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Hohenberg-Kohn theorems in electrostatic and uniform magnetostatic fields

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The Hohenberg-Kohn (HK) theorems of bijectivity between the external scalar potential and the gauge invariant nondegenerate ground state density, and the consequent Euler variational principle for the density, are proved for arbitrary electrostatic field and the constraint of fixed electron number. The HK theorems are generalized for spinless electrons to the added presence of an external uniform magnetostatic field by introducing the new constraint of fixed canonical orbital angular momentum. Thereby, a bijective relationship between the external scalar and vector potentials, and the gauge invariant nondegenerate ground state density and physical current density, is proved. A corresponding Euler variational principle in terms of these densities is also developed. These theorems are further generalized to electrons with spin by imposing the added constraint of fixed canonical orbital and spin angular momenta. The proofs differ from the original HK proof and explicitly account for the many-to-one relationship between the potentials and the nondegenerate ground state wave function. A Percus-Levy-Lieb constrained-search proof expanding the domain of validity to N -representable functions, and to degenerate states, again for fixed electron number and angular momentum, is also provided. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4934800>]

I. INTRODUCTION

The Hohenberg-Kohn (HK) theorems¹ constitute a fundamental advance in quantum mechanics. As a consequence, they have furthered our understanding of the electronic structure of matter: atoms, molecules, solids, clusters, surfaces, and lower dimensional electronic systems such as heterostructures, quantum dots, and graphene. Matter, according to HK, is described as a system of N electrons in an external electrostatic field $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$. The first HK theorem defines the concept of a *basic variable* of quantum mechanics. Knowledge of this gauge invariant property—the nondegenerate ground state density $\rho(\mathbf{r})$ —is of two-fold significance: (a) It determines the Schrödinger theory wave functions Ψ of the system, both ground and excited states, (b) as the wave function Ψ is now proved to be a functional of the basic variable, it constitutes together with the second HK theorem—the energy variational principle for arbitrary variations of the density—the basis of theories of electronic structure such as of Hohenberg-Kohn,¹ Kohn-Sham,² and quantal density functional theories^{3,4} (QDFT). The theorems are valid for arbitrary confining potential $v(\mathbf{r})$ and electron number N but are derived⁵ for the constraint of *fixed* N . In this paper, we generalize the HK theorems for spinless electrons to the added presence of an external *uniform* magnetostatic field. As the presence of the magnetic field constitutes a new degree of freedom, we introduce the further natural constraint of *fixed* canonical orbital angular momentum. Thereby, we prove that the basic variables in quantum mechanics in a uniform magnetic field are the gauge invariant nondegenerate ground state density $\rho(\mathbf{r})$ and *physical* current density $\mathbf{j}(\mathbf{r})$. These

theorems are then further generalized to electrons with spin by imposing the constraints of *fixed* canonical orbital and spin angular momentum.

The generalization is motivated by the considerable recent interest in yrast states which are states of lowest energy for fixed angular momentum. These states have been studied experimentally and theoretically for both bosons and fermions, e.g., rotating trapped Bose-Einstein condensates,⁶ and harmonically trapped electrons in the presence of a uniform perpendicular magnetic field.⁷ The theorems derived are applicable to all experimentations with a uniform magnetic field such as the magneto-caloric effect,⁸ the Zeeman effect, cyclotron resonance, magnetoresistance, the de-Haas-van Alphen effect, the Hall effect, the quantum Hall effect, the Meissner effect, and nuclear magnetic resonance.

The manner by which a basic variable is so defined is via the proof of the first HK theorem for v -representable densities. To explain this, and to contrast the present proofs with the HK proof, we first briefly describe the HK arguments. The HK theorems are proved for a nondegenerate ground state. Particularizing to electrons without any loss of generality, the Hamiltonian \hat{H} in atomic units (charge of electron $-e$; $|e| = \hbar = m = 1$) is $\hat{H} = \frac{1}{2} \sum_k p_k^2 + \frac{1}{2} \sum_{k,\ell} 1/|\mathbf{r}_k - \mathbf{r}_\ell| + \sum_k v(\mathbf{r}_k)$, where the terms correspond to the kinetic \hat{T} (with momentum $\hat{\mathbf{p}}_k = -i\nabla_{\mathbf{r}_k}$), the electron-interaction \hat{W} , and external potential \hat{V} operators, respectively. 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 $\mathbf{R} = \mathbf{r}_1, \dots, \mathbf{r}_N$, $\mathbf{X} = \mathbf{x}_1, \dots, \mathbf{x}_N$, $\mathbf{x} = \mathbf{r}\sigma$ being the spatial and spin coordinates of the electron. The energy E is the expectation $E = \langle \Psi(\mathbf{X}) | \hat{H}(\mathbf{R}) | \Psi(\mathbf{X}) \rangle$. In the first HK theorem, it is initially

proved (map C) that there is a one-to-one relationship between the external potential $v(\mathbf{r})$ and the nondegenerate ground-state wave function $\Psi(\mathbf{X})$. Employing this relationship, it is then proved (map D) that there is a one-to-one relationship between the wave function $\Psi(\mathbf{X})$ and the corresponding nondegenerate ground state density $\rho(\mathbf{r})$. Thus, knowledge of $\rho(\mathbf{r})$ determines $v(\mathbf{r})$ to within a constant. Since for a fixed electron number N , the kinetic \hat{T} and electron-interaction potential \hat{W} energy operators are known, so is the system Hamiltonian. Solution of the corresponding Schrödinger equation then leads to the wave functions Ψ of the system. *It is the one-to-one relationship between the external potential and the gauge invariant density that defines the latter as a basic variable.* As the wave function Ψ , and hence energy $E_v[\rho]$ are functionals of the density $\rho(\mathbf{r})$, the variational Euler equation for the density with fixed $v(\mathbf{r})$ follows subject to the constraint of known electron number N (see Table 1). (The lowest nondegenerate^{9,10} excited state density $\rho^e(\mathbf{r})$ of a given symmetry different from that of the ground state is also a basic variable.)

