Current- and spin-density-functional theory for inhomogeneous electronic systems in strong magnetic fields

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We formulate the current- and spin-density-functional theory for electronic systems in arbitrarily strong magnetic fields. A set of single-particle self-consistent equations which determine, in addition to the ground-state energy, the density, the spin density, the current density, and the spin-current density, is derived and is proved to be gauge invariant and to satisfy various physical requirements, including the continuity equation. For a magnetic field of constant direction in space, we prove that the exchange-correlation energy functional $E_{xc}[n_\uparrow, n_\downarrow, \mathbf{j}_{p\uparrow}, \mathbf{j}_{p\downarrow}]$ [$n_{\uparrow(\downarrow)}(\mathbf{r})$ is the $\uparrow$ ($\downarrow$) component of the density and $\mathbf{j}_{p\uparrow(\downarrow)}(\mathbf{r})$ is the $\uparrow$ ($\downarrow$) component of the "paramagnetic" current density] is actually a functional of $n_\uparrow(\mathbf{r})$, $n_\downarrow(\mathbf{r})$, $\boldsymbol{\nu}_\uparrow(\mathbf{r}) \equiv \nabla \times \mathbf{j}_{p\uparrow}(\mathbf{r})/n_\uparrow(\mathbf{r})$, and $\boldsymbol{\nu}_\downarrow(\mathbf{r}) \equiv \nabla \times \mathbf{j}_{p\downarrow}(\mathbf{r})/n_\downarrow(\mathbf{r})$. An explicit form of E_{xc}, which is local in $\boldsymbol{\nu}_\uparrow(\mathbf{r})$ and $\boldsymbol{\nu}_\downarrow(\mathbf{r})$, is derived from linear-response theory. The generalizations to finite-temperature ensembles and to magnetic fields of arbitrarily varying directions are presented.

I. INTRODUCTION

Density-functional theory[1] (DFT) in the self-consistent formulation of Kohn and Sham[2] (KS) is one of the most frequently used tools for the study of the electronic structure of condensed matter. Originally, the theory was formulated for electrons in the presence of an arbitrary external potential, but no magnetic field. Under such conditions, time-reversal invariance ensures that there is no average current density, nor spin density.[3] When a magnetic field $\mathbf{B}(\mathbf{r})$ is applied to the system—or, even in the absence of a magnetic field, in broken-symmetry systems such as ferromagnets (for an example of spin-broken symmetry) or open-shell atoms (for current-broken symmetry)—finite current and spin densities appear in the ground state. Traditionally, the presence of currents has been ignored, whereas the effects of spin polarization have been studied in detail, and incorporated in the self-consistent KS scheme,[3,4] generating the so-called spin-density-functional theory.

The above approach is only justified if one can show that the orbital currents give a negligible contribution to the energy functional. That this is not true *a priori* can be seen from the following argument. In a noninteracting, homogeneous electron gas, in the presence of a weak magnetic field, the contributions to the ground-state energy from spin polarization and orbital currents are $\sim \frac{1}{2}\chi_P^0 B^2$ and $\frac{1}{2}\chi_L^0 B^2$ respectively, where χ_P^0 is the paramagnetic Pauli susceptibility, and $\chi_L^0 = -\frac{1}{3}\chi_P^0$ is the orbital Landau susceptibility.[5] The two contributions are of the same order of magnitude. When interactions between the electrons are included, χ_P is considerably enhanced by exchange. Should a similar correction also occur in χ_L, then the spin-density-functional theory would be in error in neglecting the contribution of orbital currents to the exchange-correlation energy. Of course, broken symmetries in interacting macroscopic electron systems are only found for spins. Therefore, ferromagnets required the spin-density-functional theory more urgently. This, however, is no longer true when extremely high magnetic fields are present, or in open-shell atoms where spontaneous currents may exist.

In this paper we present the first complete formulation of a current- and spin-density-functional theory (CSDFT) for the nonrelativistic[6] (Pauli) Hamiltonian of interacting electrons in a magnetic field. There are various physical situations in which huge magnetic fields coexist with a strongly inhomogeneous electronic structure and our formulation should prove useful in all such cases. For example, we have in mind (i) broken-symmetry states (charge-density waves, spin-density waves, Wigner crystals) in three-dimensional semimetals and doped semiconductors in strong magnetic fields,[7] (ii) broken-symmetry states in the fractional quantum-Hall-effect regime of a two-dimensional electron gas,[8,9] (iii) the effect of an external potential of the fractional quantum Hall effect, and (iv) ground-state energy calculations in open-shell atoms and molecules.

Even besides the above-mentioned applications, there is an intrinsic theoretical challenge in the formulation of such a theory. It is due to the fact that the separation of the Hamiltonian into an internal and an interaction part (the latter describing the coupling to the external fields) is *not gauge invariant.* For this reason, one is forced to work with quantities which are not gauge invariant, and hence do not have a direct physical meaning. For exam-

ple, one of the basic variables in our formulation will have to be the paramagnetic current density $\mathbf{j}_p$, rather than the physical current density $\mathbf{j}$ (the latter is defined *via* the continuity equation) and the challenge is to formulate a gauge-invariant theory in terms of $\mathbf{j}_p$. In the following, we shall show how this key difficulty is overcome by sharpening our understanding of the structure of the exchange-correlation energy functional.

This paper is organized as follows. In Sec. II we introduce the basic variables and prove the two basic theorems of CSDFT, i.e., the analogue of the Hohenberg-Kohn theorem and the variational theorem.[1] In Sec. III we derive self-consistent one-electron equations which determine the density, the spin polarization, and the currents in the ground state. In Sec. IV the one-electron equations are proved to be gauge invariant, to satisfy the continuity equation, and to possess the usual magnetic-translation-group properties whenever the number of flux quanta per unit cell is a rational number p/q. In Sec. V we use diagrammatic linear-response theory to determine an approximate form of the energy functional which becomes exact for high densities, weak magnetic fields, and slowly varying currents. Section VI presents the generalizations of the theory to magnetic fields of arbitrarily varying direction and to finite-temperature ensembles. Section VII contains a discussion and summary of the results.

II. BASIC VARIABLES AND THEOREMS

A. Hohenberg-Kohn theorem

We consider the nonrelativistic Hamiltonian for N electrons (e is the absolute value of the charge)

$$H=H_0+\sum_\sigma \int n_\sigma^{\rm op}(\mathbf{r})V_\sigma(\mathbf{r})d\mathbf{r}+\frac{e}{c}\sum_\sigma \int \mathbf{j}_{p\sigma}^{\rm op}(\mathbf{r})\cdot\mathbf{A}_\sigma(\mathbf{r})d\mathbf{r} +\frac{e^2}{2mc^2}\sum_\sigma \int n_\sigma^{\rm op}(\mathbf{r})A_\sigma^2(\mathbf{r})d\mathbf{r} \ . \tag{2.1}$$

H_0 is the Hamiltonian of the homogeneous electron gas,

$$H_0=-\sum_{i=1}^{N}\frac{\hbar^2\nabla_i^2}{2m}+\tfrac{1}{2}\sum_{\substack{i,j\\ i\neq j}}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_j|} \ . \tag{2.2}$$

The remaining terms describe interactions with external scalar and vector potentials. The scalar potentials $V_\uparrow(\mathbf{r})$ and $V_\downarrow(\mathbf{r})$ couple to the density of spin-up and spin-down electrons, respectively. The symmetric combination $\frac{1}{2}[V_\uparrow(\mathbf{r})+V_\downarrow(\mathbf{r})]$ corresponds to the usual external potential $V(\mathbf{r})$, while the antisymmetric combination

$$\tfrac{1}{2}[V_\uparrow(\mathbf{r})-V_\downarrow(\mathbf{r})]\equiv\frac{e\hbar^2}{2mc}B(\mathbf{r})$$

corresponds to an external magnetic field *with a constant* $\hat{\mathbf{z}}$ *direction in space.* (The case of a magnetic field with variable direction is discussed in detail in Sec. VI.) To develop a complete current-density-functional theory we also need, as a formal tool, *two* external vector potentials $A_\uparrow(\mathbf{r})$ and $A_\downarrow(\mathbf{r})$ which couple to spin-up and spin-down electrons, respectively. The physical Hamiltonian, of course, has $\mathbf{A}_\uparrow(\mathbf{r})=\mathbf{A}_\downarrow(\mathbf{r})=\mathbf{A}(\mathbf{r})$ and $\hat{\mathbf{z}}B(\mathbf{r})=\nabla\times\mathbf{A}(\mathbf{r})$. These values will have to be reintroduced at the end of the formal manipulations. The density and paramagnetic current-density operators are defined as follows ($\sigma=\uparrow,\downarrow$):

$$n_\sigma^{\rm op}(\mathbf{r})\equiv\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}) \ , \tag{2.3a}$$

$$j_{p\sigma}^{\rm op}(r)\equiv-\frac{i\hbar}{2m}\{\psi_\sigma^\dagger(\mathbf{r})\nabla\psi_\sigma(\mathbf{r})-[\nabla\psi_\sigma^\dagger(\mathbf{r})]\psi_\sigma(\mathbf{r})\} \ . \tag{2.3b}$$

