Rigorous formulation of the Kohn and Sham theory

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The theory of Kohn and Sham treats a system of interacting electrons by establishing a correspondence between this system and a noninteracting system. In this paper we develop a new formulation of this theory, which differs from the original by its rigor and by the more correct treatment of the kinetic energy term. This new formulation has the additional advantage that it bypasses the v representability requisite of the original Hohenberg-Kohn-Sham theory.

I. INTRODUCTION

The attempts to simplify the many-electron problem in terms of physical quantities or equations conceptually simpler and easier to calculate go back to 1927 with the works of Thomas[1] and Fermi,[2] who realized the central role of the density in such problems. Their approach was intuitive rather than mathematical.

Eliminating the many variables of the many-electron Schrödinger equation was not an easy task. Thus the search for simplification led to another direction, the effective potential theories, i.e., to substitute the electron interaction term, which was the source of the difficulties, by an effective potential.[3,4] In fact, the volume of atomic, molecular, and solid-state physics calculations was based on these theories. Local-exchange potentials were preferred instead of the nonlocal potential of the Hartree-Fock theory.

A sound theoretical formulation of the problem with the density as basic variable came with the work of Hohenberg and Kohn[5] in 1964. This led after one year to the work of Kohn and Sham[6] which justified the effective-field approximations and gave impetus to improvements of such theories. This work stimulated many investigations for reasonably accurate exchange and correlation energy-density functionals.[7–9] The fact that a kinetic energy correction term should be involved in the Kohn-Sham equations was overlooked for years, and only recently did this deficiency of the Hohenberg-Kohn-Sham (HKS) theory appear in literature.[10–14]

The success of the Kohn-Sham theory for the ground state led to attempts of generalization to excited states and to development of functional theories for such states. Recently many excited-state theories appeared, some along the lines of the initial HKS theory. One of these was the transition-state theory of Slater,[15] who performed calculations that compared well with the experimental data. This theory found a sound mathematical basis with the work of one of us,[10,16] whose subspace functional theory led to equations similar to those of the KS theory, with fractional occupation numbers. These equations nearly coincide with those of Slater's theory. Other less traditional approaches for the excited-state problem appeared, like those of Valone and Capitani.[17] Still the KS theory is the most popular in applications. Therefore, we believe that it is worth looking for a rigorous formulation of this theory. Such a formulation is presented in this paper.

II. HOHENBERG-KOHN THEORY

We shall now review some recent developments on the Hohenberg-Kohn theory, which will be used for our formulation of the KS theory. In what follows, we shall use $|\psi\rangle$ to denote an arbitrary N-fermion state, while $|\phi\rangle$ will be reserved to Slater determinants. Furthermore, we shall make use of the symbol $\Longrightarrow$ as in $\psi\Longrightarrow\rho$ to denote that the state $|\psi\rangle$ has the density $\rho(\vec{r})$, i.e., $\langle\psi|\hat{\rho}(\vec{r})|\psi\rangle=\rho(\vec{r})$.

Suppose now that the Hamiltonian $H=H_0+\hat{V}$ of a system of fermions is given. The symbols used are expressed in terms of the fermion field operators and

$$\hat{V}=\int V(\vec{r})\hat{\rho}(\vec{r})d^3r \tag{1}$$

is the external potential. By H_0 we shall denote the kinetic energy operator T when we refer to the noninteracting system, and $H_0=T+H_{\rm int}$ for the interacting system:

$$T=\tfrac{1}{2}\int\nabla\Psi^\dagger(\vec{r})\nabla\Psi(\vec{r})d^3r\ , \tag{2}$$

$$H_{\rm int}=\tfrac{1}{2}\int\frac{\Psi^\dagger(\vec{r})\hat{\rho}(\vec{r}')\Psi(\vec{r})}{|\vec{r}-\vec{r}'|}d^3r\,d^3r'\ . \tag{3}$$