In the added presence of an external magnetostatic field $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, where $\mathbf{A}(\mathbf{r})$ is the vector potential, the Hamiltonian when the interaction of the field is only with the orbital angular momentum is

$$\hat{H} = \frac{1}{2} \sum_k \left[\hat{\mathbf{p}}_k + \frac{1}{c} \mathbf{A}(\mathbf{r}_k) \right]^2 + \hat{W} + \hat{V}. \quad (1)$$

When the interaction of the magnetic field is with both the orbital and spin angular momenta, the Hamiltonian is

$$\hat{H} = \frac{1}{2} \sum_k \left[\hat{\mathbf{p}}_k + \frac{1}{c} \mathbf{A}(\mathbf{r}_k) \right]^2 + \hat{W} + \hat{V} + \frac{1}{c} \sum_k \mathbf{B}(\mathbf{r}_k) \cdot \mathbf{s}_k, \quad (2)$$

where \mathbf{s} is the electron spin angular momentum vector. In deriving the Hamiltonians of Eqs. (1) and (2), we have hewed to the philosophy¹¹ that the only “fundamental” interactions are those that can be generated by the substitution $\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} + \frac{1}{c} \mathbf{A}$. (This then defines the physical momentum operator in the presence of a magnetic field, and thereby the physical current density $\mathbf{j}(\mathbf{r})$.) In non-relativistic quantum mechanics, the Hamiltonian of Eq. (2) is derived¹¹ by Schrödinger-Pauli theory for spin $\frac{1}{2}$ particles via the kinetic energy operator $\frac{1}{2} \boldsymbol{\sigma} \cdot (\mathbf{p} + \mathbf{A}) \boldsymbol{\sigma} \cdot (\mathbf{p} + \mathbf{A})$, where $\boldsymbol{\sigma}$ is the Pauli matrix and $\mathbf{s} = \frac{1}{2} \boldsymbol{\sigma}$. The spin magnetic moment generated in this way has the correct gyromagnetic ratio $g = 2$.

It would appear that one could prove a one-to-one relationship between the gauge invariant properties $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ and the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ along the lines of the HK proof. However, no such proof is possible as the relationship between the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the nondegenerate ground state wave function $\Psi(\mathbf{X})$ can be *many-to-one*¹² and even *infinite-to-one*.¹³ Hence, in these cases, there is no equivalent of map C, and therefore, the original HK path is not possible. The proof that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ are the basic variables must then differ from the original HK proof. Furthermore, the proof must account for the many-to-one relationship between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and $\Psi(\mathbf{X})$.

In the literature,^{2,12,14} the proofs of what properties constitute the basic variables are not rigorous in the HK sense of the one-to-one relationship between the basic variables and the external potentials $\{v, \mathbf{A}\}$. Further, they do not account

for the many-to-one relationship between $\{v, \mathbf{A}\}$ and Ψ . Additionally, the system angular momentum is not considered. The choice of the basic variables is arrived at solely on the basis of a map D-type proof between these assumed properties and the nondegenerate ground state Ψ , thereby the claim that Ψ is a functional of these properties. In these proofs, the existence of a bijective map C is implicitly assumed^{15,16} (see also the last reference of 12). For example, in spin-DFT^{2,12,14} for which the Hamiltonian is that of Eq. (2) with the field component of the momentum absent, the basic variables are assumed to be $\{\rho(\mathbf{r}), \mathbf{m}(\mathbf{r})\}$, where $\mathbf{m}(\mathbf{r})$ is the magnetization density. In current-DFT,¹⁴ corresponding to the Hamiltonian of Eq. (1), the basic variables are assumed to be $\rho(\mathbf{r})$ and the gauge variant paramagnetic current density $\mathbf{j}_p(\mathbf{r})$. For the Hamiltonian of Eq. (2), the basic variables are assumed to be $\{\rho(\mathbf{r}), \mathbf{m}(\mathbf{r}), \mathbf{j}_p(\mathbf{r})\}$ or $\{\rho(\mathbf{r}), \mathbf{m}(\mathbf{r}), \mathbf{j}_p(\mathbf{r}), \mathbf{j}_{p,m}(\mathbf{r})\}$, where $\mathbf{j}_{p,m}(\mathbf{r})$ are the gauge variant paramagnetic currents of each component of the magnetization density. Subsequently, a map D proof is provided. Additionally, with the basic variables now assumed known, a Percus-Levy-Lieb (PLL)-type proof^{17,18} can then be formulated.¹⁹ More recently, we gave a derivation^{15,20} which purported to prove that $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ were the basic variables but the proof was in error.²¹ Subsequently, we proved Ref. 22 for the Hamiltonian of Eq. (1) that for the significant subset of systems^{13,23} for which the ground state wave function Ψ is real, the basic variables are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. Our proof of bijectivity between $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ and $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ explicitly accounts for the many-to-one $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ to Ψ relationship. This proof then constitutes a special case of the more general proof for Ψ complex presented in this work.