The corresponding ground-state expectation values are denoted by $n_\sigma(\mathbf{r})$ and $\mathbf{j}_{p\sigma}(\mathbf{r})$. The physical current densities $\mathbf{j}_\sigma(\mathbf{r})$ are related to the paramagnetic current densities by the equation

$$\mathbf{j}_\sigma^{\rm op}(\mathbf{r})=\mathbf{j}_{p\sigma}^{\rm op}(\mathbf{r})+\frac{e}{mc}n_\sigma^{\rm op}(\mathbf{r})\mathbf{A}_\sigma(\mathbf{r}) \ . \tag{2.4}$$

They satisfy the continuity equations

$$\frac{\partial n_\sigma^{\rm op}(\mathbf{r};t)}{\partial t}+\nabla\cdot\mathbf{j}_\sigma^{\rm op}(\mathbf{r},t)=0 \ .$$

Summing over σ gives the continuity equation for the number density, while taking the difference between spin up and spin down gives the continuity equation for the z component of the spin density. The constancy of the total number of electrons and the static continuity equations [$\nabla\cdot\mathbf{j}_\sigma(\mathbf{r})=0$] impose the constraints

$$\sum_\sigma\int n_\sigma(\mathbf{r})d\mathbf{r}=N \ , \tag{2.5a}$$

$$\nabla\cdot\mathbf{j}_{p\sigma}(\mathbf{r})=-\frac{e}{mc}\nabla\cdot[n_\sigma(\mathbf{r})\mathbf{A}_\sigma(\mathbf{r})] \ . \tag{2.5b}$$

We shall denote by C the class of densities and current densities $n_\sigma(\mathbf{r})$ and $\mathbf{j}_{p\sigma}(\mathbf{r})$ which can be realized in a nondegenerate ground state corresponding to some external fields $V_\sigma(\mathbf{r})$ and $\mathbf{A}_\sigma(\mathbf{r})$. All our subsequent considerations are logically restricted to densities in this class. Experience with the usual DFT indicates that this restriction is not of practical importance.

The generalized Hohenberg-Kohn theorem states that $V_\sigma(\mathbf{r})$ and $\mathbf{A}_\sigma(\mathbf{r})$, and the nondegenerate ground-state wave functions ψ are uniquely determined (apart from a common additive constant in the scalar potentials V_σ) by the knowledge of the distributions $n_\sigma(\mathbf{r})$ and $\mathbf{j}_{p\sigma}(\mathbf{r})$.

The proof of the theorem is by *reductio ad absurdum.* Suppose there were two different sets of fields V_σ, $\mathbf{A}_\sigma$, and V'_σ, $\mathbf{A}'_\sigma$ giving the same ground-state distributions n_σ and $\mathbf{j}_{p\sigma}$. Let $|\psi\rangle$ and $|\psi'\rangle$ be the two different ground states corresponding to the two sets of fields. Let us denote by H and H' the two corresponding Hamiltonians, and by E and E' the two corresponding ground-state energies. Then, from the variational principle for the ground state of H we obtain the inequality

$$E=\langle\psi\,|\,H\,|\,\psi\rangle<\langle\psi'\,|\,H\,|\,\psi'\rangle$$
$$=E'+\sum_\sigma\int d\mathbf{r}\,n_\sigma(\mathbf{r})[V_\sigma(\mathbf{r})-V'_\sigma(\mathbf{r})]$$
$$+\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}_{p\sigma}(\mathbf{r})\cdot[\mathbf{A}_\sigma(\mathbf{r})-\mathbf{A}'_\sigma(\mathbf{r})]$$
$$+\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n_\sigma(\mathbf{r})[\mathbf{A}^2_\sigma(\mathbf{r})-\mathbf{A}'^2_\sigma(\mathbf{r})]\ .$$

Another inequality is obtained by interchanging the primed and unprimed variables. Summing the two inequalities we come to the inconsistent result

$$E+E'<E+E'\ .$$

Thus, it is not possible to have the same density distributions in two essentially different sets of fields. Hence, the fields, the ground state, and the ground-state energy are uniquely determined by the densities, and paramagnetic current density. This result would have not been true if we had attempted to work with the physical current densities j as basic variable. In that case one would still have the freedom of operating a gauge transformation on the vector potential, and hence multiplying the ground-state wave function by a coordinate-dependent phase factor, *without changing* the physical current density. Therefore, the ground-state wave function is *not* a unique functional of j. Working with the paramagnetic current density $\mathbf{j}_p$ eliminates this ambiguity.

B. Variational principle

The ground-state energy functional can be written as

$$E[n_\sigma,\mathbf{j}_{p\sigma}]=F[n_\sigma,\mathbf{j}_{p\sigma}]+\sum_\sigma\int d\mathbf{r}\,n_\sigma(\mathbf{r})V_\sigma(\mathbf{r})$$
$$+\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}_{p_\sigma}(\mathbf{r})\cdot\mathbf{A}_\sigma(\mathbf{r})$$
$$+\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n_\sigma(\mathbf{r})A^2_\sigma(\mathbf{r})\ . \tag{2.6}$$

The functional F is defined as

$$F[n_\sigma,\mathbf{j}_{p\sigma}]\equiv\langle\psi[n_\sigma,\mathbf{j}_{p\sigma}]\,|\,H_0\,|\,\psi[n_\sigma,\mathbf{j}_{p\sigma}]\rangle \tag{2.7}$$

and does not contain any reference to the external fields. Thus, it is possible to define a functional

$$E_{V_\sigma\mathbf{A}_\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]=F[n'_\sigma,\mathbf{j}'_{p\sigma}]+\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})V_\sigma(\mathbf{r})$$
$$+\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}'_{p\sigma}(\mathbf{r})\cdot\mathbf{A}_\sigma(\mathbf{r})$$
$$+\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})A^2_\sigma(\mathbf{r}) \tag{2.8}$$

in which the external fields are fixed, and the densities are varied independently.

The variational principle now states that the functional $E_{V_\sigma\mathbf{A}_\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]$ has a minimum when $(n'_\sigma,\mathbf{j}'_{p\sigma})=(n_\sigma,\mathbf{j}_{p\sigma})$, the true density and current-density distributions corresponding to the given external fields. This theorem follows from the variational principle for the ground-state wave function, which allows us to write

$$E_{V_\sigma\mathbf{A}_\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]\equiv\langle\psi[n'_\sigma,\mathbf{j}'_{p\sigma}]\,|\,H\,|\,\psi[n'_\sigma,\mathbf{j}'_{p\sigma}]\rangle$$
$$\geq\langle\psi[n_\sigma,\mathbf{j}_{p\sigma}]\,|\,H\,|\,\psi[n_\sigma,\mathbf{j}_{p\sigma}]\rangle$$
$$\equiv E_{V_\sigma\mathbf{A}_\sigma}[n_\sigma,\mathbf{j}_{p\sigma}]\ .$$

[H is the Hamiltonian of Eq. (2.1) with the given external fields V_σ and $\mathbf{A}_\sigma$.] The minimum must be found subject to the constraints of Eq. (2.5).

III. SELF-CONSISTENT EQUATIONS

In this section we show that the minimization of $E_{V_\sigma\mathbf{A}_\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]$ is formally equivalent to the self-consistent solution of a one-electron Schrödinger-like equation.

We first decompose the internal energy functional $F[n'_\sigma,\mathbf{j}'_{p\sigma}]$ as follows:

$$F[n'_\sigma,\mathbf{j}'_{p\sigma}]=T_s[n'_\sigma,\mathbf{j}'_{p\sigma}]$$
$$+\frac{e^2}{2}\int\int\frac{n'(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}\,d\mathbf{r}'$$
$$+E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]\ . \tag{3.1}$$

The first term, T_s, is the noninteracting version of the functional F. More precisely,

$$T_s[n'_\sigma,\mathbf{j}'_{p\sigma}]=\left\langle\psi^0[n'_\sigma,\mathbf{j}'_{p\sigma}]\left|-\sum_{i=1}^N\frac{\hbar^2\nabla_i^2}{2m}\right|\psi^0[n'_\sigma,\mathbf{j}'_{p\sigma}]\right\rangle \tag{3.2}$$

where $\psi^0[n'_\sigma,\mathbf{j}'_{p\sigma}]$ is the ground-state wave function of N *noninteracting electrons* with the given density and current-density distributions.[10] The second term, where $n(\mathbf{r})\equiv n_\uparrow(\mathbf{r})+n_\downarrow(\mathbf{r})$, is the usual electrostatic energy. The third term, $E_{\rm xc}$, is the exchange-correlation energy functional.