The theorem of Hohenberg and Kohn states that for any density $\rho(\vec{r})$, $\rho(\vec{r})\geq 0$, $\int\rho(\vec{r})d^3r=N$ there exists *at most* one potential $V_\rho(\vec{r})$ such that its ground state $|\psi_\rho\rangle$ has the density ρ: $\psi_\rho\Longrightarrow\rho$. Consequently for all ρ for which V_ρ and $|\psi_\rho\rangle$ exist, we can define a functional

$$G_H(\rho)=\langle\psi_\rho|H_0+\hat{V}|\psi_\rho\rangle\ ,$$

where $\hat{V}$ is the external potential. This functional has the property that $\min_\rho G_H(\rho)=E_0$ (the ground-state energy of the Hamiltonian H). In addition, the minimum is attained when ρ is the correct ground-state density. Thus, at least in principle, the ground-state energy can be obtained by a minimization procedure involving just one function ρ of the position variable $\vec{r}$.

The above theorem of Hohenberg and Kohn is rigorous. However, a problem remains: $G_H(\rho)$ is defined only for some densities ρ, namely those corresponding to some

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ground state. Indeed, it can be proved[18,19] that there exist reasonable densities ρ for which there is no ground state $|\psi\rangle$ such that $\psi \Rightarrow \rho$, so $G_H(\rho)$ is not defined for those ρ. This is annoying, for one needs to vary ρ freely in order to obtain the Euler condition for the minimization of $G_H(\rho)$. That is, the domain of definition of $G_H(\rho)$ should be extended. This has been done by Percus and Levy[20–22] who defined, for any $\rho(\vec{r})$ with finite kinetic energy, $\rho(\vec{r}) \geq 0$, $\int \rho(\vec{r}) d^3r = N$, and $\int (\nabla \sqrt{\rho})^2 d^3r < \infty$ the following functionals:

$$Q_{H_0}(\rho) = \inf\{\langle \psi | H_0 | \psi \rangle \text{ for all } \psi \Rightarrow \rho\} , \tag{4}$$

$$Q_H(\rho) = Q_{H_0}(\rho) + \int V(\vec{r}) \rho(\vec{r}) d^3r . \tag{5}$$

(For the noninteracting case, the infimum is taken over all Slater determinants $|\phi\rangle$ for which $\phi \Rightarrow \rho$.)

As Levy proved, $Q_H(\rho)$ is the desired extension of $G_H(\rho)$; indeed, he proved the following.

(a) $Q_H(\rho)$ is an extension of $G_H(\rho)$. To be precise, for all ρ for which $G_H(\rho)$ is defined, one has $Q_H(\rho) = G_H(\rho)$.

(b) $\min_\rho Q_H(\rho) = E_0$. The minimum is attained for the correct ground-state density.

In addition, Lieb[18] proved that the infimum of the functional defined by Eq. (4) is actually a minimum.

Theorem 1 (Lieb). Let $\rho(\vec{r}) \geq 0$, $\int \rho(\vec{r}) d^3r = N$, $\int (\nabla \sqrt{\rho})^2 d^3r < \infty$. Then

(1) there exist N-fermion states $|\phi\rangle, |\psi\rangle$ such that

$$\langle \phi | T | \phi \rangle < \infty ,$$

$$\langle \psi | T + H_{\text{int}} | \psi \rangle < \infty ,$$

and

$$\phi \Rightarrow \rho, \psi \Rightarrow \rho ;$$

(2) the infima

$$\inf\{\langle \phi | T | \phi \rangle \text{ for all } \phi \Rightarrow \rho\} ,$$

$$\inf\{\langle \psi | T + H_{\text{int}} | \psi \rangle \text{ for all } \psi \Rightarrow \rho\}$$

are well defined and finite; and

(3) the above infima are minima, i.e., they are attained by some states $|\phi_\rho\rangle, |\psi_\rho\rangle$, respectively.