Here, we extend the HK theorems to systems of electrons in external electrostatic $\mathcal{E}(\mathbf{r}) = -\nabla v(\mathbf{r})$ and magnetostatic $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ fields with known electron number N and angular momentum \mathbf{J} . The proofs are for a uniform magnetostatic field and for Hamiltonians in which the interaction of the magnetic field is (i) solely with the orbital angular momentum ($\mathbf{J} = \mathbf{L}$) and (ii) with both the orbital and spin angular momenta ($\mathbf{J} = [\mathbf{L}$ and $\mathbf{S}]$). We prove, in the *rigorous* HK sense, that for fixed N and \mathbf{J} , the basic variables are the gauge invariant nondegenerate ground state density $\rho(\mathbf{r})$ and *physical* current density $\mathbf{j}(\mathbf{r})$. In other words, knowledge of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ determines the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ to within a constant and the gradient of a scalar function, respectively. Hence, with the Hamiltonians known, solution of the respective Schrödinger and Schrödinger-Pauli equations leads to the wave functions of each system. The proof is for (v, \mathbf{A}) -representable $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. The extension to the PLL^{17,18} constrained-search path for N -representable and degenerate states readily follows. As the wave function Ψ is a functional of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, theories of electronic structure based on $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ as the basic variables can then be formulated.

II. PROOF OF GENERALIZED HOHENBERG-KOHN THEOREMS

To accentuate the role of the density $\rho(\mathbf{r})$ and physical current density $\mathbf{j}(\mathbf{r})$, we rewrite the Hamiltonians of Eqs. (1) and (2) in terms of operators representative of these gauge invariant properties. The Hamiltonians can then be written,

respectively, as

$$\hat{H} = \hat{T} + \hat{W} + \hat{V}_A \quad (3)$$

and

$$\hat{H} = \hat{T} + \hat{W} + \hat{V}_A - \int \hat{\mathbf{m}}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r}) d\mathbf{r}, \quad (4)$$

where the total external potential operator \hat{V}_A is

$$\hat{V}_A = \hat{V} + \frac{1}{c} \int \hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} - \frac{1}{2c^2} \int \hat{\rho}(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r}, \quad (5)$$

and the corresponding energy expectations $E = \langle \Psi(\mathbf{X}) | \hat{H} | \Psi(\mathbf{X}) \rangle$ as

$$E = T + E_{ee} + V_A \quad (6)$$

and

$$E = T + E_{ee} + V_A - \int \mathbf{m}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r}) d\mathbf{r}, \quad (7)$$

where the total external potential energy V_A is

$$\begin{aligned} V_A &= \langle \Psi(\mathbf{X}) | \hat{V}_A | \Psi(\mathbf{X}) \rangle \\ &= \int \rho(\mathbf{r}) v(\mathbf{r}) d\mathbf{r} + \frac{1}{c} \int \mathbf{j}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} \\ &\quad - \frac{1}{2c^2} \int \rho(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r} \end{aligned} \quad (8)$$

and where T and E_{ee} are the kinetic and electron-interaction energy expectations. In the above equations, the physical current density $\mathbf{j}(\mathbf{r})$ is defined in terms of the physical momentum operator ($\hat{\mathbf{p}} + \frac{1}{c} \mathbf{A}$) as

$$\begin{aligned} \mathbf{j}(\mathbf{r}) &= N \Re \sum_{\sigma} \int \Psi^*(\mathbf{r}\sigma, \mathbf{X}^{N-1}) \left(\hat{\mathbf{p}} + \frac{1}{c} \mathbf{A}(\mathbf{r}) \right) \\ &\quad \times \Psi(\mathbf{r}\sigma, \mathbf{X}^{N-1}) d\mathbf{X}^{N-1}, \end{aligned} \quad (9)$$

or equivalently as the expectation of the current density operator $\hat{\mathbf{j}}(\mathbf{r})$,

$$\mathbf{j}(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\mathbf{j}}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle, \quad (10)$$

where

$$\hat{\mathbf{j}}(\mathbf{r}) = \hat{\mathbf{j}}_p(\mathbf{r}) + \hat{\mathbf{j}}_d(\mathbf{r}), \quad (11)$$

with the paramagnetic $\hat{\mathbf{j}}_p(\mathbf{r})$ and diamagnetic $\hat{\mathbf{j}}_d(\mathbf{r})$ operator components defined, respectively, as

$$\hat{\mathbf{j}}_p(\mathbf{r}) = \frac{1}{2} \sum_k [\hat{\mathbf{p}}_k \delta(\mathbf{r}_k - \mathbf{r}) + \delta(\mathbf{r}_k - \mathbf{r}) \hat{\mathbf{p}}_k] \quad (12)$$

and

$$\hat{\mathbf{j}}_d(\mathbf{r}) = \hat{\rho}(\mathbf{r}) \mathbf{A}(\mathbf{r}) / c, \quad (13)$$

with the density operator $\hat{\rho}(\mathbf{r})$ being

$$\hat{\rho}(\mathbf{r}) = \sum_k \delta(\mathbf{r}_k - \mathbf{r}). \quad (14)$$

The magnetization density $\mathbf{m}(\mathbf{r})$ is the expectation

$$\mathbf{m}(\mathbf{r}) = \langle \Psi(\mathbf{X}) | \hat{\mathbf{m}}(\mathbf{r}) | \Psi(\mathbf{X}) \rangle, \quad (15)$$

with the local magnetization density operator $\hat{\mathbf{m}}(\mathbf{r})$ defined as

$$\hat{\mathbf{m}}(\mathbf{r}) = -\frac{1}{c} \sum_k \mathbf{s}_k \delta(\mathbf{r}_k - \mathbf{r}). \quad (16)$$

(The current density operator $\hat{\mathbf{j}}(\mathbf{r})$ can also be defined in terms of the Hamiltonian \hat{H} as $\hat{\mathbf{j}}(\mathbf{r}) = c \partial \hat{H} / \partial \mathbf{A}$. This confirms that for both the Hamiltonians of Eqs. (3) and (4), the physical current density is the orbital current density.)