By definition $\psi^0[n'_\sigma,\mathbf{j}'_{p\sigma}]$ is a Slater determinant of N one-electron wave functions, $\psi'_{i\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]$, which are the N lowest-lying solutions of either spin of a Schrödinger equation with some appropriate external fields $V'_\sigma[n'_\sigma,\mathbf{j}'_{p\sigma}]$ and $\mathbf{A}'_\sigma[n'_\sigma,\mathbf{j}'_{p\sigma}]$:

$$\left[\frac{1}{2m}\left[-i\hbar\nabla+\frac{e}{c}\mathbf{A}'_\sigma(\mathbf{r})\right]^2+V'_\sigma(\mathbf{r})\right]\psi'_{i\sigma}(\mathbf{r})=\varepsilon'_{i\sigma}\psi'_{i\sigma}(\mathbf{r})\ . \tag{3.3}$$

The densities n'_σ and $\mathbf{j}'_{p\sigma}$, are related to the one-electron wave functions by the equations

$$n'_\sigma(\mathbf{r})=\sum_{i=1}^{N_\sigma}|\psi'_{i\sigma}(\mathbf{r})|^2 ,$$

$$\mathbf{j}'_{p\sigma}(\mathbf{r})=\frac{-i\hbar}{2m}\sum_{i=1}^{N_\sigma}\{\psi'^{*}_{i\sigma}(\mathbf{r})\nabla\psi'_{i\sigma}(\mathbf{r})-[\nabla\psi'^{*}_{i\sigma}(\mathbf{r})]\psi'_{i\sigma}(\mathbf{r})\} . \tag{3.4}$$

Here N_σ is the number of the highest occupied orbital of spin σ, defined by the condition $\varepsilon'_{N_\sigma,\sigma}\le\mu$, $\varepsilon'_{N_\sigma+1,\sigma}>\mu$, and μ is the chemical potential. The functional $T_s[n'_\sigma,\mathbf{j}'_{p\sigma}]$ defined in Eq. (3.2) can now be expressed in terms of the one-electron eigenvalues $\varepsilon'_{i\sigma}$. Multiplying Eq. (3.3) to the left by $\psi^{*}_{i\sigma}(\mathbf{r})$, integrating over $\mathbf{r}$, and summing over i and σ, we find

$$T_s[n'_\sigma,\mathbf{j}'_{p\sigma}]=\sum_\sigma\sum_{i=1}^{N_\sigma}\varepsilon'_{i\sigma}-\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})V'_\sigma(\mathbf{r})-\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}'_{p\sigma}(\mathbf{r})\cdot\mathbf{A}'_\sigma(\mathbf{r})-\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})A'^{2}_\sigma(\mathbf{r}) . \tag{3.5}$$

Combining Eqs. (2.8), (3.1), and (3.5) we find the functional to be minimized:

$$E_{V_\sigma\mathbf{A}_\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]=\sum_\sigma\sum_{i=1}^{N_\sigma}\varepsilon'_{i\sigma}+\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})[V_\sigma(\mathbf{r})-V'_\sigma(\mathbf{r})]+\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}'_{p\sigma}(\mathbf{r})\cdot[\mathbf{A}_\sigma(\mathbf{r})-\mathbf{A}'_\sigma(\mathbf{r})]+\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})[A^2_\sigma(\mathbf{r})-A'^{2}_\sigma(\mathbf{r})]+\frac{e^2}{2}\int\int d\mathbf{r}\,d\mathbf{r}'\frac{n'(\mathbf{r})n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}+E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}] . \tag{3.6}$$

In calculating the functional derivatives of Eq. (3.6) with respect to n'_σ and $\mathbf{j}'_{p\sigma}$ one must keep in mind that $\varepsilon'_{i\sigma}$, V'_σ, and $\mathbf{A}'_\sigma$ are functionals of these distributions. However, as a consequence of Eq. (3.3), the derivatives of $\varepsilon'_{i\sigma}$ are exactly canceled by the derivatives of V'_σ and $\mathbf{A}'_\sigma$. Thus, the variational principle leads to the equations

$$V'_\sigma(\mathbf{r})=V_\sigma(\mathbf{r})+V_H(\mathbf{r})+V_{{\rm xc}\,\sigma}(\mathbf{r})+\frac{e^2}{2mc^2}\{A^2_\sigma(\mathbf{r})-[\mathbf{A}_\sigma(\mathbf{r})+\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r})]^2\} , \tag{3.7a}$$

$$\mathbf{A}'_\sigma(\mathbf{r})=\mathbf{A}_\sigma(\mathbf{r})+\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r}) . \tag{3.7b}$$

We have defined

$$V_H(\mathbf{r})=e^2\int d\mathbf{r}'\frac{n'(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} , \tag{3.8a}$$

$$V_{{\rm xc}\,\sigma}(\mathbf{r})=\left.\frac{\delta E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]}{\delta n'_\sigma(\mathbf{r})}\right|_{\{\mathbf{j}'_{p\sigma}\},n'_{-\sigma}} , \tag{3.8b}$$

$$\frac{e}{c}\mathbf{A}_{{\rm xc}\sigma}(\mathbf{r})=\left.\frac{\delta E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]}{\delta\mathbf{j}'_{p\sigma}(\mathbf{r})}\right|_{\{n'_\sigma\},\mathbf{j}'_{p-\sigma}} . \tag{3.8c}$$

Equations (3.7) and (3.8) determine the fields V'_σ and A'_σ as functionals of n'_σ and $\mathbf{j}'_{p\sigma}$. The latter are in turn determined by V'_σ and $\mathbf{A}'_\sigma$, via Eqs. (3.3) and (3.4). Thus we have obtained, at least formally, a self-consistent one-electron equation, from which the ground-state properties can be calculated. Its explicit form is

$$\left[\frac{1}{2m}\left[-i\hbar\nabla+\frac{e}{c}[\mathbf{A}(\mathbf{r})+\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r})]\right]^2+\frac{e^2}{2mc^2}\{A^2(\mathbf{r})-[\mathbf{A}(\mathbf{r})+\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r})]^2\}+V_\sigma(\mathbf{r})+V_H(\mathbf{r})+V_{{\rm xc}\,\sigma}(\mathbf{r})\right]\psi'_{i\sigma}(\mathbf{r})=\varepsilon'_{i\sigma}\psi'_{i\sigma}(\mathbf{r}),\quad i=1,\ldots,N_\sigma . \tag{3.9}$$

The external fields have now been assigned their physical values, i.e., $\mathbf{A}_\uparrow(\mathbf{r})=\mathbf{A}_\downarrow(\mathbf{r})=\mathbf{A}(\mathbf{r})$ and $B(\mathbf{r})\hat{\mathbf{z}}=\nabla\times\mathbf{A}(\mathbf{r})$. We emphasize the fact that the "effective" vector potential $\mathbf{A}+\mathbf{A}_{{\rm xc}\,\sigma}$ appears *linearly* in this equation. The quadratic term remains $(e^2/2mc^2)A^2$, as in the non interacting case.

The ground-state energy can be obtained from Eq. (3.6), inserting the expressions for V'_σ and $\mathbf{A}'_\sigma$ given in Eq. (3.7). The result is

$$E_G=\sum_\sigma\sum_{i=1}^{N_\sigma}\varepsilon_{i\sigma}-\tfrac{1}{2}\int\int d\mathbf{r}\,d\mathbf{r}'\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}-\sum_\sigma\int d\mathbf{r}\,n_\sigma(\mathbf{r})V_{{\rm xc}\,\sigma}(\mathbf{r})-\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}_{p\sigma}(\mathbf{r})\cdot\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r})+E_{\rm xc}[n_\sigma,\mathbf{j}_{p\sigma}] . \tag{3.10}$$

We note, in passing, that the chemical potential μ, determined by occupying the N lowest-lying states of either spin is the exact chemical potential (Koopman's theorem of DFT). This completes the construction of the self-consistent one-electron scheme.

We conclude this section with several observations concerning the fictitious continuation of the physical $\mathbf{A}$ to two nonphysical independent components $\mathbf{A}_\sigma$. This trick was necessary to generate a Schrödinger-type equation which determines self-consistently *both* components $\mathbf{j}_{p\sigma}$ of the paramagnetic-current density. We could have obtained a simpler formulation using $\mathbf{j}_p=\sum_\sigma \mathbf{j}_{p\sigma}$ as the basic variable. Since the physical Hamiltonian depends only on $\mathbf{j}_p$, the Hohenberg-Kohn theorem and the variational principle would still be valid in terms of $\mathbf{j}_p$, but now there would be only *one* vector potential. The Schrödinger-type equation would still have the form of Eq. (3.9), but now with a single

$$(e/c)\,\mathbf{A}_{\rm xc}=\delta E_{\rm xc}[n_\sigma,\mathbf{j}_p]/\delta \mathbf{j}_p \ ,$$

a functional of $\mathbf{j}_p$. A limitation of this simpler formulation is that $j_{p\uparrow}$ and $j_{p\downarrow}$ determined from the self-consistent equations have no physical meaning when considered separately. Only their sum corresponds to the actual paramagnetic current density. Furthermore, an advantage of the formulation in terms of two currents and two vector potentials is that it exposes some internal symmetries of $E_{\rm xc}[n_\sigma,\mathbf{j}_{p\sigma}]$ which would not be accessible in the $\mathbf{j}_p$ formulation (see Sec. IV). We shall return to these questions in Sec. VI, where the theory is generalized to magnetic fields of arbitrarily varying directions.

