha(\mathbf{R})]$. (For a constant magnetic field, the above Hamiltonian can be shown to correspond to the interaction of the magnetic field with the orbital angular momentum.)

The question which arises is what properties constitute the basic variables in quantum mechanics when a magnetostatic field is present. The answer, originally provided a quarter of a century ago [11], is that the basic variables are the ground-state density $\rho(\mathbf{r})$ and the gauge-variant *paramagnetic* current density $\mathbf{j}_p(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\mathbf{j}}_p(\mathbf{r}) | \Psi(\mathbf{X}) \rangle$. With this choice of basic variables, a constrained-search proof is readily constructed [12]. One searches over all antisymmetric functions $\Psi_{\rho, \mathbf{j}_p}(\mathbf{X})$ that yield the ground state $\{\rho, \mathbf{j}_p\}$. The true ground-state wave function $\Psi(\mathbf{X})$ is that which minimizes the expectation value of $\hat{T} + \hat{U}$. Although such a proof with these basic variables appears logical, it is fundamentally in error as explained below.

In our recent work [5,6] we have explained why $\{\rho, \mathbf{j}_p\}$ cannot be the basic variables. Among the several reasons given, the most significant one is that the proof for $\{\rho, \mathbf{j}_p\}$ being the basic variables ignores a fundamental physical fact intrinsic to this case. In contrast to the $\mathbf{B}(\mathbf{r}) = 0$ case, where the relationship between the external potential $v(\mathbf{r})$ and the nondegenerate ground-state wave function $\Psi(\mathbf{X})$ is one to one, in the $\mathbf{B}(\mathbf{r})$ finite case the relationship between the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the nondegenerate ground state $\Psi(\mathbf{X})$ can be *many to one*. Hence,

$$\begin{matrix} \{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\} & \searrow & \\ \{v'(\mathbf{r}), \mathbf{A}'(\mathbf{r})\} & \longrightarrow & \\ \{v''(\mathbf{r}), \mathbf{A}''(\mathbf{r})\} & \longrightarrow & \Psi(\mathbf{X}) \\ \cdots & \nearrow & \end{matrix} \qquad (5)$$

The *many-to-one* relationship is exhibited, for example, by the two-dimensional Hooke's atom in a magnetic field [13]. In this example there exists an *infinite* number of $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ that generate the same ground state $\Psi(\mathbf{X})$. A consequence of the many-to-one relationship is that knowledge of $\{\rho, \mathbf{j}_p\}$ is inadequate to determine the physical current density $\mathbf{j}(\mathbf{r})$ *uniquely*. The constrained-search proof with $\{\rho, \mathbf{j}_p\}$ as the basic variables is thus in error.

As a result of the many-to-one relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and $\Psi(\mathbf{X})$, it is evident that there can be no equivalent of map C of the original HK proof. The proof [11] that $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ are the basic variables relies *solely* on a map-D-type argument of a one-to-one relationship between $\Psi(\mathbf{X})$ and $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$. The claim is that since the wave function $\Psi(\mathbf{X})$ is then known, the many-to-one relationship

between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and $\Psi(\mathbf{X})$ can be ignored. However, the solely map D argument *presupposes* [5,14] the existence of the generalization of map C and is therefore fundamentally flawed. Consequently, one does not know the wave function $\Psi(\mathbf{X})$. For other reasons why $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ cannot be the basic variables, we refer the reader to [5,6].