We first present the proof of bijectivity between $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ and $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ for spinless electrons corresponding to the Hamiltonian of Eq. (1) or (3) for fixed electron number N and angular momentum \mathbf{L} . The proof is by *reductio ad absurdum*. Let us consider two different physical systems $\{v, \mathbf{A}\}$ and $\{v', \mathbf{A}'\}$ that generate different nondegenerate ground state wave functions Ψ and Ψ' . We assume the gauges of the unprimed and primed systems to be the same. Let us further assume that these systems lead to the *same* nondegenerate ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. We prove this cannot be the case. From the variational principle for the energy for a nondegenerate ground state, one obtains the inequality

$$E = \langle \Psi | \hat{H} | \Psi \rangle < \langle \Psi' | \hat{H} | \Psi' \rangle. \quad (17)$$

Now,

$$\begin{aligned} \langle \Psi' | \hat{H} | \Psi' \rangle &= \langle \Psi' | \hat{T} + \hat{W} + \hat{V}' + \frac{1}{c} \int \hat{\mathbf{j}}'(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r}) d\mathbf{r} - \frac{1}{2c^2} \int \hat{\rho}(\mathbf{r}) A'^2(\mathbf{r}) d\mathbf{r} | \Psi' \rangle \\ &\quad + \langle \Psi' | \hat{V} - \hat{V}' | \Psi' \rangle \\ &\quad + \frac{1}{c} \langle \Psi' | \int [\hat{\mathbf{j}}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) - \hat{\mathbf{j}}'(\mathbf{r}) \cdot \mathbf{A}'(\mathbf{r})] d\mathbf{r} | \Psi' \rangle - \frac{1}{2c^2} \langle \Psi' | \int \hat{\rho}(\mathbf{r}) [A^2(\mathbf{r}) - A'^2(\mathbf{r})] d\mathbf{r} | \Psi' \rangle. \end{aligned} \quad (18)$$

Employing the above assumptions and following the same steps as in Ref. 22, one obtains the inequality

$$E + E' < E + E' + \int [\hat{\mathbf{j}}'_p(\mathbf{r}) - \hat{\mathbf{j}}_p(\mathbf{r})] \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})] d\mathbf{r}, \quad (19)$$

where $E' = \langle \Psi' | \hat{H} | \Psi' \rangle$. The inequality of Eq. (19) is a general result.

As the majority of the experimental and consequent theoretical work is performed for uniform magnetic fields, our proof too is for such fields.

Consider next the third term on the right hand side of Eq. (19). With $\mathbf{B}(\mathbf{r}) = B \hat{\mathbf{i}}_z$, $\mathbf{B}'(\mathbf{r}) = B' \hat{\mathbf{i}}_z$, and the symmetric gauge $\mathbf{A}(\mathbf{r}) = \frac{1}{2} \mathbf{B} \times \mathbf{r}$, $\mathbf{A}'(\mathbf{r}) = \frac{1}{2} \mathbf{B}' \times \mathbf{r}$, this term may be written as

$$I = \frac{1}{2} \Delta \mathbf{B} \cdot \int \mathbf{r} \times [\mathbf{j}'_p - \mathbf{j}_p(\mathbf{r})] d\mathbf{r}, \quad (20)$$

where $\Delta \mathbf{B} = (B - B') \hat{\mathbf{i}}_z$. First, consider the integral

$$I_1 = \int \mathbf{r} \times \mathbf{j}_p(\mathbf{r}) d\mathbf{r} \quad (21)$$

$$= -\frac{i}{2} \sum_k \int d\mathbf{X} \int d\mathbf{r} \Psi^*(\mathbf{X}) \times [\mathbf{r} \times \nabla_{\mathbf{r}_k} \delta(\mathbf{r} - \mathbf{r}_k) + \delta(\mathbf{r} - \mathbf{r}_k) \mathbf{r} \times \nabla_{\mathbf{r}_k}] \Psi(\mathbf{X}). \quad (22)$$

Next consider the second integral of I_1 of Eq. (22),

$$I_{12} = \frac{1}{2} \int d\mathbf{X} \Psi^*(\mathbf{X}) \left(\sum_k \mathbf{r}_k \times \hat{\mathbf{p}}_k \right) \Psi(\mathbf{X}) \quad (23)$$

$$= \frac{1}{2} \int d\mathbf{X} \Psi^*(\mathbf{X}) \sum_k \hat{\mathbf{L}}_k \Psi(\mathbf{X}) = \frac{1}{2} \mathbf{L}, \quad (24)$$

where $\hat{\mathbf{L}}_k = \mathbf{r}_k \times \hat{\mathbf{p}}_k$ is the canonical orbital angular momentum operator, with $\hat{\mathbf{p}}$ the canonical momentum operator ($\hat{\mathbf{p}} = \hat{\mathbf{p}}_{kinetic} + \hat{\mathbf{p}}_{field} = m\mathbf{v} + \frac{q}{c}\mathbf{A}$) and \mathbf{L} the total canonical orbital angular momentum defined by Eq. (24). Note that the canonical angular momentum is gauge variant.