IV. GAUGE INVARIANCE

In this section we demonstrate that the self-consistent equation formulation is a gauge-invariant one, and that it satisfies the continuity equation for the currents. Consider the gauge transformation

$$\mathbf{A}(\mathbf{r})\rightarrow \mathbf{A}_{\rm new}(\mathbf{r})=\mathbf{A}(\mathbf{r})-\nabla\Lambda(\mathbf{r}) \ , \tag{4.1}$$

where Λ is an arbitrary function. The requirement of gauge invariance is that if $n_\sigma(\mathbf{r})$, $\mathbf{j}_{p\sigma}(\mathbf{r})$, and E_G are the densities, current densities and ground-state energy corresponding to the physical external fields $V(\mathbf{r})$, $\mathbf{A}(\mathbf{r})$, and $\mathbf{B}(\mathbf{r})$, then the new densities and ground-state energy corresponding to $V(\mathbf{r})$, $\mathbf{A}_{\rm new}(\mathbf{r})$, and $\mathbf{B}(\mathbf{r})$ are

$$\begin{aligned} &n_{\sigma\,\rm new}(\mathbf{r})=n_\sigma(\mathbf{r}) \ , \\ &\mathbf{j}_{p\sigma\,\rm new}(\mathbf{r})=\mathbf{j}_{p\sigma}(\mathbf{r})+\frac{e}{mc}n_\sigma(\mathbf{r})\nabla\Lambda(\mathbf{r}) \ , \\ &E_{G\,\rm new}=E_G \ . \end{aligned} \tag{4.2}$$

The second of these equations states that the physical currents, Eq. (2.4), are invariant under the transformation. To prove the gauge invariance of our scheme and also the validity of the continuity equations for particle and spin currents, it is essential to determine the properties of the various functionals under the transformation

$$\mathbf{j}'_{p\sigma}\rightarrow \mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma \ . \tag{4.3}$$

($\Lambda_\uparrow$ and $\Lambda_\downarrow$ are now *two* independent functions.) We begin with the functional $F[n'_\sigma,\mathbf{j}'_{p\sigma}]$, which is defined by Eq. (2.7). Clearly, the ground-state wave function transforms according to the rule

$$\psi\left[n'_\sigma,\mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma\right]=\exp\left[i\frac{e}{\hbar c}\sum_{i=1}^{N}[\Lambda_\uparrow(\mathbf{r}_i)P_{i\uparrow}+\Lambda_\downarrow(\mathbf{r}_i)P_{i\downarrow}]\right]\psi[n'_\sigma,\mathbf{j}'_{p\sigma}] \ , \tag{4.4}$$

where

$$P_{i\atop\downarrow}=\frac{1\pm\sigma_{iz}}{2}$$

is the projector for the state of spin $\uparrow$ ($\downarrow$) of the ith electron. The validity of this equation can be directly checked by calculating the expectation value of $\mathbf{j}_{p\sigma}$ with the transformed wave function. From this, the transformation of F is immediately derived:

$$F\left[n'_\sigma,\mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma\right]=F[n'_\sigma,\mathbf{j}'_{p\sigma}]+\frac{e}{c}\sum_\sigma\int d\mathbf{r}\,\mathbf{j}'_{p\sigma}(\mathbf{r})\cdot\nabla\Lambda_\sigma(\mathbf{r})+\frac{e^2}{2mc^2}\sum_\sigma\int d\mathbf{r}\,n'_\sigma(\mathbf{r})\,|\,\nabla\Lambda_\sigma(\mathbf{r})\,|^2 \ . \tag{4.5}$$

The crucial fact about this equation, is that the transformation depends only on $\mathbf{j}'_{p\sigma}$ and n'_σ, not on the ground-state wave function. The same transformation rule applies, therefore, also to the noninteracting functional $T_s[n'_\sigma,\mathbf{j}'_{p\sigma}]$. Taking the difference of F and T_s, and using Eq. (3.1) leads to the important result

$$E_{\rm xc}\left[n'_\sigma,\mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma\right]=E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}] \ . \tag{4.6}$$

This is an *exact* property of the exchange-correlation functional which, as we now show, guarantees the gauge invariance of the self-consistent equations.

Differentiating both sides of Eq. (4.6) with respect to n'_σ and $\mathbf{j}'_{p\sigma}$, and using the definitions of Eqs. (3.8b)–(3.8d) we find the following transformations:

$$V_{\mathrm{xc}\sigma}\left[n'_\sigma, \mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma\right]=V_{\mathrm{xc}\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]-\frac{e^2}{mc^2}\sum_\sigma \mathbf{A}_{\mathrm{xc}\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]\cdot\nabla\Lambda_\sigma\ , \tag{4.7a}$$

$$\mathbf{A}_{\mathrm{xc}\sigma}\left[n'_\sigma, \mathbf{j}'_{p\sigma}+\frac{e}{mc}n'_\sigma\nabla\Lambda_\sigma\right]=\mathbf{A}_{\mathrm{xc}\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]\ . \tag{4.7b}$$

In particular, we see that the combination

$$V_{\mathrm{xc}\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]-\frac{e^2}{mc^2}\mathbf{A}_{\mathrm{xc}\sigma}[n'_\sigma,\mathbf{j}'_{p\sigma}]\cdot\mathbf{A}\ , \tag{4.8}$$

which appears as a scalar potential term in Eq. (3.9), is invariant under the simultaneous transformations (4.1) and (4.3) (the latter with $\Lambda_\uparrow=\Lambda_\downarrow=\Lambda$).

Thus, we see that Eq. (3.9) satisfies the requirements of gauge invariance. For, suppose we have found the self-consistent solution corresponding to the vector potential $\mathbf{A}(\mathbf{r})$. Let us multiply each of the self-consistent ψ_i's by a phase factor $\exp[i(e/\hbar)\Lambda(r_i)]$, so that the new densities and current densities are given by Eq. (4.2). Let us insert the new densities and current densities in $V_{\mathrm{xc}\sigma}$ and $\mathbf{A}_{\mathrm{xc}\sigma}$, and let us also replace $\mathbf{A}$ by $\mathbf{A}_{\mathrm{new}}$. Then, using Eq. (4.7) we can easily verify that the scalar potential term in the Schrödinger-like equation is invariant, while the vector potential is changed by the subtraction of $\nabla\Lambda$. Then, the new ψ_i's and the new densities are the self-consistent solutions corresponding to $\mathbf{A}_{\mathrm{new}}$. Furthermore, the ground-state energy, which is given by Eq. (3.10), is invariant, because the ε_i's do not change, while the variation of $V_{\mathrm{xc}\sigma}$ is exactly canceled by the variation of the $\mathbf{j}_{p\sigma}$'s. Thus, the proof of gauge invariance is complete.

We now prove that Eq. (4.6) also guarantees

$$\nabla\cdot[n'_\sigma(\mathbf{r})\,\mathbf{A}_{\mathrm{xc}\sigma}(\mathbf{r})]=0\ . \tag{4.9}$$

Since the structure of the Schrödinger-like equation (3.9) already guarantees

$$\nabla\cdot\left[\mathbf{j}_{p\sigma}(\mathbf{r})+\frac{e}{mc}n_\sigma(\mathbf{r})[A(\mathbf{r})+\mathbf{A}_{\mathrm{xc}\sigma}(\mathbf{r})]\right]=0\ ,$$

it is clear that Eq. (4.9) is equivalent to the continuity equation for the physical particle and spin currents. To prove this, note that if E_{xc} satisfies Eq. (4.6) for any $\Lambda_\sigma(\mathbf{r})$, then it can only depend on the combination

$$\boldsymbol{\nu}'_\sigma(\mathbf{r})\equiv\nabla\times\frac{\mathbf{j}'_{p\sigma}(\mathbf{r})}{n'_\sigma(\mathbf{r})}\ . \tag{4.10}$$

Thus, we can write

$$E_{\mathrm{xc}}[n'_\sigma,\mathbf{j}'_{p\sigma}]\equiv\bar{E}_{\mathrm{xc}}[n'_\sigma,\boldsymbol{\nu}'_\sigma]\ , \tag{4.11}$$

where $\bar{E}_{\mathrm{xc}}$ is a functional of n'_σ and $\boldsymbol{\nu}'_\sigma$. Taking the functional derivative of E_{xc} with respect to $\mathbf{j}'_{p\sigma}$ at constant n'_σ's we find, after simple transformations,

$$\frac{e}{c}A_{\mathrm{xc}\sigma}(\mathbf{r})=-\frac{1}{n'_\sigma(\mathbf{r})}\nabla\times\frac{\delta\bar{E}_{\mathrm{xc}}[n'_\sigma,\boldsymbol{\nu}'_\sigma]}{\delta\boldsymbol{\nu}'_\sigma(\mathbf{r})}\bigg|_{\{n'_\sigma\},\boldsymbol{\nu}'_{-\sigma}}\ . \tag{4.12}$$

Hence, Eq. (4.9) follows at once. It is interesting to express the exchange-correlation potential in terms of $\bar{E}_{\mathrm{xc}}$. The result is

$$V_{\mathrm{xc}\sigma}(\mathbf{r})=\frac{\delta\bar{E}_{\mathrm{xc}}[n'_\sigma,\boldsymbol{\nu}'_\sigma]}{\delta n'_\sigma(\mathbf{r})}\bigg|_{\{\boldsymbol{\nu}'_\sigma\},n'_{-\sigma}}-\frac{e}{c}\mathbf{A}_{\mathrm{xc}\sigma}(\mathbf{r})\cdot\frac{\mathbf{j}'_{p\sigma}(\mathbf{r})}{n'_\sigma(\mathbf{r})}\ , \tag{4.13}$$

which clearly exhibits the transformation property of Eq. (4.7a). Incidentally, the same functional form of Eq. (4.11) applies to the full ground-state energy E_G.