In the following we shall show that since the minimum of $Q_{H_0}(\rho)$ exists, a potential $V_\rho(\vec{r})$ exists such that $|\psi_\rho\rangle$ is an eigenstate of $H_0 + \hat{V}_\rho$, i.e.,

$$\left[H_0 + \int \hat{\rho}(\vec{r}) V_\rho(\vec{r}) d^3r\right] |\psi_\rho\rangle = E |\psi_\rho\rangle . \tag{6}$$

In fact, the potential enters as a Lagrange multiplier, or rather as a set of Lagrange multipliers in finding the extrema of $\langle \psi | H_0 | \psi \rangle$ under the density constraint.

It is preferable to work with the density operators $\hat{\rho}_n$,

$$\hat{\rho}_n = \int \hat{\rho}(\vec{r}) \phi_n(\vec{r}) d^3r ,$$

where $\varphi_n(\vec{r})$ is any orthonormal set of square integrable functions, which are chosen real so that $\hat{\rho}_n$ is a Hermitian operator. Then the conditions $\langle \psi | \hat{\rho}(\vec{r}) | \psi \rangle = \rho(\vec{r})$ become

$$\langle \psi | \hat{\rho}_n | \psi \rangle = \rho_n, \quad n = 1,2, \ldots .$$

For the derivation of Eq. (6) we note that since the minimum of $\langle \psi | H_0 | \psi \rangle$ under the conditions

$$\langle \psi | \hat{\rho}_n | \psi \rangle = \rho_n, \quad \langle \psi | \psi \rangle = 1$$

exists, the expression

$$G(\psi) = \langle \psi | H_0 | \psi \rangle + \sum \lambda_n \langle \psi | \hat{\rho}_n | \psi \rangle - E \langle \psi | \psi \rangle ,$$

where λ_n are Lagrange multipliers for the density constraints, has at least one extremum. The resulting equation under the variation of $|\psi\rangle$ is

$$H_0 |\psi\rangle + \sum_n \lambda_n \hat{\rho}_n |\psi\rangle = E |\psi\rangle . \tag{7}$$

The solution of Eq. (7) depends on the parameters λ_n and has to satisfy the conditions

$$\langle \psi(\lambda_1, \lambda_2, \ldots) | \hat{\rho}_n | \psi(\lambda_1, \lambda_2, \ldots) \rangle = \rho_n, \quad n = 1,2, \ldots . \tag{8}$$

As there is always at least one solution, there is at least one set of parameters λ_n which satisfies Eq. (8). Next we write the explicit expression for $\hat{\rho}_n$ in Eq. (7) and the expression $\sum_n \lambda_n \hat{\rho}_n$ becomes

$$\sum_n \lambda_n \hat{\rho}_n = \sum_n \int \lambda_n \varphi_n(\vec{r}) \hat{\rho}(\vec{r}) d^3r .$$

Under the hypothesis that the integration and summation signs can change order, we have

$$\sum \lambda_n \hat{\rho}_n = \int \sum_n \lambda_n \varphi_n(\vec{r}) \hat{\rho}(\vec{r}) d^3r$$

$$= \int V_\rho(\vec{r}) \hat{\rho}(\vec{r}) d^3r$$

for some function $V_\rho(\vec{r})$.

Thus Eq. (7) becomes

$$H_0 |\psi\rangle + \int V_\rho(\vec{r}) \hat{\rho}(\vec{r}) d^3r |\psi\rangle = E |\psi\rangle; \quad \text{Q.E.D.}$$

[The hypothesis of the interchange of the summation and integration signs does not always hold. Then a local $V(r)$ may not exist. Such examples are given by Englisch and Englisch.[23] A derivation of this equation was also given by Levy and others.[14,24]] Thus we conclude that the potential plays the role of a Lagrange multiplier for the extrema of H_0 under the density constraints. When the constraints are relaxed, the minimum gets lower.

It is useful to know the relation of the set of $|\psi\rangle$ for which the minima of $\langle \psi | H_0 | \psi \rangle$ under the condition $\langle \psi | \hat{\rho}(\vec{r}) | \psi \rangle = \rho(\vec{r})$ are obtained to the set of ground states.