The first integral of I_1 of Eq. (22) is

$$I_{11} = -\frac{i}{2} \sum_k \int d\mathbf{X} \int d\mathbf{r} \Psi^*(\mathbf{X}) \epsilon_{\alpha\beta\gamma} \times \frac{\partial}{\partial r_{k\gamma}} (r_{\beta} \delta(\mathbf{r} - \mathbf{r}_k) \Psi(\mathbf{X})). \quad (25)$$

On integrating the inner integral by parts and dropping the surface term, one obtains

$$I_{11} = -\frac{i}{2} \sum_k \int d\mathbf{X} \times [-\epsilon_{\alpha\beta\gamma} \int d\mathbf{r} \frac{\partial \Psi^*(\mathbf{X})}{\partial r_{k\gamma}} r_{\beta} \delta(\mathbf{r} - \mathbf{r}_k) \Psi(\mathbf{X})] \quad (26)$$

$$= -\frac{i}{2} \sum_k \int d\mathbf{X} [-\epsilon_{\alpha\beta\gamma} \frac{\partial \Psi^*(\mathbf{X})}{\partial r_{k\gamma}} r_{k\beta} \Psi(\mathbf{X})]. \quad (27)$$

On integrating by parts again, one obtains

$$I_{11} = -\frac{i}{2} \sum_k \epsilon_{\alpha\beta\gamma} \int d\mathbf{X} \Psi^*(\mathbf{X}) \frac{\partial}{\partial r_{k\gamma}} (r_{k\beta} \Psi(\mathbf{X})) \quad (28)$$

$$= -\frac{i}{2} \sum_k \int d\mathbf{X} \Psi^*(\mathbf{X}) (\mathbf{r}_k \times \nabla_{\mathbf{r}_k}) \Psi(\mathbf{X}) = \frac{1}{2} \mathbf{L}. \quad (29)$$

Hence, the integral I of Eq. (20) is

$$I = \frac{1}{2} \Delta \mathbf{B} \cdot (\mathbf{L}' - \mathbf{L}). \quad (30)$$

If one imposes the condition that the total canonical orbital angular momentum is *fixed* so that $\mathbf{L} = \mathbf{L}'$, then the integral I vanishes so that the third term on the right hand side of Eq. (19) vanishes.

For states with fixed orbital angular momentum \mathbf{L} , Eq. (19) then reduces to the contradiction

$$E + E' < E + E'. \quad (31)$$

What this means is that the original assumption that Ψ and Ψ' differ is erroneous and that there can exist a $\{v, \mathbf{A}\}$ and

a $\{v', \mathbf{A}'\}$ with the same nondegenerate ground state wave function. The fact that $\Psi = \Psi'$ means that $\rho(\mathbf{r})|_{\Psi} = \rho'(\mathbf{r})|_{\Psi'}$. However, the corresponding physical current densities are not the same, $\mathbf{j}(\mathbf{r})|_{\Psi} \neq \mathbf{j}'(\mathbf{r})|_{\Psi'}$, because $\mathbf{j}_d(\mathbf{r})|_{\Psi} \neq \mathbf{j}'_d(\mathbf{r})|_{\Psi'}$ if one hews with the original assumption that $\mathbf{A}(\mathbf{r})$ is different from $\mathbf{A}'(\mathbf{r})$. This proves that the assumption that there exists a different $\{v', \mathbf{A}'\}$ (with the same N and \mathbf{L}) that leads to the same $\{\rho, \mathbf{j}\}$ as that due to $\{v, \mathbf{A}\}$ is incorrect. This step takes into account the fact that there could exist many $\{v, \mathbf{A}\}$ that lead to the same nondegenerate ground state Ψ . Hence, there exists only one $\{v, \mathbf{A}\}$ for fixed N and \mathbf{L} that leads to a nondegenerate ground state $\{\rho, \mathbf{j}\}$. The one-to-one relationship between $\{\rho, \mathbf{j}\}$ and $\{v, \mathbf{A}\}$ is therefore proved for the case when the interaction of the magnetic field is solely with the orbital angular momentum.

With $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ as the basic variables, the wave function Ψ is a functional of these properties. By a density and physical current density *preserving* unitary transformation,^{4,15,24} it can be 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: $\Psi = \Psi[\rho, \mathbf{j}, \alpha]$ is gauge variant. However, as the physical system remains unchanged for different gauge functions, the choice of vanishing gauge function is valid.

As the ground state energy is a functional of the basic variables: $E = E_{v, \mathbf{A}}[\rho, \mathbf{j}]$, a variational principle for $E_{v, \mathbf{A}}[\rho, \mathbf{j}]$ exists for arbitrary variations of (v, \mathbf{A}) -representable densities $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. The corresponding Euler equations for $\rho(\mathbf{r})$ and $\mathbf{j}(\mathbf{r})$ follow, and these must be solved self-consistently with the constraints $\int \rho(\mathbf{r}) d\mathbf{r} = N$, $\int \mathbf{r} \times (\mathbf{j}(\mathbf{r}) - \frac{1}{c} \rho(\mathbf{r}) \mathbf{A}(\mathbf{r})) d\mathbf{r} = \mathbf{L}$, and $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$. Implicit in this variational principle, as in all such energy variational principles, is that the external potentials remain fixed throughout the variation. (See Table I.)