As a final issue related to gauge invariance, we comment on the possibility of applying Bloch's theorem to the solution of the Kohn-Sham–like equation in a periodic crystal potential and a uniform magnetic field. It is known that this presents considerable difficulties, even in a one-particle picture, since the external vector potential $\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{B}\times\mathbf{r}$ does not have the periodicity of the lattice. In general, the translation by a lattice vector can be viewed as a gauge transformation, whose generating function is $\Lambda(\mathbf{r})=\frac{1}{2}(\mathbf{B}\times\mathbf{a})\cdot\mathbf{r}$. This transformation multiples the wave function $\psi(\mathbf{r})$ by a phase factor

$$\exp[\tfrac{1}{2}i(\mathbf{B}\times\mathbf{a})\cdot\mathbf{r}]\ . \tag{4.14}$$

It can be shown that the result of two successive translations $T_{\mathbf{a}}T_{\mathbf{a}'}$ differs, in general, from the result of the composite translation $T_{\mathbf{a}+\mathbf{a}'}$ by the appearance of a phase factor depending on $\mathbf{a}$ and $\mathbf{a}'$. In mathematical terms, this means that the electronic wave functions give not an ordinary, but a *projective,* representation[11] of the translation group, i.e., they are not Bloch waves. A complete classification of the irreducible projective representations of the translation group can still be made if the magnetic field is along one of the three basis vectors of the lattice, and the number of magnetic flux quanta per unit cell is rational. In this case a Bloch-wave representation of the wave function is still possible (see Ref. 11 for details). The point we want to make here is that if we translate $\mathbf{r}\rightarrow\mathbf{r}+\mathbf{a}$ in our effective one-particle equations the transformation of the wave function will still be given by (4.14). This can be easily verified by noting that under this transformation $\nabla\times(\mathbf{j}_{p\sigma}/n_\sigma)$, $A_{\mathrm{xc}\sigma}(\mathbf{r})$, and the scalar-potential combination of Eq. (4.8) are invariant. In other words, both the effective vector potential and the effective scalar potential have the same periodicity as the lattice. Therefore, their presence does not modify the conditions for the applicability of Bloch's theorem which were obtained in a truly noninteracting system.

V. APPROXIMATE FORM OF THE EXCHANGE-CORRELATION ENERGY FUNCTIONAL

For the above formulation to be of practical use, it is still necessary to provide a reasonably simple approximate expression for $E_{\rm xc}[n_\sigma,\mathbf{j}_{p\sigma}]$. In the usual spin-density-functional theory,[4] which ignores the orbital currents, this need is satisfied by the local-density approximation (LDA), i.e.,

$$E_{\rm xc}^{\rm LDA}[n_\sigma]\cong\int d\mathbf{r}\, n(\mathbf{r})\varepsilon_{\rm xc}[n_\uparrow(\mathbf{r}),n_\downarrow(\mathbf{r})]\ , \tag{5.1}$$

where $\varepsilon_{\rm xc}[n_\uparrow,n_\downarrow]$ is the exchange-correlation energy, per electron, of a uniform electron gas, evaluated at the local values of the spin densities. At first sight, it seems that one could easily extend the LDA to the currents, i.e., write $E_{\rm xc}$ as an integral of a function of the local paramagnetic current density. However, this is not possible, because, according to Eq. (4.11), $E_{\rm xc}$ must depend on the *curl* of $\mathbf{j}_{p\sigma}/n_\sigma$. Thus, we conclude that the LDA vanishes identically for the currents. The simplest approximation beyond the LDA corresponds to a local approximation in the new variables $\boldsymbol{\nu}_\sigma(\mathbf{r})$. To determine the coefficient of the lowest-order term in this expansion we resort, as usual, to perturbation theory.

We consider small, but otherwise arbitrary current densities $\mathbf{j}'_{p\sigma}(r)$ in a uniform electron gas. The functional $F[n'_\sigma,\mathbf{j}'_{p\sigma}]$ is expanded to second order in $\mathbf{j}'_p$, i.e.,

$$F[n'_\sigma,\mathbf{j}'_{p\sigma}]\cong F[n'_\sigma,0]+\tfrac{1}{2}\sum_{\mathbf{q},\sigma}\mathbf{j}_{p\sigma}(\mathbf{q})\cdot\vec{\vec{F}}_{2\sigma}(\mathbf{q})\cdot\mathbf{j}_{p\sigma}(-\mathbf{q})\ , \tag{5.2}$$

where $\vec{\vec{F}}_{2\sigma}(\mathbf{q})$ is an as yet undetermined tensor which depends on the uniform densities $n_\uparrow$ and $n_\downarrow$. Anticipating the RPA form of the result we have ignored here possible crossterms of the form $\mathbf{j}_{p\uparrow}\cdot\mathbf{j}_{p\downarrow}$. From the variational principle, the current induced by a weak vector potential is calculated:

$$\mathbf{j}_{p\sigma}(\mathbf{q})=-\frac{e}{c}[\vec{\vec{F}}_{2\sigma}(\mathbf{q})]^{-1}\cdot\mathbf{A}(\mathbf{q})\ .$$

This leads to the identification

$$[\vec{\vec{F}}_{2\sigma}(\mathbf{q})]^{-1}=-\vec{\vec{P}}_\sigma(\mathbf{q})\ , \tag{5.3}$$

where

$$P_{\sigma,ij}(\mathbf{q})=P_\sigma(\mathbf{q})\left[\delta_{ij}-\frac{q_iq_j}{q^2}\right]-\frac{n_\sigma}{m}\frac{q_iq_j}{q^2}\ , \tag{5.4a}$$

$$P_\sigma(q)=-2\sum_n\frac{|\langle n\,|\,j_{p\sigma\perp}(q)\,|\,0\rangle|^2}{E_n-E_0} \tag{5.4b}$$

is the usual response function of linear-response theory.[12] $j_{p\sigma\perp}(\mathbf{q})$ is a transverse component of $\mathbf{j}_{p\sigma}(\mathbf{q})$. $|\,n\,\rangle$ and E_n are exact eigenstates and eigenvalues of the uniform electron gas ($n=0$ is the ground state).

Inverting Eq. (5.4a) we obtain

$$[F_{2\sigma}(\mathbf{q})]_{ij}=-P_\sigma^{-1}(q)\left[\delta_{ij}-\frac{q_iq_j}{q^2}\right]+\frac{m}{n_\sigma}\frac{q_iq_j}{q^2}\ .$$

Similarly, the second-order coefficient in the expansion of T_s is

$$[T_{s2\sigma}(\mathbf{q})]_{ij}=-P_{0\sigma}^{-1}(q)\left[\delta_{ij}-\frac{q_iq_j}{q^2}\right]+\frac{m}{n_\sigma}\frac{q_iq_j}{q^2}\ .$$

(P_0 is the noninteracting response function.) The difference $F_{2\sigma}(\mathbf{q})-T_{s2\sigma}(\mathbf{q})$ is the second-order coefficient in the current expansion of $E_{\rm xc}$. Note that it is a purely transverse tensor because the longitudinal components cancel out in the difference. Hence, the expansion of $E_{\rm xc}$ reads

$$E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]\cong E_{\rm xc}[n'_\sigma,0]-\tfrac{1}{2}\sum_{\mathbf{q},\sigma}\mathbf{j}_{p\sigma\perp}(\mathbf{q})[P_\sigma^{-1}(q)-P_{0\sigma}^{-1}(q)]\cdot\mathbf{j}_{p\sigma\perp}(-\mathbf{q})\ , \tag{5.5}$$

where $\mathbf{j}_{p\sigma\perp}(\mathbf{q})$ is the transverse part of $\mathbf{j}_{p\sigma}(\mathbf{q})$.

We consider the limit of slowly varying currents, i.e., $q\to0$. In this limit the behavior of $P_\sigma(q)$ has been the subject of a recent study,[13] based on the random-phase approximation. We refer to this work for technical details. For small q, P_σ has the form

$$P_\sigma(q)=-\frac{n_\sigma}{m}-\frac{c^2\chi_{L\sigma}}{e^2}q^2\ , \tag{5.6}$$

where $\chi_{L\sigma}$ is the contribution of spin σ to the orbital magnetic susceptibility. For the noninteracting electron gas $c^2\chi^0_{L\sigma}/e^2=-v_{F\sigma}/24\pi^2\hbar$, where $v_{F\sigma}$ is the Fermi velocity. Hence, we can rewrite Eq. (5.5) as follows:

$$E_{\rm xc}[n_\sigma,\mathbf{j}_{p\sigma}]\cong E_{\rm xc}[n_\sigma,0]+\sum_\sigma\int d\mathbf{r}\frac{mk_{F\sigma}}{48\pi^2}\left[\frac{\chi_{L\sigma}}{\chi^0_{L\sigma}}-1\right]\left|\nabla\times\frac{\mathbf{j}_{p\sigma}(\mathbf{r})}{n_\sigma}\right|^2 \tag{5.7}$$

($k_{F\sigma}$ is the Fermi momentum).

In Ref. 13 we have calculated the value of χ_L/χ^0_L for a *paramagnetic* electron gas in the random-phase approximation (RPA). The calculation parallels the calculation of Ma and Brueckner[14] of the exchange-correlation energy of a weakly inhomogeneous electron gas, but now is applied to the current-current correlation function. The values of the paramagnetic χ_L/χ^0_L are tabulated in Ref.

