because F_{12} is not the driving force on the fluxon in the primary.

IV. CONCLUSION

The coupling force for an isolated fluxon in a dual-film system [Eq. (20)] is not identical with the coupling force on a fluxon in a superconducting dc transformer. The force F_c is, however, responsible for the operation of the transformer and probably represents the maximum coupling which can exist in a transformer. In the transformer the fluxons are not isolated and overlap of their current and field distributions serves to decrease the coupling. The transformer coupling is destroyed by perpendicular magnetic fields close to the critical field which may be only about 10 G (10^{-3} T). When there is no applied magnetic field and when the thin-film approximation ($d < \lambda$) is valid Eq. (20) may represent the transformer coupling reasonably well. For type-I films such as tin, the approximations should be reasonably accurate for film thicknesses up to about 10^{-7} m (1000 Å) and somewhat better for alloy films.

The film-thickness dependence of the coupling force predicted by Eqs. (20) and (21) agrees qualitatively with experiment. With the secondary thickness fixed the transformer coupling parameter (the ratio of secondary voltage to primary voltage) decreases with decreasing primary film thickness.[4] Since the coupling parameter is not simply related to the coupling force it is impossible to make a quantitative comparison between the calculation and these experiments.

ACKNOWLEDGMENTS

I have profited by discussions with J. R. Manson, M. J. Skove, and other associates during the course of this work.

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PHYSICAL REVIEW B VOLUME 7, NUMBER 5 1 MARCH 1973

Inhomogeneous Electron Gas*

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(Received 17 May 1972)

This work is a generalization of the Hohenberg–Kohn–Sham theory of the inhomogeneous electron gas, with emphasis on spin effects. An argument based on quantum electrodynamics is used to express the ground-state energy of a system of interacting electrons as a functional of the current density. Expressions are derived for coefficients appearing in an expansion of the correlation functional in terms of the linear-response functions of the homogeneous system, for a gas of almost constant four-current density. The current density contains a spin-dependent term which leads, in the nonrelativistic limit, to a local potential which is also spin dependent. This potential is applied to the problems of spin splitting of energy bands in ferromagnets and spin-density-wave antiferromagnets. The relations between the present approach, that of Slater, and the collective electron theory of ferromagnetism of Stoner are described.

I. INTRODUCTION

Hohenberg and Kohn[1] (HK) and subsequently Kohn and Sham (KS)[2,3] developed a theory of the ground state of an interacting electron gas in the presence of an external potential $V(r)$. The essential concept of their treatment is that the energy is a universal functional of the density of the system $n(r)$ plus a linear functional of the potential $V(r)$. The functional of density $F[n]$ applies to all electronic systems in their ground state regardless of the specific form of the external potential $V(r)$.

The approach of HK does not include spin explicitly and therefore is not immediately useful in problems in which an external magnetic field is involved or in which magnetic order is present. This work presents a generalization of the treatment of

HK. We start from the equations of quantum electrodynamics for an electron field in interaction with an electromagnetic field. A formal expression is derived for the ground-state energy of a system of interacting electrons, which indicates this energy is a universal functional of the four-current density. In a nonrelativistic limit, this functional depends on the charge density $n(r)$, the spin density $\vec{s}(r)$, and the ordinary current density $\vec{j}(r)$ (Sec. II).[4] In Sec. III we extend the procedure of HK for a gas of almost constant four-current density and relate the linear-response functions of the homogeneous system to the coefficients appearing in an expansion of the functional in terms of the four-current densities.[5]

We consider in Sec. IV a situation in which the ordinary current can be neglected. A variational argument leads to a local spin-dependent effective potential, in accord with Stoddart and March.[6] The exchange potential for electrons of spin σ depends on the number density of electrons of spin σ, n_σ in the usual way: $\sim n_\sigma^{1/3}$, with a coefficient of proportionality which is two-thirds of the Slater value. Although this is not surprising, it fills a gap in the formal theory in that it shows that the $n_\sigma^{1/3}$ approach should also apply to spin splittings when the electron density is not rapidly varying. These results are applied to ferromagnetic systems and to spin-density-wave antiferromagnets.