We next consider electrons with spin corresponding to the Hamiltonian of Eq. (2) or (4). In this case, with the same assumptions made regarding the two different physical systems $\{v, \mathbf{A}; \psi\}$ and $\{v', \mathbf{A}'; \psi'\}$ leading to the same $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ as before, the inequality of Eq. (19) is replaced by

$$E + E' < E + E' + \int [\mathbf{j}'_p(\mathbf{r}) - \mathbf{j}_p(\mathbf{r})] \cdot [\mathbf{A}(\mathbf{r}) - \mathbf{A}'(\mathbf{r})] d\mathbf{r} - \int [\mathbf{m}'(\mathbf{r}) - \mathbf{m}(\mathbf{r})] \cdot [\mathbf{B}(\mathbf{r}) - \mathbf{B}'(\mathbf{r})] d\mathbf{r}. \quad (32)$$

The inequality is once again a general result. The third term on the right hand side vanishes if one imposes the constraint that the orbital angular momentum \mathbf{L} of the unprimed and primed systems is the same. Hence, next consider the last term of Eq. (32). For a uniform magnetic field with $\mathbf{B}(\mathbf{r}) = B \hat{\mathbf{i}}_z$ and $\mathbf{B}'(\mathbf{r}) = B' \hat{\mathbf{i}}_z$, we have

$$\int \mathbf{m}(\mathbf{r}) \cdot \mathbf{B}(\mathbf{r}) d\mathbf{r} = B \int m_z(\mathbf{r}) d\mathbf{r}, \quad (33)$$

where¹⁹

$$m_z(\mathbf{r}) = -\frac{1}{2c} [\rho_\alpha(\mathbf{r}) - \rho_\beta(\mathbf{r})], \quad (34)$$

TABLE I. Comparison of Hohenberg-Kohn and generalized Hohenberg-Kohn theories.

Theory	Hohenberg-Kohn DFT	Generalized HK DFT
Parameters characterizing ground state	Electron number N	Electron number N Angular momentum \mathbf{L}
Relationship between potentials and wave function	One-to-one between $v(\mathbf{r})$ and Ψ	Many-to-one between $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and Ψ
Properties characterizing ground state	Electron density $\rho(\mathbf{r})$	Electron density $\rho(\mathbf{r})$ Physical current density $\mathbf{j}(\mathbf{r})$
Bijectivity theorem	For fixed N $\rho(\mathbf{r}) \leftrightarrow v(\mathbf{r})$	For fixed N and \mathbf{L} $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\} \leftrightarrow \{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$
Wave function and energy functionals	$\Psi = \Psi[\rho, \alpha]$ For fixed $v : E = E_v[\rho]$	$\Psi = \Psi[\rho, \mathbf{j}, \alpha]$ For fixed $\{v, \mathbf{A}\} : E = E_{v, \mathbf{A}}[\rho, \mathbf{j}]$
Euler equations and constraints	Variational principle for fixed v and known N : $\frac{\delta E_v[\rho]}{\delta \rho} = 0$ $\int \rho(\mathbf{r}) d\mathbf{r} = N$	Variational principle for fixed $\{v, \mathbf{A}\}$ and known N, \mathbf{L} : $\frac{\delta E_{v, \mathbf{A}}[\rho, \mathbf{j}]}{\delta \rho} \Big _{\mathbf{j}} = 0$ $\frac{\delta E_{v, \mathbf{A}}[\rho, \mathbf{j}]}{\delta \mathbf{j}} \Big _{\rho} = 0$ $\int \rho(\mathbf{r}) d\mathbf{r} = N$ $\int \mathbf{r} \times (\mathbf{j}(\mathbf{r}) - \frac{1}{c} \rho(\mathbf{r}) \mathbf{A}(\mathbf{r})) d\mathbf{r} = \mathbf{L}$ $\nabla \cdot \mathbf{j}(\mathbf{r}) = 0$

with $\rho_\alpha(\mathbf{r}), \rho_\beta(\mathbf{r})$ being the spin-up and spin-down spin densities. The last term of the inequality is then

$$\begin{aligned} & \int [\mathbf{m}'(\mathbf{r}) - \mathbf{m}(\mathbf{r})] \cdot \Delta \mathbf{B}(\mathbf{r}) d\mathbf{r} \\ &= -\frac{1}{2c} \Delta B \int [\{\rho'_\alpha(\mathbf{r}) - \rho'_\beta(\mathbf{r})\} - \{\rho_\alpha(\mathbf{r}) - \rho_\beta(\mathbf{r})\}] d\mathbf{r}, \end{aligned} \quad (35)$$

with $\Delta B = B - B'$. If the z -component of the total spin angular momentum S_z for the unprimed and primed systems is the same, the corresponding spin densities are the same. The last term of Eq. (35) thus vanishes leading once again to the contradiction $E + E' < E + E'$. More generally, the magnetization densities $\mathbf{m}(\mathbf{r})$ and $\mathbf{m}'(\mathbf{r})$ are the same if the total spin angular momentum \mathbf{S} is the same. Hence, once again, the bijective relationship between the nondegenerate ground state densities $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ and the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ is proved, provided one imposes the constraint that the total orbital \mathbf{L} and spin \mathbf{S} angular momentum are fixed.