13, for a wide range of densities. In the general spin-polarized case, numerical results for $\chi_{L\sigma}/\chi^0_{L\sigma}$ in the RPA are not yet available. The final step in the construction of our approximate $E_{\rm xc}$ is to replace the n_σ's by the local densities $n_\sigma(\mathbf{r})$ in Eq. (5.7). The Fermi momenta and the orbital susceptibilities are now calculated at the local densities. We can still use the LDA for the remaining part, $E_{\rm xc}[n_\sigma,0]$, of the functional. Our approximate expression for $E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]$ is therefore

$$E_{\rm xc}[n'_\sigma,\mathbf{j}'_{p\sigma}]\cong\int n'(\mathbf{r})\varepsilon_{\rm xc}[n'_\uparrow(\mathbf{r}),n'_\downarrow(\mathbf{r})]d\mathbf{r}+\sum_\sigma\int b_\sigma[n'_\sigma(\mathbf{r})]\left|\nabla\times\frac{\mathbf{j}'_{p\sigma}(\mathbf{r})}{n'_\sigma(\mathbf{r})}\right|^2 d\mathbf{r} \tag{5.8}$$

where

$$b_\sigma[n'_\sigma(r)]\cong\frac{mk_{F\sigma}(\mathbf{r})}{48\pi^2}\left[\frac{\chi_{L\sigma}}{\chi^0_{L\sigma}}-1\right].$$

This expression has the form of Eq. (4.11) and, therefore, leads to gauge-invariant equations. The exchange-correlation vector potential $\mathbf{A}_{{\rm xc}\,\sigma}$ is given by (neglecting derivatives of b_σ with respect to $\mathbf{r}$)

$$\frac{e}{c}A_{{\rm xc}\,\sigma}(\mathbf{r})\cong-\frac{\bar b_\sigma}{n_\sigma(\mathbf{r})}\nabla\times\left[\nabla\times\frac{\mathbf{j}_{p\sigma}(\mathbf{r})}{n_\sigma(\mathbf{r})}\right] \tag{5.9a}$$

($\bar b_\sigma$ is an average value of b_σ). Similarly we find

$$V_{{\rm xc}\,\sigma}(\mathbf{r})=V^{\rm LDA}_{{\rm xc}\,\sigma}(\mathbf{r})-\frac{e}{c}\mathbf{A}_{{\rm xc}\,\sigma}(\mathbf{r})\cdot\frac{\mathbf{j}_{p\sigma}(\mathbf{r})}{n_\sigma(\mathbf{r})}\ , \tag{5.9b}$$

where $V^{\rm LDA}_{{\rm xc}\,\sigma}$ is the usual exchange-correlation potential in local-spin-density-functional theory. Note that the right-hand sides of Eqs. (5.9a) and (5.9b) are actually *independent of the electron charge.* This is expected since the effect of the current on the exchange-correlation energy is not an electromagnetic one, but a purely quantum one, due to the distortion of the wave function in the presence of currents.

VI. GENERALIZATIONS

A. Magnetic field of arbitrarily varying direction

We have assumed in our treatment thus far that the magnetic field $B\propto V_\uparrow-V_\downarrow$ has a constant direction in space. This guarantees the existence of two conserved currents: the particle current and the z component of the spin current. What happens if $\mathbf{B}$ is allowed to have an arbitrary direction in space? The most general approach describes the system in terms of the following variables:

$$n_{\alpha\beta}(\mathbf{r})=\langle\psi^\dagger_\beta(\mathbf{r})\psi_\alpha(\mathbf{r})\rangle=n^*_{\beta\alpha}(\mathbf{r}) \tag{6.1a}$$

and

$$\mathbf{j}_{p\alpha\beta}(\mathbf{r})=\frac{-i\hbar}{2m}\langle\psi^\dagger_\beta(\mathbf{r})\nabla\psi_\alpha(\mathbf{r})-[\nabla\psi^\dagger_\beta(\mathbf{r})]\psi_\alpha(\mathbf{r})\rangle$$
$$=\mathbf{j}^*_{p\beta\alpha}(\mathbf{r}) \tag{6.1b}$$

(α and β are spin indices). Expanding these variables in terms of Pauli matrices, i.e.,

$$n_{\alpha\beta}(\mathbf{r})=n(\mathbf{r})\delta_{\alpha\beta}+\sum_{\lambda=1}^{3}n_\lambda(\mathbf{r})\sigma^\lambda_{\alpha\beta}\ , \tag{6.2a}$$

$$\mathbf{j}_{p\alpha\beta}(\mathbf{r})=\mathbf{j}_p(\mathbf{r})\delta_{\alpha\beta}+\sum_{\lambda=1}^{3}\mathbf{j}_{p\lambda}(\mathbf{r})\sigma^\lambda_{\alpha\beta}\ , \tag{6.2b}$$

we obtain quantities of direct physical significance. For example, $n(\mathbf{r})$ is the density, $n_\lambda(\mathbf{r})$ ($\lambda=1,2,3$) are the components of the spin density (times $2/\hbar$), $\mathbf{j}_p(\mathbf{r})$ is the paramagnetic current density, and $\mathbf{j}_{p\lambda}(\mathbf{r})$ are the components (times $2/\hbar$) of the paramagnetic spin-current density. We can now introduce external fields

$$V_{\alpha\beta}(\mathbf{r})=V(\mathbf{r})\delta_{\alpha\beta}+\sum_{\lambda=1}^{3}V_\lambda(\mathbf{r})\sigma^\lambda_{\alpha\beta}\ , \tag{6.3a}$$

$$\mathbf{A}_{\alpha\beta}(\mathbf{r})=\mathbf{A}(\mathbf{r})\delta_{\alpha\beta}+\sum_{\lambda=1}^{3}\mathbf{A}_\lambda(\mathbf{r})\sigma^\lambda_{\alpha\beta} \tag{6.3b}$$

which couple to $n_{\alpha\beta}$ and $\mathbf{j}_{p\alpha\beta}$, respectively. The Hohenberg-Kohn theorem and the variational principle can now be proved in the usual way. Note that the vector part of $V_{\alpha\beta}(\mathbf{r})$ corresponds to a magnetic field: $V_\lambda(\mathbf{r})=-(e\hbar^2/2mc)B_\lambda(\mathbf{r})$. The physical Hamiltonian, of course, contains only the first component $\mathbf{A}(\mathbf{r})$ of the vector potential. The three spin components $\mathbf{A}_\lambda(\mathbf{r})$ are fictitious, and must be regarded as a mathematical necessity to formulate complete self-consistent equations.

The Schrödinger-type equation takes the form

$$\frac{1}{2m}\sum_\beta\left[-i\hbar\nabla+\frac{e}{c}\mathbf{A}^{\rm eff}(\mathbf{r})\right]^2_{\alpha\beta}\psi_\beta(\mathbf{r})+\frac{e^2}{2mc^2}\sum_\beta\{A^2(\mathbf{r})\delta_{\alpha\beta}-[(A^{\rm eff})^2(\mathbf{r})]_{\alpha\beta}\}\psi_\beta(\mathbf{r})+\sum_\beta V^{\rm eff}_{\alpha\beta}(\mathbf{r})\psi_\beta(\mathbf{r})=\varepsilon\psi_\alpha(\mathbf{r})\ . \tag{6.4}$$

The effective fields are given by

$$V^{\rm eff}_{\alpha\beta}(\mathbf{r})=V_{\alpha\beta}(\mathbf{r})+V_H(\mathbf{r})\delta_{\alpha\beta}+V^{\rm xc}_{\alpha\beta}(\mathbf{r})\ , \tag{6.5a}$$

$$\mathbf{A}^{\rm eff}_{\alpha\beta}(\mathbf{r})=\mathbf{A}(\mathbf{r})\delta_{\alpha\beta}+\mathbf{A}^{\rm xc}_{\alpha\beta}(\mathbf{r})\ , \tag{6.5b}$$

and the exchange-correlation components are defined as

functional derivatives of the E_{xc} functional,

$$V^{xc}_{\alpha\beta}(\mathbf{r})=\frac{\delta E_{xc}[n_{\alpha\beta},\mathbf{j}_{p\alpha\beta}]}{\delta n_{\beta\alpha}(\mathbf{r})} , \tag{6.6a}$$

$$\frac{e}{c}\mathbf{A}^{xc}_{\alpha\beta}(\mathbf{r})=\frac{\delta E_{xc}[n_{\alpha\beta},\mathbf{j}_{p\alpha\beta}]}{\delta \mathbf{j}_{p\beta\alpha}(\mathbf{r})} . \tag{6.6b}$$

The "intensive fields" $n_{\alpha\beta}(\mathbf{r})$ and $\mathbf{j}_{p\alpha\beta}(\mathbf{r})$ are calculated self-consistently from the N lowest-lying one-electron eigenfunctions as follows:

$$n_{\alpha\beta}(\mathbf{r})=\sum_{i=1}^{N}\psi^{*}_{i\beta}(\mathbf{r})\psi_{i\alpha}(\mathbf{r}) , \tag{6.7a}$$

$$\mathbf{j}_{p\alpha\beta}(\mathbf{r})=\frac{-i\hbar}{2m}\sum_{i=1}^{N}\{\psi^{*}_{i\beta}(\mathbf{r})\nabla\psi_{i\alpha}(\mathbf{r})-[\nabla\psi^{*}_{i\beta}(\mathbf{r})]\psi_{i\alpha}(\mathbf{r})\} . \tag{6.7b}$$

Equations (6.4)–(6.7) are, therefore, our set of self-consistent equations.