It is a somewhat unexpected result of some recent band calculations for ferromagnetic nickel[7,8] that use of a local effective exchange potential proportional to $n_\sigma^{1/3}$ leads to values of the spin splitting, magneton number, and spin-wave effective mass that do not differ radically from corresponding results obtained from treatments of the electron interaction of this situation by more sophisticated methods.[9,10] We attempt an explanation of this situation in Sec. V by making an estimate of the spin splitting on the basis of the local effective potential and also by using a t-matrix approach applied to a many-band form of the Hubbard Hamiltonian. Although the results are not identical there is a substantial degree of agreement. Section VI contains a summary of the results.

II. GENERAL FORMULATION

Quantum electrodynamics (QED) furnishes a fundamental basis on which the quantum theory of a system of interacting electrons can be based. This point of view has been applied on occasion in atomic theory with the intent of studying relativistic effects and many-body potentials.[11] We are not aware of similar attempts in the theory of solids. It seems to us that the formalism of QED is particularly convenient for our present purpose because all the interaction between a charged particle and an electromagnetic field, which must be expressed in a relatively cumbersome manner in ordinary nonrelativistic quantum mechanics, is contained in a single simple term.

Our discussion will be based on the QED formalism as given by Schweber.[12] We consider a system of an arbitrary number of electrons in a large box under the influence of a four-vector potential $A_\mu(x) = [v(r, t), \vec{A}(r, t)]$. However, we are not significantly concerned with relativistic effects and will proceed to the nonrelativistic limit after the general principles have been described.

We begin with the Schrödinger equation for quantum electrodynamics in Fock space,

$$\left(it\frac{\partial}{\partial t} - H\right)|\Psi\rangle = 0. \tag{2.1}$$

The Hamiltonian used contains four parts:

$$H = H_0 + H_C + H_I + H_{\text{ext}} \ . \tag{2.2}$$

The operator H_0 describes noninteracting Dirac and electromagnetic fields

$$H_0 = H_{\text{em}} + \int d^3x\, \tilde{\psi}(x)\, h(x)\, \psi(x) \ , \tag{2.3}$$

in which H_{em} describes a free radiation field and $h(x)$ is the Dirac Hamiltonian for a single particle,

$$h(x) = (i\gamma^\mu \partial_\mu - m) \ .$$

We will use the radiation gauge so that a Coulomb interaction between electrons appears explicitly,

$$H_C = \tfrac{1}{2}\int d^3x\, d^3x'\, \tilde{\psi}(x)\gamma_0\psi(x) \times (e^2/|x - x'|)\tilde{\psi}(x')\gamma_0\psi(x') \ . \tag{2.4}$$

The interaction between matter and the tranverse portion of the radiation field is contained in H_I:

$$H_I = -\int j_\mu(x) A^\mu(x)\, d^3x. \tag{2.5}$$

Finally, H_{ext} describes the interaction of the electrons with an external nonquantized electromagnetic field A^μ_{ext}. It is convenient to include in A^μ_{ext} the Coulomb field produced by the nuclei of the system which, for our purposes, may be assumed to be fixed:

$$H_{\text{ext}} = -\int j_\mu(x) A^\mu_{\text{ext}}(x)\, d^3x \ . \tag{2.6}$$

Now let $|G\rangle$ be the actual ground state of the system of matter and electromagnetic fields. We define the current density in the ground state as

$$J_\mu(x) = \langle G|j_\mu(x)|G\rangle \ . \tag{2.7}$$

The expectation value is taken with respect to the Fock-space operators: The resulting $J_\mu(x)$ is an ordinary function of position. The four components of J_μ are not all independent, since the equation of continuity must be satisfied:

$$\partial_\mu J^\mu(x) = 0. \tag{2.8}$$

It is now possible to repeat the arguments of

Hohenberg and Kohn to show that the ground-state energy is a unique functional of $J_\mu(x)$. The proof is by *reductio ad absurdum*.