This may be seen in a different manner by accentuating the role of the spin angular momentum. With the z -component of the total spin \mathbf{S} being $S_z = \sum_k s_{z,k}$, the density $m_z(\mathbf{r})$ may be written as

$$m_z(\mathbf{r}) = -\frac{1}{cN} \sum_{\sigma} S_z \gamma(\mathbf{r}\sigma, \mathbf{r}\sigma), \quad (36)$$

with $\gamma(\mathbf{x}\mathbf{x}') = N \int \Psi^*(\mathbf{r}\sigma, \mathbf{X}^{N-1}) \Psi(\mathbf{r}'\sigma', \mathbf{X}^{N-1}) d\mathbf{X}^{N-1}$, the density matrix. Since in the primed system, the spin vectors are different, i.e., some s'_k , we have

$$\begin{aligned} & \int [\mathbf{m}'(\mathbf{r}) - \mathbf{m}(\mathbf{r})] \cdot \Delta \mathbf{B}(\mathbf{r}) d\mathbf{r} \\ &= \Delta B \int [m'_z(\mathbf{r}) - m_z(\mathbf{r})] d\mathbf{r} \end{aligned} \quad (37)$$

$$= \frac{\Delta B}{cN} \sum_{\sigma} \int [S'_z \gamma'(\mathbf{r}\sigma, \mathbf{r}\sigma) - S_z \gamma(\mathbf{r}\sigma, \mathbf{r}\sigma)] d\mathbf{r}. \quad (38)$$

Employing the original assumption that the diagonal matrix elements $\gamma(\mathbf{r}\sigma, \mathbf{r}\sigma)$ of the density matrix $\gamma(\mathbf{x}\mathbf{x}')$ are the same for the unprimed and primed systems, we have the right hand side of Eq. (38) to be

$$\frac{\Delta B}{cN} \sum_{\sigma} \int [S'_z - S_z] \gamma(\mathbf{r}\sigma, \mathbf{r}\sigma) = 0, \quad (39)$$

provided $S'_z = S_z$.

In the above proofs for the Hamiltonians of Eqs. (3) and (4), the definition of the current density $\mathbf{j}(\mathbf{r})$ employed is that of Eq. (10). However, for finite systems, the Hamiltonian of Eq. (4) can also be written as²⁵

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{W} + \hat{V} + \frac{1}{c} \int \hat{\mathbf{j}}_p(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r} \\ &+ \frac{1}{2c^2} \int \hat{\rho}(\mathbf{r}) A^2(\mathbf{r}) d\mathbf{r} \\ &+ \frac{1}{c} \int \hat{\mathbf{j}}_m(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) d\mathbf{r}, \end{aligned} \quad (40)$$

where the magnetization current density operator $\hat{\mathbf{j}}_m(\mathbf{r})$ is defined as

$$\hat{\mathbf{j}}_m(\mathbf{r}) = -c \nabla \times \mathbf{m}(\mathbf{r}). \quad (41)$$

Hence, the physical current density $\mathbf{j}(\mathbf{r})$ may also be defined as²⁵

$$\mathbf{j}(\mathbf{r}) = c \frac{\partial \hat{H}}{\partial \mathbf{A}(\mathbf{r})} = \mathbf{j}_p(\mathbf{r}) + \mathbf{j}_d(\mathbf{r}) + \mathbf{j}_m(\mathbf{r}), \quad (42)$$

the sum of the paramagnetic, diamagnetic, and magnetization current densities. Even for this definition of the physical current density $\mathbf{j}(\mathbf{r})$, the proof of bijectivity between $\{\rho, \mathbf{j}\}$ and $\{v, \mathbf{A}\}$ is valid provided the angular momenta \mathbf{L} and \mathbf{S} are fixed. For spin-compensated systems, the magnetization current density $\mathbf{j}_m(\mathbf{r})$ vanishes.

The above proofs, that nondegenerate ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ are the basic variables, are valid for the subset of

(v, \mathbf{A}) -representable densities for fixed (N, \mathbf{L}) or fixed $(N, \mathbf{L}, \mathbf{S})$ as the case may be. With the knowledge of the properties that constitute the basic variables, it is then possible to generalize this conclusion to the broader subset of N -representable densities for fixed (N, \mathbf{L}) or $(N, \mathbf{L}, \mathbf{S})$, and to degenerate states, via the PLL constrained-search framework. We present here the constrained-search argument as applied to the Schrödinger Hamiltonian of Eq. (3).

Suppose there exist antisymmetric functions $\Psi_{\rho, \mathbf{j}}(N, \mathbf{L})$ for fixed (N, \mathbf{L}) that lead to the ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. How then does one distinguish these functions from the true ground state wave function Ψ ? Following PLL, on application of the variational principle to the Hamiltonian of Eq. (3), we have (for fixed external potentials $v(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$)

$$\langle \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) | \hat{H} | \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rangle \geq \langle \Psi | \hat{H} | \Psi \rangle = E \quad (43)$$

or equivalently

$$\langle \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) | \hat{T} + \hat{W} | \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rangle \geq \langle \Psi | \hat{T} + \hat{W} | \Psi \rangle. \quad (44)$$

Hence, of all the N -representable $\Psi_{\rho, \mathbf{j}}(N, \mathbf{L})$ that lead to the ground state $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, the true wave function Ψ is that which minimizes the expectation $\langle \hat{T} + \hat{W} \rangle$. This is the constrained-search over all $\Psi_{\rho, \mathbf{j}}(N, \mathbf{L})$ to arrive at Ψ .