Theorem 2. The set of ground states is a proper subset of the set of $|\psi_\rho\rangle$, where

$$\langle \psi_\rho | H_0 | \psi_\rho \rangle = \min\{\langle \psi | H_0 | \psi \rangle \text{ for all } \psi \Rightarrow \rho\} .$$

Proof. If $|\psi_0\rangle$ is a ground state for some potential $\hat{V}$ and $\psi_0 \Rightarrow \rho$, then for any other $|\psi\rangle$ such that $\psi \Rightarrow \rho$,

$$\langle \psi_0 | H_0 + \hat{V} | \psi_0 \rangle \leq \langle \psi | H_0 + \hat{V} | \psi \rangle$$

and

$$\langle\psi_0|\hat{V}|\psi_0\rangle=\langle\psi|\hat{V}|\psi\rangle=\int V(r)\rho(r)d^3r\ .$$

Hence,

$$\langle\psi_0|H_0|\psi_0\rangle\leq\langle\psi|H_0|\psi\rangle\ ,$$

that is, $|\psi_0\rangle$ minimizes $\langle\psi|H_0|\psi\rangle$ under the condition $\psi\Rightarrow\rho$, i.e., $|\psi_0\rangle=|\psi_\rho\rangle$.

On the other hand, as Lieb[18] and Levy[19] showed, there exist densities ρ which cannot be realized by any ground state. For such ρ, $\min_{\psi\Rightarrow\rho}\langle\psi|H_0|\psi\rangle$ has a minimizing $|\psi_\rho\rangle$, which will be an eigenstate of $H_0+\hat{V}$ for some $\hat{V}$, but not a ground state. Thus the set of $|\psi_\rho\rangle$ is greater than the set of ground states; Q.E.D.

III. RIGOROUS KS THEORY

The advantage of the KS scheme is that instead of having to search for the real ground state of the interacting system which is a linear combination of infinite number of Slater determinants, one has to solve a system of N one-particle Schrödinger equations in an effective potential, $V_{\text{eff}}(\vec{r})$. By means of these one-particle wave functions one can form the Slater determinant, that is, the wave function of an equivalent N-particle noninteracting system. The initial formulation of Kohn and Sham relied on the density variational principle of Hohenberg and Kohn, discussed in the preceding sections. In the formulation that follows no such variational principle will be necessary. The various functionals will be defined by Slater determinants and the minima of the energy will be obtained by doing variations in the set of states corresponding to Slater determinants. These states will be denoted by $|\phi\rangle$ and the corresponding set by S_{SI}. One must note that S_{SI} is not a linear space, i.e., a linear combination of Slater determinants is not a Slater determinant apart from very special cases. In this section $|\psi\rangle$ will denote a general state in the Hilbert space.

As we aim to derive a minimum principle for a functional having $|\phi\rangle$ as variable, it is necessary to define a functional over $|\phi\rangle$ whose value is either (a) always equal to the expectation value of the Hamiltonian of the interacting system for some state $|\psi\rangle$ belonging to the set of ground states as is tacitly implied in the initial KS theory, i.e., $G(\phi)=\langle\psi|H|\psi\rangle$, or (b) one can define $G(\phi)\neq\langle\psi|H|\psi\rangle$, but the minimum value of $G(\phi)$ must coincide with the minimum value of $\langle\psi|H|\psi\rangle$. The second case will be used here. The procedure is as follows.

For any N-particle Slater determinant with finite kinetic energy, i.e., for every $|\phi\rangle$ in S_{SI} with $\langle\phi|T|\phi\rangle<\infty$, a non-negative function $\rho_\phi(\vec{r})$ is defined by means of the relation $\rho_\phi(\vec{r})=\langle\phi|\hat{\rho}(\vec{r})|\phi\rangle$.