Suppose that there should exist another external potential A'^{μ}_{ext}, such that the ground state with this potential, $|G'\rangle$, gave rise to the same current density J_μ. The ground-state vectors $|G\rangle$ and $|G'\rangle$ must be different, since they satisfy different Schrödinger equations unless A^{μ}_{ext} and A'^{μ}_{ext} differ by a constant. The effect of a gauge transformation is discussed subsequently.

Let H, H', E, and E' be the Hamiltonians and energies pertaining to $|G\rangle$ and $|G'\rangle$, respectively. Then, according to the minimum property of the ground-state energy,

$$E' = \langle G'|H'|G'\rangle < \langle G|H'|G\rangle$$

$$= \langle G|H - \int d^3x j_\mu (A'^{\mu}_{\text{ext}} - A^{\mu}_{\text{ext}})|G\rangle \ . \qquad (2.9)$$

Since A^{μ}_{ext} is not quantized,

$$\langle G|\int d^3x j_\mu A^{\mu}_{\text{ext}}|G\rangle = \int J_\mu A^{\mu}_{\text{ext}} d^3x \ ,$$

and we have

$$E' < E - \int d^3x J_\mu (A'^{\mu}_{\text{ext}} - A^{\mu}_{\text{ext}}) \ . \qquad (2.10)$$

If we now assume that $J_\mu = \langle G'|j_\mu|G'\rangle$ also, we may simply repeat the argument leading to (2.10) with primed and unprimed quantities interchanged. Thus

$$E < E' - \int d^3x J_\mu (A^{\mu}_{\text{ext}} - A'^{\mu}_{\text{ext}}) \ . \qquad (2.11)$$

Addition of (2.10) and (2.11) leads to

$$E + E' < E' + E \ ,$$

which is a contradiction.

The argument indicates that A^{μ}_{ext} must be a unique functional of J_μ. But H is determined if A^{μ}_{ext} is given, and so the ground state must be a unique functional of J_μ, and we can write

$$E = E[J] \ . \qquad (2.12)$$

The preceding argument did not consider explicitly the possibility of a gauge transformation of A^{μ}_{ext}. In this case, one must obtain $E' = E$, since as a consequence of the equation of continuity, the interaction term in the Lagrangian from which (2.1) is derived as a specialization is unaltered.[13] We will henceforth discard this possibility, and consider such A's to be equivalent. Our detailed calculations will be performed in the radiation gauge.

It can now be established that $E[J]$ will possess a minimum for the correct $J^\mu(x)$ for fixed A^{μ}_{ext} if the admissible state vectors are restricted by the condition

$$\langle G|\int j^0(x) d^3x|G\rangle = \int J^0(x) d^3x = \text{const.} \qquad (2.13)$$

This equation is derived by integrating the equation of continuity (2.8) over a spacelike surface in the standard way that one derives the integral form of the transformation laws. Equation (2.13) is the familiar constraint on the total number of particles in the system.

It is convenient to define

$$F[J] = \langle G|H_0 + H_C + H_I|G\rangle \ , \qquad (2.14)$$

so that

$$E[J] = F[J] - \int J_\mu(x) A^{\mu}_{\text{ext}}(x) d^3x \ . \qquad (2.15)$$

Since E is a unique functional of J, it follows from (2.15) that F is also a unique functional of J. Again, let $|G'\rangle$ be the ground-state vector associated with a different external field A'^{μ}_{ext}. We construct the energy functional using this object (but using A, not A'):

$$E[G'] = F[J'] - \int J'_\mu(x) A^{\mu}_{\text{ext}} d^3x \ .$$

However, the energy is a minimum if $|G'\rangle = |G\rangle$. Thus

$$E[G'] > E[G] = F[J] - \int J_\mu(x) A^{\mu}_{\text{ext}} d^3x \ . \qquad (2.16)$$

Thus $E[J]$ is a minimum with respect to all current-density functionals associated with other possible external potentials A'^{μ}_{ext}, provided that such other current densities also satisfy the equation of continuity.