Again, in the usual manner, it is possible to describe the energy minimization by two nested minimizations. As the wave function is a functional of $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, one first defines the universal functional

$$F_{N, \mathbf{L}}[\rho, \mathbf{j}] = \min_{\Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rightarrow \rho, \mathbf{j}} \langle \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) | \hat{T} + \hat{W} | \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rangle \quad (45)$$

such that searching over all N -representable $\Psi_{\rho, \mathbf{j}}(N, \mathbf{L})$, the functional $F_{N, \mathbf{L}}[\rho, \mathbf{j}]$ delivers the minimum of the expectation $\langle \hat{T} + \hat{W} \rangle$. The functional is equally valid for degenerate states. The ground state energy E may then be written as

$$E = \min_{\rho, \mathbf{j}} \left\{ \min_{\Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rightarrow \rho, \mathbf{j}} [\langle \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) | \hat{T} + \hat{W} + \hat{V}_A | \Psi_{\rho, \mathbf{j}}(N, \mathbf{L}) \rangle] \right\} \quad (46)$$

$$= \min_{\rho, \mathbf{j}} \{ F_{N, \mathbf{L}}[\rho, \mathbf{j}] + V_A \} \quad (47)$$

$$= \min_{\rho, \mathbf{j}} E_{v, \mathbf{A}}[\rho, \mathbf{j}]. \quad (48)$$

The variations in Eq. (48) are over all N -representable $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ for fixed (N, \mathbf{L}) . The stringent (v, \mathbf{A}) -representability requirement and the restriction to nondegenerate ground states are thereby overcome. The extension of these arguments to the Schrödinger-Pauli Hamiltonian of Eq. (4) follows similarly.

III. CONCLUDING REMARKS

In conclusion, we have generalized the HK theorems to the added presence of a uniform magnetic field. We have considered the cases of the interaction of the magnetic field with the orbital angular momentum as well as when the interaction is with both the orbital and spin angular momenta. In this work, we have proved a one-to-one relationship between the external potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the nondegenerate ground state densities $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. The proof differs from that of the original HK theorem and explicitly accounts for the many-to-one relationship between

the potentials $\{v(\mathbf{r}), \mathbf{A}(\mathbf{r})\}$ and the nondegenerate ground state wave function Ψ . To account for the presence of the magnetic field, which constitutes an added degree of freedom, one must then impose a further constraint beyond that of fixed electron number N as in the original HK theorems. For the Hamiltonian corresponding to spinless electrons, the added constraint is that of fixed canonical orbital angular momentum \mathbf{L} . For that corresponding to electrons with spin, the constraints imposed are those of fixed canonical orbital \mathbf{L} and spin \mathbf{S} angular momenta. (The gauge employed for the canonical angular momentum \mathbf{L} can be chosen to be the same as that employed for the Hamiltonian.) It is the further constraint on the angular momentum that makes a rigorous HK-type proof of bijectivity between the gauge invariant basic variables and the external scalar and vector potentials possible. Additionally, the HK-type proofs are possible because the Hamiltonians considered are rigorously derived from the tenets of nonrelativistic quantum mechanics. (The Hamiltonian of spin-DFT is not so derivable. It is *ad hoc*.)

With the knowledge that the basic variables are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, a variational principle for the energy functional $E_{v, \mathbf{A}}[\rho, \mathbf{j}]$ for arbitrary variations of (v, \mathbf{A}) -representable densities $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$ is then developed for each Hamiltonian considered. The constraints on the corresponding Euler equations are those of fixed electron number and angular momentum, and the satisfaction of the equation of continuity.

Having proved that the basic variables are $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$, it is then possible to replace the stringent (v, \mathbf{A}) -representability constraint for fixed electron number and angular momentum by the broader subset of N -representable functions, and to extend the conclusions to degenerate states, via a Percus-Levy-Lieb constrained-search argument.

Again, knowing what the basic variables are, it is possible to map the interacting system defined by the Hamiltonians of Eqs. (1) and (2) to one of the noninteracting fermions with the same $\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})$, and \mathbf{J} . Such a mapping has been derived within QDFT.²⁶ The theory has been applied to map an interacting system¹³ (in two-dimensions) of two electrons in a magnetic field and a harmonic trap $v(\mathbf{r}) = \frac{1}{2}\omega_0 r^2$ for which the ground state wave function is $\Psi(\mathbf{r}_1, \mathbf{r}_2) = C(1 + r_{12})e^{-\frac{1}{2}(r_1^2 + r_2^2)}$, where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ and $C^2 = 1/\pi^2(3 + \sqrt{2}\pi)$, to one of the noninteracting fermions with the same $\{\rho(\mathbf{r}), \mathbf{j}(\mathbf{r})\}$. This example corresponds to the special case of zero angular momentum. However, the QDFT mapping for finite angular momentum is straightforward. A Kohn-Sham-type mapping is, of course, also possible. Work towards the mathematical and physical properties of the energy functional $E_{v, \mathbf{A}}[\rho, \mathbf{j}]$ is in progress. The approximate energy functionals subsequently developed will then be compared with the exact QDFT mappings for the quantum dot.²⁶ For other recent work, see Refs. 27 and 28. The conclusions in the latter are based on the assumption of existence of a HK theorem but one without the requirement of the constraint on the angular momentum.

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