Consider next the space of all Slater determinants $|\phi'\rangle$ having the same density as $|\phi\rangle$. Then by theorem 1 the minimum of the kinetic energy in this space exists. By means of this minimum one can define the following functional:

$$G_T(\phi)=\min\{\langle\phi'|T|\phi'\rangle \text{ for all } \phi'\Rightarrow\rho_\phi\}\ . \tag{9a}$$

The state or states for which this minimum is attained will be denoted by $|\phi'_\phi\rangle$. Then it follows that

$$G_T(\phi)=\langle\phi'_\phi|T|\phi'_\phi\rangle\ . \tag{9b}$$

In a similar way one can define a functional for states in S_{SI} by means of the minimum of the kinetic energy plus the interaction energy in the space of all states $|\psi\rangle$ with the same density as $|\phi\rangle$, i.e.,

$$G_{H_0}(\phi)=\min\{\langle\psi|T+H_{\text{int}}|\psi\rangle \text{ for all } \psi\Rightarrow\rho\}\ . \tag{10a}$$

The existence of this minimum follows from theorem 1. The minimizing state or states will be denoted by $|\psi_\phi\rangle$. As the search for the minimum is in a space which contains S_{SI}, $|\psi_\phi\rangle$ does not necessarily belong to S_{SI}. The following equality holds for $|\psi_\phi\rangle$:

$$\langle\psi_\phi|T+H_{\text{int}}|\psi_\phi\rangle=G_{H_0}(\phi)\ . \tag{10b}$$

By means of the functionals defined by Eqs. (9a) and (10a), one can define the following functionals:

$$\Delta T(\phi)=\langle\psi_\phi|T|\psi_\phi\rangle-\langle\phi'_\phi|T|\phi'_\phi\rangle \tag{11}$$

and

$$E_{\text{xc}}(\phi)=\langle\psi_\phi|H_{\text{int}}|\psi_\phi\rangle-\tfrac{1}{2}\int\frac{\rho_\phi(\vec{r})\rho_\phi(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r\,d^3r'\ , \tag{12}$$

where E_{xc} is the exchange and correlation energy. Finally we define

$$G_H(\phi)=\langle\phi|T|\phi\rangle+\Delta T(\phi)+\int V(\vec{r})\rho_\phi(\vec{r})d^3r+E_{\text{xc}}(\phi)+\tfrac{1}{2}\int\frac{\rho_\phi(\vec{r})\rho_\phi(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r\,d^3r'\ . \tag{13}$$

Evidently, $G_H(\phi)$ is well defined, since each term of the expression for this functional is well defined by Eqs. (9)—(12). As the following theorem shows, $G_H(\phi)$ has all the desired properties.

Theorem 3. (a) The minimum of the functional $G_H(\phi)$ in S_{SI} exists and its value is equal to the ground-state energy, E_0 of H. (b) If the minimum of $G_H(\phi)$ is attained for some $|\phi_0\rangle$, then the density $\rho_{\phi_0}=\langle\phi_0|\hat{\rho}(\vec{r})|\phi_0\rangle$ is the correct ground-state density of H.

Proof. (a) First, rewrite Eq. (13) in the form

$$G_H(\phi)=\langle\phi|T|\phi\rangle-\langle\phi'_\phi|T|\phi'_\phi\rangle+\langle\psi_\phi|T+H_{\text{int}}+V|\psi_\phi\rangle\ , \tag{14}$$

where $|\phi'_\phi\rangle$, $|\psi_\phi\rangle$ are defined by Eqs. (9) and (10) and use was made of (11) and (12). From Eq. (9) it follows that

$$\langle\phi|T|\phi\rangle\geq\langle\phi'_\phi|T|\phi'_\phi\rangle \tag{15}$$

and since

$$\langle\psi_\phi|T+H_{\text{int}}+V|\psi_\phi\rangle\geq E_0\ , \tag{16}$$

Eq. (14) gives

$$G_H(\phi)\geq E_0\ . \tag{17}$$

To show that the minimum of $G_H(\phi)$ equals E_0 consider $|\psi_0\rangle$, i.e., the ground state of H and set

$\rho_0(\vec{r})=\langle\psi_0|\hat{\rho}(\vec{r})|\psi_0\rangle$. By theorem 1, $\min\{\langle\phi|T|\phi\rangle$ for all $\phi\Longrightarrow\rho_0\}$ is well defined, and attained by some $|\phi_0\rangle$.