The physical content of the current operator can be made more explicit through the Gordon decomposition[14]

$$j^0 = -e\psi^\dagger\psi \ , \qquad (2.17a)$$

$$j^k = \frac{e}{2mi}\left(\tilde{\psi}\frac{\partial\psi}{\partial x_k} - \frac{\partial\tilde{\psi}}{\partial x_k}\psi\right) - \frac{e^2}{m}A^k\tilde{\psi}\psi$$

$$+ \frac{e}{2m}\epsilon^{kjl}\frac{\partial}{\partial x^j}(\tilde{\psi}\sigma^l\psi) - \frac{ie}{2m}\frac{\partial}{\partial t}(\tilde{\psi}\alpha^k\psi), \qquad (2.17b)$$

$$k = 1, 2, 3 \ .$$

Here ϵ^{kjl} is the Levi-Civita symbol $\epsilon^{123} = 1$, $\epsilon^{213} = -1$; a summation over repeated indices is understood.

We can now define the following functions:

$$n(x) = \langle G|\psi^\dagger(x)\psi(x)|G\rangle \ , \qquad (2.18a)$$

$$s^l(x) = \langle G|\tilde{\psi}(x)\sigma^l\psi(x)|G\rangle \ , \qquad (2.18b)$$

$$\mathcal{J}_l(x) = \frac{e}{2m}\langle G|\tilde{\psi}(x)(p_l - eA_l)\psi(x)$$

$$- (p_l + eA_l)\tilde{\psi}(x)\psi(x)|G\rangle \ , \qquad (2.18c)$$

$$g^l(x) = -\frac{ie}{2m}\langle G|\tilde{\psi}(x)\alpha^l\psi(x)|G\rangle \ . \qquad (2.18d)$$

The quantity n describes the electron density in the system, $s^l(x)$ represents the spin density, $\mathcal{J}_l(x)$ represents the combination of ordinary and (displacement) polarization currents, and g^l, which couples small and large components of the Dirac field, has no obvious nonrelativistic analog. The contribution to the interaction energy from the spin current can be transformed with the aid of Stokes's theorem,

$$\int \frac{e}{2m}\,\epsilon^{klj}\,\frac{\partial s^l}{\partial x^j}\,A_k(x)\,d^3x = -\frac{e}{2m}\int \vec{s}(x)\cdot\vec{B}(x)\,d^3x\ , \qquad (2.19)$$

in which $\vec{s}$ is the ordinary spin vector corresponding to s^l and $\vec{B}=\vec{\nabla}\times\vec{A}_{\rm ext}$. The ground-state energy of the system can be written by substituting Eqs. (2.17)–(2.19) into (2.15):

$$E=F[J]+\int d^3x\left(en(x)v(x)+\frac{e}{2m}\vec{s}(x)\cdot\vec{B}(x) + \frac{e}{2m}i\frac{\partial}{\partial t}\,\vec{g}\cdot\vec{A}-\vec{J}(x)\cdot\vec{A}(x)\right) \qquad (2.20)$$

This equation shows that when the energy is considered as a functional of the current density there are four contributions, independent except for the restriction imposed by Eq. (2.8). These involve the charge density, spin density, ordinary current, and polarization current. This result is a generalization of the expression of Kohn and Sham, who considered only the charge density. We note that it is possible now to invoke the variational argument of HK to show that the field components V, $\vec{B}$, and $\vec{A}$ are unique functions of n, $\vec{s}$, $\vec{g}$, and $\vec{J}$.