In our work [5,6], we have proved the bijective relationship between the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the gauge-invariant properties $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ of the N-electron system in a nondegenerate ground state. In other words,

$$\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\} \longleftrightarrow \{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}. \tag{6}$$

Thus, knowledge of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ determines $v(\mathbf{r})$ to within a constant and $\mathbf{A}(\mathbf{r})$ to within the gradient of a scalar function, and thereby determines uniquely the Hamiltonian $\hat{H}$ of the system. Our proof of this bijectivity explicitly accounts for the many-to-one relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the non-degenerate ground state $\Psi(\mathbf{X})$. Hence, the basic variables in the presence of a magnetostatic field are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. With this knowledge, a constrained-search proof for the determination of the ground-state wave function $\Psi(\mathbf{X})$ follows [5,6]. One searches over all antisymmetric functions $\Psi_{\rho,\mathbf{j}}(\mathbf{X})$ that yield the ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. These functions lead to rigorous upper bounds to the ground-state energy. The true ground-state wave function $\Psi(\mathbf{X})$ is that which yields $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ and which minimizes the expectation value of $\hat{T} + \hat{U}$:

$$\min_{\Psi_{\rho,\mathbf{j}} \to \rho, \mathbf{j}} \langle \Psi_{\rho,\mathbf{j}}(\mathbf{X}) | \hat{T} + \hat{U} | \Psi_{\rho,\mathbf{j}}(\mathbf{X}) \rangle. \tag{7}$$

This expectation value is independent of the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$. Once again, as $\Psi(\mathbf{X})$ cannot be an eigenfunction of more than one $\hat{H}$ with a multiplicative scalar potential and vector potential, it follows that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ determines $\hat{H}$ uniquely to within an additive constant and the gradient of a scalar function:

$$\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\} \to \Psi(\mathbf{X}) \to \hat{H}. \tag{8}$$

If more than one $\Psi(\mathbf{X})$ satisfies Eq. (7), then these functions all give the same ground-state energy. Thus, degenerate ground states are accounted for in Eq. (8). In going from $\Psi(\mathbf{X})$ to $\hat{H}$, the external potential $v(\mathbf{r})$ may again be obtained from the corresponding "quantal Newtonian" first law [15,16]: $\mathcal{F}^{\text{ext}} + \mathcal{F}^{\text{int}} = 0$, where $\mathcal{F}^{\text{ext}} = \mathcal{E}(\mathbf{r}) - \mathcal{L}(\mathbf{r})$ with $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$ and $\mathcal{L}(\mathbf{r}) = \mathbf{j}(\mathbf{r}) \times \mathbf{B}(\mathbf{r})/\rho(\mathbf{r})$ the magnetic field component of the Lorentz field, and $\mathcal{F}^{\text{int}}(\mathbf{r}) = \mathcal{E}_{ee}(\mathbf{r}) - \mathcal{D}(\mathbf{r}) - \mathcal{Z}(\mathbf{r}) - \mathcal{I}(\mathbf{r})$ with $\mathcal{I}(\mathbf{r})$ the contribution of the magnetic field to the internal field of the electrons. (For the definitions of the fields and their quantal sources, we refer the reader to [15].) This constrained-search proof for the determination of the ground-state wave function $\Psi(\mathbf{X})$, and simultaneously the energy E, is the correct counterpart to our proof via bijectivity. Once again, it is possible to construct antisymmetric functions $\Psi_{\rho,\mathbf{j}}(\mathbf{X})$ [17–19] that reproduce a given $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. [We note that in the construction of the Slater determinant in [17], the bijective relationship of Eq. (6) must be employed.]

The conclusion, based on the above discussion, is that knowledge of what constitutes the basic variables in quantum mechanics is arrived at via a (HK-type) proof of bijectivity between the basic variables and the external potentials. It

is with this knowledge that a PLL proof becomes possible, because only then is the subspace over which the constrained search is to be performed defined. The search over this subspace then leads to the true ground-state wave function and energy.

For completeness, we note that according to the Gunnarsson-Lundqvist theorem [20,21], there also exists a one-to-one relationship between the density $\rho^e(\mathbf{r})$ of the lowest excited state of a given symmetry and the external potential $v(\mathbf{r})$. Thus such a density is also a basic variable of quantum mechanics. With this knowledge, a constrained-search proof for the determination of the excited-state wave function $\Psi^e(\mathbf{X})$ and energy E^e may then be constructed. One searches over all antisymmetric functions $\Psi_{\rho^e}(\mathbf{X})$ of the given symmetry that yield the density $\rho^e(\mathbf{r})$. The wave function $\Psi^e(\mathbf{X})$ is that which yields the density $\rho^e(\mathbf{r})$ and which minimizes the expectation value of $\hat{T} + \hat{U}$. The functions $\Psi_{\rho^e}(\mathbf{X})$ yield rigorous upper bounds to the excited-state energy, with $\Psi^e(\mathbf{X})$ leading to the true value E^e.