From the exact Hamiltonian of interacting electrons in a magnetic field, the following exact equations for the divergence of the ground-state currents are derived:

$$\nabla\cdot\left[\mathbf{j}_p(\mathbf{r})+\frac{e}{mc}n(\mathbf{r})\mathbf{A}(\mathbf{r})\right]=0 , \tag{6.8a}$$

$$\nabla\cdot\left[\mathbf{j}_{p\lambda}(\mathbf{r})+\frac{e}{mc}n_\lambda(\mathbf{r})\mathbf{A}(\mathbf{r})\right]=\frac{2}{\hbar}(\mathbf{V}\times\mathbf{n})_\lambda . \tag{6.8b}$$

The first is the usual continuity equation for the particle current. The second represents a modified continuity equation for the spin current, where the right-hand side accounts for the fact that the spin density is not conserved, but precesses around the direction of the local magnetic field. Equations (6.8a) and (6.8b) must also be satisfied by our one-particle equations. However, close inspection of the Schrödinger-type equation reveals that it only assures the following relationships:

$$\nabla\cdot\left[\mathbf{j}_p(\mathbf{r})+\frac{e}{mc}[n(\mathbf{r})\mathbf{A}(\mathbf{r})+n(\mathbf{r})\mathbf{A}_{xc}(\mathbf{r})]+\sum_{\lambda=1}^{3}n_\lambda(\mathbf{r})\mathbf{A}_{xc\lambda}(\mathbf{r})\right]=0 \tag{6.9a}$$

and

$$\nabla\cdot\mathbf{j}_{p\lambda}(\mathbf{r})+\frac{e}{mc}\nabla\cdot[n_\lambda(\mathbf{r})\mathbf{A}(\mathbf{r})+n_\lambda(\mathbf{r})\mathbf{A}_{xc}(\mathbf{r})+n(\mathbf{r})\mathbf{A}_{xc\lambda}(\mathbf{r})] -\frac{2}{\hbar}[\mathbf{V}(\mathbf{r})\times\mathbf{n}(\mathbf{r})]_\lambda-\frac{2}{\hbar}[\mathbf{V}_{xc}(\mathbf{r})\times\mathbf{n}(\mathbf{r})]_\lambda-\frac{2e}{\hbar c}\sum_{\mu,\nu}\varepsilon_{\lambda\mu\nu}\mathbf{A}_{xc\mu}(\mathbf{r})\cdot\mathbf{j}_{p\nu}(\mathbf{r})=0 . \tag{6.9b}$$

The two sets of relations (6.8) and (6.9) are compatible if and only if

$$\nabla\cdot\left[n(\mathbf{r})\mathbf{A}_{xc}(\mathbf{r})+\sum_{\lambda=1}^{3}n_\lambda(\mathbf{r})\mathbf{A}_{xc\lambda}(\mathbf{r})\right]=0 \tag{6.10a}$$

and

$$\frac{e}{mc}\nabla\cdot[n_\lambda(\mathbf{r})\mathbf{A}_{xc}(\mathbf{r})+n(\mathbf{r})\mathbf{A}_{xc\lambda}(\mathbf{r})]-\frac{2}{\hbar}\sum_{\mu,\nu}\varepsilon_{\lambda\mu\nu}V^{xc}_{\mu}(\mathbf{r})n_\nu(\mathbf{r})-\frac{2e}{\hbar c}\sum_{\mu,\nu}\varepsilon_{\lambda\mu\nu}\mathbf{A}_{xc\mu}(\mathbf{r})\cdot\mathbf{j}_{p\nu}(\mathbf{r})=0 . \tag{6.10b}$$

These "compatibility relations" will now be shown to follow from the symmetry of the E_{xc} functional. For this, we note that, by a straightforward generalization of the arguments produced in Sec. IV, the E_{xc} functional, regarded now as functional of n, n_λ, $\mathbf{j}_p$, and $\mathbf{j}_{p_\lambda}$, must be invariant under a transformation of its arguments corresponding to the following transformation of the wave function:

$$\psi(\mathbf{r}_1,\ldots,\mathbf{r}_n;\sigma_1,\ldots,\sigma_N)\rightarrow\exp\left[i\frac{e}{\hbar c}\Lambda(r_1,\sigma_1)\right]\cdots\exp\left[i\frac{e}{\hbar c}\Lambda(r_N,\sigma_N)\right]\psi(\mathbf{r}_1,\ldots,\mathbf{r}_N;\sigma_1,\ldots,\sigma_N) , \tag{6.11}$$

where

$$\Lambda(\mathbf{r},\sigma)=\Lambda_0(\mathbf{r})+\boldsymbol{\Lambda}(\mathbf{r})\cdot\boldsymbol{\sigma} \tag{6.12}$$

is a matrix in spin space. The invariance group of the E_{xc} functional following from this transformation is easily obtained from the definitions (6.1) and (6.2). We find

$$E_{xc}[n',n'_\lambda,\mathbf{j}'_p,\mathbf{j}'_{p\lambda}]=E_{xc}[n,n_\lambda,\mathbf{j}_p,\mathbf{j}_{p\lambda}] , \tag{6.13}$$

where

$$\begin{aligned} n'&=n ,\\ n'_\lambda&=\sum_{\mu=1}^{3}R_{\lambda\mu}n_\mu,\quad \lambda=1,2,3\\ \mathbf{j}'_p&=\mathbf{j}_p+\frac{e}{mc}\left[n\nabla\Lambda_0+\sum_{\lambda=1}^{3}n_\lambda\nabla\Lambda_\lambda\right] ,\\ \mathbf{j}'_{p\lambda}&=\sum_{\mu=1}^{3}R_{\lambda\mu}\left[\mathbf{j}_{p\mu}+\frac{e}{mc}(n_\mu\nabla\Lambda_0+n\nabla\Lambda_\mu)\right] , \end{aligned} \tag{6.14}$$

$\lambda=1,2,3$.

$R_{\lambda\mu}$ is the matrix corresponding to a rotation by $2|\Lambda|e/\hbar c$ along the direction of Λ. Now to proceed as in Sec. IV, we should determine the functional form of E_{xc} which is equivalent to the symmetry relation (6.13), and prove that it implies the compatibility relations (6.10). Due to the complexity of the transformation group (6.14) this method is not used here. However, we can prove equations (6.10) by an alternative method which does not rely on the explicit form of the E_{xc} functional. We consider an *infinitesimal transformation* $\delta\Lambda_0+\delta\boldsymbol{\Lambda}\cdot\boldsymbol{\sigma}$, such that

$$\delta n_\lambda=\frac{2e}{\hbar c}\sum_{\mu,\nu}\varepsilon_{\lambda\mu\nu}n_\mu\delta\Lambda_\nu\ ,$$

$$\delta\mathbf{j}_p=\frac{e}{mc}\left[n\nabla\delta\Lambda_0+\sum_{\nu=1}^{3}n_\nu\nabla\delta\Lambda_\nu\right]\ , \tag{6.15}$$

$$\delta\mathbf{j}_{p\lambda}=\frac{2e}{\hbar c}\sum_{\mu,\nu}\varepsilon_{\lambda\mu\nu}\mathbf{j}_{p\mu}\delta\Lambda_\nu+\frac{e}{mc}(n\nabla\delta\Lambda_\lambda+n_\lambda\nabla\delta\Lambda_0)\ .$$

Then, from Eq. (6.13) it follows

$$\int d\mathbf{r}\left[\sum_{\lambda=1}^{3}\frac{\delta E_{xc}}{\delta n_\lambda(\mathbf{r})}\delta n_\lambda(\mathbf{r})+\frac{\delta E_{xc}}{\delta\mathbf{j}_p(\mathbf{r})}\cdot\delta\mathbf{j}_p(\mathbf{r})+\sum_{\lambda=1}^{3}\frac{\delta E_{xc}}{\delta\mathbf{j}_{p\lambda}(\mathbf{r})}\cdot\delta\mathbf{j}_{p\lambda}(\mathbf{r})\right]=0\ . \tag{6.16}$$

Inserting Eq. (6.15) in Eq. (6.16), using the definitions $\delta E_{xc}/\delta n_\lambda(\mathbf{r})=V_\lambda^{xc}(\mathbf{r})$, $\delta E_{xc}/\delta\mathbf{j}_p(\mathbf{r})=(e/c)\mathbf{A}^{xc}(\mathbf{r})$, etc., and integrating by parts wherever necessary, it is easily seen that Eq. (6.16) implies precisely the compatibility relations (6.10). This is a very important result. It tells us that the self-consistent-equation scheme for arbitrary directions of the magnetic field satisfies the continuity equation for the particle current and the modified continuity equation for the spin current, provided the exchange-correlation energy functional is invariant under the group of transformations specified in Eqs. (6.13) and (6.14). It may be hard, in practice, to find the most general form of E_{xc} which satisfies this invariance. An example of a functional which has this property is

$$E_{xc}[n,n_\lambda,\mathbf{j}_p,\mathbf{j}_{p\lambda}]=\bar{E}_{xc}\left[n_{\hat{\mathbf{s}}},n_{-\hat{\mathbf{s}}},\nabla\times\frac{\mathbf{j}_{p\hat{\mathbf{s}}}}{n_{\hat{\mathbf{s}}}},\nabla\times\frac{\mathbf{j}_{p-\hat{\mathbf{s}}}}{n_{-\hat{\mathbf{s}}}}\right]\ . \tag{6.17}$$

In this equation, $\hat{\mathbf{s}}$ denotes the direction of the local spin polarization, and the symbols are defined as follows:

$$|\mathbf{n}(\mathbf{r})|=\left[\sum_\lambda n_\lambda(\mathbf{r})^2\right]^{1/2}\ ,$$

$$n_{\pm\hat{\mathbf{s}}}(\mathbf{r})=n(\mathbf{r})\pm|\mathbf{n}(\mathbf{r})|\ ,$$

$$\mathbf{j}_{p\pm\hat{\mathbf{s}}}(\mathbf{r})=\mathbf{j}_p(\mathbf{r})\pm\mathbf{j}_{p\parallel}(\mathbf{r})\ ,$$

and the longitudinal (in spin-space) current $\mathbf{j}_{p\parallel}(\mathbf{r})$ is given by

$$\mathbf{j}_{p\parallel}(\mathbf{r})=\sum_{\lambda=1}^{3}\mathbf{j}_{p\lambda}(\mathbf{r})n_\lambda(\mathbf{r})/|\mathbf{n}(\mathbf{r})|\ .$$