Consider now $G_H(\phi_0)$. By the definition of $|\phi_0\rangle$, we have $\rho_{\phi_0}=\rho_{\psi_0}$. On the other hand, the $|\phi'_{\phi_0}\rangle$ and $|\psi_{\phi_0}\rangle$ defined by Eqs. (9) and (10) are nothing but $|\phi_0\rangle$ and $|\psi_0\rangle$, since we have

$$\langle\psi_0|T+H_{\text{int}}|\psi_0\rangle = \min\{\langle\psi|T+H_{\text{int}}|\psi\rangle \text{ for all } \psi\Longrightarrow\rho_{\psi_0}\}$$

and

$$\langle\phi_0|T|\phi_0\rangle=\min\{\langle\phi|T|\phi\rangle \text{ for all } \phi\Longrightarrow\rho_{\psi_0}\}\ .$$

Then Eq. (14) becomes

$$G_H(\phi_0)=\langle\phi_0|T|\phi_0\rangle-\langle\phi_0|T|\phi_0\rangle + \langle\psi_0|T+H_{\text{int}}+V|\psi_0\rangle=E_0\ .$$

Thus part (a) of the theorem is proven.

(b) Suppose now that for some $|\phi_0\rangle$ we have $G_H(\phi_0)=E_0$. Equality in relation (17) holds if and only if relations (15) and (16) are equalities. Thus we have

$$\langle\psi_{\phi_0}|T+H_{\text{int}}+V|\psi_{\phi_0}\rangle=E_0\ , \tag{18}$$

where $|\psi_{\phi_0}\rangle$, by Eq. (10), is a state such that

$$\langle\psi_{\phi_0}|\hat{\rho}(\vec{r})|\psi_{\phi_0}\rangle=\langle\phi_0|\hat{\rho}(\vec{r})|\phi_0\rangle\ .$$

But (18) implies that $|\psi_{\phi_0}\rangle$ is the ground state of H. Thus $\langle\phi_0|\hat{\rho}(\vec{r})|\phi_0\rangle$ is the correct ground-state density; Q.E.D.

Thus there is a way of formulating the KS theory without the need of variational principles on functionals defined on the space of densities, i.e., it is possible to bypass the Hohenberg and Kohn theory. The theory developed here defines energy functionals on the space of Slater determinants $|\phi\rangle$. The value of these functionals is not equal to the expectation value of the Hamiltonian of a ground state of some interacting system having the same density as $|\phi\rangle$. However, the minimum value of this functional is equal to the ground-state energy of the system considered. The equation resulting from the minimization of $G_H(\phi)$ given by Eq. (13) is

$$T|\phi\rangle+\int V_{\text{eff}}(\vec{r})\hat{\rho}(\vec{r})d^3r\,|\phi\rangle=E|\phi\rangle\ , \tag{19a}$$

where

$$V_{\text{eff}}(\vec{r})=V(\vec{r})+V_{\text{xt}}(\vec{r})+\int\frac{\rho(\vec{r}')dr'^3}{|\vec{r}-\vec{r}'|} \tag{19b}$$

with

$$V_{\text{xt}}(\vec{r})=\frac{\delta}{\delta\rho}[E_{\text{xc}}(\rho)+\Delta T(\rho)]\ . \tag{19c}$$

These equations are equivalent to those of the KS theory.

The dependence of $E_{\text{xc}}(\phi)$ and $\Delta T(\phi)$ on ρ follows from the fact that for a given $|\phi\rangle$ a $\rho(r)$ is defined, and by Eqs. (9)—(12), to all $|\phi\rangle$ having the same density, the same value of these functionals corresponds. Hence these functionals can be defined as functionals of ρ. We believe that further rigorous investigation of the KS theory will help in the search for the determination of the functionals $\Delta T(\phi)$ and $E_{\text{xc}}(\phi)$ which enter the HKS equations.

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