Are all solely map-D-type proofs of what constitutes a basic variable flawed? In addition to the case of current-density-functional theory as discussed above, such proofs also exist for spin-density-functional theory [22], for current-density-functional theory when the added interaction between the magnetic field and the spin angular momentum is also considered, and for other Hamiltonians [23]. The corresponding PLL proofs exist [18,19,24] for the *assumed* basic variables. We discuss these individual cases in future work. We note, however, that ignoring the natural fact of the many-to-one relationship between the external potentials and the nondegenerate ground-state wave function voids these proofs. Furthermore, solely map-D-type proofs can be applied to *any* property, making it unclear as to what the true basic variables are. For example, in current DFT, the map D proof [11] given for $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ has also been given [25] for the variables $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. What is done in map-D-type proofs is that arbitrarily chosen properties are put on the right-hand side of the map, a map C between external potentials and the wave function presupposed, and then a one-to-one relationship "proved" between the wave function $\Psi(\mathbf{X})$ and the property. Lastly, the principal manner by which DFT is applied is via the assumption of noninteracting v representability. That is via the construction of a model system of noninteracting fermions or bosons that possess values of the basic variables that are identical to those of the interacting electronic system. Knowledge of the *true* basic variables then permits the construction of the *unique* model system that reproduces these variables. For example, in current DFT it is possible to construct [5,15] model noninteracting fermion and boson systems that reproduce the basic variables $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. This shows that these densities are noninteracting v representable. It is not possible to construct such a unique local effective potential system with $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ as the basic variables because knowledge of $\{\rho(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ cannot uniquely determine $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. We also note that the optimized potential method has been proposed [26] as a means to circumvent the many-to-one relationship between the external potentials and the ground-state wave function, but the underlying formal issues still persist.

Finally, as discussed above, the PLL constrained-search proofs for the determination of the wave function $\Psi(\mathbf{X})$ for

the cases for which $\mathbf{B}(\mathbf{r}) = 0$ and $\mathbf{B}(\mathbf{r}) \neq 0$ are *explicitly* independent of the respective external potentials $v(\mathbf{r})$ and $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$. This is a key attribute of the PLL-type proof. But these proofs require *a priori* knowledge of the basic variables $\rho(\mathbf{r})$ and $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, respectively. As a consequence, there is an *implicit* dependence of the proofs on the external potentials. This follows from the bijective relationship between the external potentials and the basic variables: knowledge of the ground-state density $\rho(\mathbf{r})$ uniquely determines $v(\mathbf{r})$ to within a constant, and knowledge of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ determines $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ to within a constant and a gauge transformation. Thus, the PLL proof is intrinsically connected to the specific physical system of interest as defined by the external potentials, in spite of the fact that one is minimizing the expectation value only of the operators $\hat{T} + \hat{U}$. In this manner, the HK theorem provides a deeper perspective into the PLL constrained-search proof.

In conclusion, there are many attributes of the PLL constrained-search proof over the HK-type proof for the determination of the wave function of a system of electrons:

the stringent v-representability constraint is reduced to one of N representability; there is the generalization in the proof to degenerate states; and lastly, there is the explicit independence from external potentials in the proof. However, these attributes only accrue as a result of preknowledge of what the basic variables are. What properties constitute the basic variables of quantum mechanics can only be determined via the rigorous HK-type bijectivity proofs which *explicitly* involve the external potentials that define the Hamiltonian. The external potentials play the key role of defining the physical system and *thereby* the basic variables. Therefore, in spite of the restriction to v-representable densities and to nondegenerate ground states, it is the HK-type proof that is the more fundamental.

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