Then, it is easily seen that $n(\mathbf{r})$ and $|\mathbf{n}(\mathbf{r})|$ are invariants of the group, while $\mathbf{j}_p(\mathbf{r})$ and $\mathbf{j}_{p\parallel}(\mathbf{r})$ transform according to

$$\mathbf{j}_p\rightarrow\mathbf{j}_p+\frac{e}{mc}(n\nabla\Lambda_0+|\mathbf{n}|\nabla\Lambda_\parallel)\ ,$$

$$\mathbf{j}_{p\parallel}\rightarrow\mathbf{j}_{p\parallel}+\frac{e}{mc}(n\nabla\Lambda_\parallel+|\mathbf{n}|\nabla\Lambda_0)\ .$$

From these equations it follows that all the arguments of $\bar{E}_{xc}$ in Eq. (6.17) are invariant under the group, and hence $\bar{E}_{xc}$ is invariant. This form of the functional is a natural generalization of the exact one derived in Sec. IV for a magnetic field of constant direction, and it is particularly suitable for the construction of a local-density approximation in $\nu_{\pm\hat{\mathbf{s}}}(\mathbf{r})$ of the type discussed in Sec. V. However, it is only approximate here, since, for instance, it does not include the contribution to E_{xc} of a twist in the relative orientation of the spin polarization at two different points.

As pointed out at the end of Sec. III, we could have saved much effort by choosing to work in a restricted formulation, where j_p rather than $(\mathbf{j}_p,\mathbf{j}_{p\lambda})$ is the basic variable, and there is only one vector potential. The resulting Schrödinger-type equation would be gauge invariant and satisfy the usual continuity equation, but the components of the spin current resulting from its solution would be entirely devoid of physical meaning.

B. Finite-temperature ensembles

Mermin's generalization[15] of DFT to finite temperature ensembles can be extended without difficulties to the present CSDFT. The one-particle equations retain their form [Eq. (3.9)] and the self-consistent expressions for the density and paramagnetic-current density become

$$n_\sigma(\mathbf{r})=\sum_i f(\varepsilon_i-\mu)|\psi_{i\sigma}(\mathbf{r})|^2\ ,$$

$$\mathbf{j}_{p\sigma}(\mathbf{r})=\sum_i f(\varepsilon_i-\mu)\{\psi_{i\sigma}^*(\mathbf{r})\nabla\psi_{i\sigma}(\mathbf{r})-[\nabla\psi_{i\sigma}^*(\mathbf{r})]\psi_{i\sigma}(\mathbf{r})\}\ , \tag{6.18}$$

where $f(\varepsilon_i-\mu)=\{1+\exp[(\varepsilon_i-\mu)/k_BT]\}^{-1}$ is the thermal occupation factor. The exchange-correlation energy functional is now replaced by the exchange-correlation contribution to the grand-canonical potential, but still it must depend on $\nabla\times(\mathbf{j}_{p\sigma}/n_\sigma)$. Thus, all the formal properties of $\mathbf{A}_{xc\sigma}$ and $V_{xc\sigma}$ are retained, and gauge invariance and continuity equations are assured.

C. Relativistic questions

Finally, we wish to make a few comments on the requirements for a relativistic extension of the theory. If we take this assignment seriously we must start with the Hamiltonian of *electrons and positrons* interacting with the electromagnetic field and subject to an additional static external field. The electromagnetic field must be treated classically, in order to prevent recombination of electrons and positrons into the true ground state of quantum electrodynamics, i.e., a vacuum. The electromagnetic interaction takes now a simple form

$$H_{\rm int}=e\int d\mathbf{r}\, j_\mu(\mathbf{r})A^\mu_{\rm ext}(\mathbf{r}) ,$$

where the fermion current, expressed in terms of Dirac four-component spinors is

$$\bar{\psi}(\mathbf{r})\gamma^\mu\psi(\mathbf{r}) .$$

The interaction does not contain the cumbersome A^2 term which was so problematic in the nonrelativistic formulation, and this is what makes the relativistic formulation so deceptively attractive. However, the price paid for this simplification is that one must now work with four-component spinors, i.e., electrons and positrons on the same footing. When the nonrelativistic limit is taken and the four-component Dirac spinors are folded back into two-component Pauli spinors (for example, by application of the Foldy-Wouthuysen transformation), the A^2 terms will reappear, and the relativistic current will go over to the nonrelativistic one. Since the external potential is kept fixed in the variational procedure, it is clear that the minimization will have to be with respect to $\mathbf{j}_p$. In other words, if the nonrelativistic limit is taken correctly the final Schrödinger-type equation and the form of the $E_{\rm xc}$ functional must reduce to what we have derived in this paper. It is then clear that in practice the CSDFT presented here is the only realistic single-particle-like theory for interacting-electron systems in strong magnetic fields.

VII. SUMMARY AND DISCUSSION

The CSDFT presented above is a rigorous formulation of a many-body problem of nonrelativistic interacting fermions in a gauge field. In addition to spin polarization, it includes for the first time the effect of orbital currents. A central result is the Schrödinger-type equation [Eq. (3.9)], showing that the replacement of the external vector potential by an effective one (including exchange-correlation effects) must be done in the linear term, but not in the quadratic one. Although at first sight this appears to violate gauge invariance and hence the continuity equation, a careful consideration of the transformation properties of $\mathbf{A}_{\rm xc}$ and $V_{\rm xc}$, based on the symmetry of $E_{\rm xc}$, reveals that there is no such violation.

We emphasize that the appearance of an exchange-correlation contribution to the vector potential has nothing to do with the fact that the circulating current generates, according to Maxwell equations, a "classical" contribution to the magnetic field. This effect is extremely small $[O(v_F^2/c^2)]$ and could be accounted for, if necessary, by replacing the external $\mathbf{A}(r)$ by the self-consistent potential

$$\mathbf{A}_{\rm sc}(\mathbf{r})=\mathbf{A}(\mathbf{r})+\frac{e}{c}\int\frac{\mathbf{j}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}' .$$

The origin of $\mathbf{A}_{\rm xc}(\mathbf{r})$, on the other hand, is purely quantum mechanical, and does not depend on the electron charge. It would also be present in a system of neutral particles (e.g., ^{3}He atoms) if the ground-state wave function carried a finite orbital current.

In Sec. V we have proposed a simple approximation for the exchange-correlation energy functional which is local in

$$\nu_\sigma(\mathbf{r})\equiv\nabla\times[\mathbf{j}_{p\sigma}(\mathbf{r})/n_\sigma(\mathbf{r})] ,$$

and does have the appropriate symmetry. The limits of validity of the approximation are specified as follows. (i) The current density should be slowly varying in space:

$$\frac{|\nabla\times\mathbf{j}_{p\sigma}(\mathbf{r})|}{|\mathbf{j}_{p\sigma}(\mathbf{r})|}\ll k_{F\sigma}(\mathbf{r}) ,$$

where $k_{F\sigma}(\mathbf{r})$ is the local Fermi momentum. (ii) The density should be high, (i.e., r_s should be small). (iii) The magnetic field should be "small" in the sense that $\hbar\omega_c(\mathbf{r})\ll E_F(\mathbf{r})$, where $\omega_c(\mathbf{r})=e\hbar B(\mathbf{r})/mc$ is the local cyclotron frequency and $E_F(\mathbf{r})$ is the local Fermi energy. Condition (ii) is needed to guarantee the applicability of the random-phase approximation to the uniform electron-gas model. Condition (iii) is very well satisfied in systems in which E_F is of the order of 1 eV, even if the magnetic field is as large as 10 T ($\hbar\omega_c\cong 1$ meV). These systems include the majority of three-dimensional metals and semiconductors. Our approximate form of the exchange-correlation energy functional does not include quantum oscillations. It can be viewed either as an average over the fast quantum oscillations, or as a form which is valid for temperatures $k_BT\gg\hbar\omega_c$ (but $k_BT\ll E_F$). In any case, the form is inappropriate for systems in which $\hbar\omega_c$ is comparable to E_F.

In order to derive a local form of the $E_{\rm xc}$ functional valid for strong magnetic fields, one will have the calculate the exchange-correlation energy of an electron gas in a uniform magnetic field such that only few (or even less than one) Landau levels are occupied. To the extent that the system is uniform $[n(\mathbf{r})=\text{const}]$ and the physical current vanishes $[\mathbf{j}(\mathbf{r})=\mathbf{0}]$, the combination $\nu(\mathbf{r})=\nabla\times[\mathbf{j}_p(\mathbf{r})/n(\mathbf{r})]$ coincides with the magnetic field and hence is constant. From the knowledge of $\varepsilon_{\rm xc}$ for uniform n and ν we can then derive a local-density approximation, letting $n\to n(\mathbf{r})$ and $\nu\to\nu(\mathbf{r})$. In other words, the results for $\varepsilon_{\rm xc}$ of a uniform electron gas in the integral, or fractional quantum-Hall-effect regime, constitute an input for the formulation of the LDA in our theory, in much the same way as $\varepsilon_{\rm xc}$ of a uniform electron gas is an input for the usual LDA.

We plan to exploit such results in various limits of magnetic field strength, in two and three dimensions, as a guide for more general forms of $E_{\rm xc}$.

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