III. GAS OF ALMOST CONSTANT CURRENT DENSITY

We follow HK and separate out the classical self-energy of the Coulomb charge distribution from $F[J]$ in Eq. (2.15) in accord with Eq. (2.4):

$$F[J]=\tfrac{1}{2}e^2\int\int d^3r\,d^3r'\,\frac{n(r)n(r')}{|\vec{r}-\vec{r}'|}+G[J]\ . \qquad (3.1)$$

Following HK, we now consider a gas for which

$$J_\mu(r)=J_\mu^{(0)}+\tilde{J}_\mu(r)\ , \qquad (3.2)$$

where $J_\mu^{(0)}$ is independent of position. Further, let $J^2=J_\mu^{(0)}J^{(0)\mu}$ and $|\tilde{J}_\mu(r)|$ be slowly varying;

$$|J_\mu(r)/J|\ll 1 \qquad (3.3)$$

as well as

$$\int \tilde{J}_\mu(r)\,d^3r=0\ . \qquad (3.4)$$

Then a formal expansion exists:

$$G[J]=G[J^0]+\int\int d^3r\,d^3r'\,K^{\mu\nu}(r-r') \times\tilde{J}_\mu(r)\tilde{J}_\nu(r')+\cdots\ . \qquad (3.5)$$

No linear term appears in this equation as a result of (3.4) and the translation invariance of the constant current system. We will now relate the coefficient $K^{\mu\nu}(r-r')$ to the linear-response functions of the homogeneous system. In the limit considered by HK, the only nonvanishing element is K^{00}, which is the particle-density response function. The current density $J_\mu(r)$ in the above includes the spin current as in (2.17). So we write

$$E[J]=F[J]-\int d^3r\,J^\mu(r)a_\mu(r)\ . \qquad (3.6)$$

We now proceed exactly as in HK. The response of $J_\mu(r)$ to an *externally varying* $a^\mu(r)$ $(=A^\mu_{\rm ext})$ is calculated by the standard procedure and one obtains the result

$$\tilde{J}_\mu(r)=\int d^3r'\,\mathcal{K}_{\mu\nu}(rr')a^\nu(r')\ , \qquad (3.7)$$

where $\mathcal{K}_{\mu\nu}(rr')$ is the familiar static linear-response function. (See, for instance, Ref. 15, where all the spin-response functions, excluding orbit effects, are calculated.) If E_n are the eigenenergies associated with the Hamiltonian of the system in the absence of the external fields, then one has the familiar expression for the static response function,

$$\mathcal{K}_{\mu\nu}(rr')=-2\sum_n\frac{(0|j_\mu(r)|n)(n|j_\nu(r')|0)}{E_0-E_n}\ . \qquad (3.8)$$

In second-order perturbation theory, one then obtains

$$E[a]=E_0+\sum_n\int\int d^3r\,d^3r'\,\frac{(0|j_\mu(r)|n)(n|j_\nu(r')|0)}{E_0-E_n} \times a^\mu(r)a^\nu(r')$$

and hence

$$E[a]=E_0-\tfrac{1}{2}\int\int d^3r\,d^3r'\,\mathcal{K}_{\mu\nu}(rr')a^\mu(r)a^\nu(r') =E_0-\tfrac{1}{2}\int\int d^3r\,d^3r'\,[\mathcal{K}^{-1}(rr')]^{\mu\nu}\tilde{J}_\mu(r)\tilde{J}_\nu(r') \qquad (3.9)$$

after inverting (3.7).

On the other hand, one has, from (3.6), another expression for $E[a]$:

$$E[a]=E_0-\int d^3r\,\tilde{J}_\mu(r)a^\mu(r)+\tfrac{1}{2}\int\int d^3r\,d^3r'\,(e^2/|\vec{r}-\vec{r}'|)\tilde{J}_0(r)\tilde{J}_0(r')+\int\int d^3r\,d^3r'\,K^{\mu\nu}(r-r')\tilde{J}_\mu(r)\tilde{J}_\nu(r')\ .$$

Using (3.7) again, we obtain

$$E[a]=E_0+\int\int d^3r\,d^3r'\,(\tfrac{1}{2}e^2/|\vec{r}-\vec{r}'|)\tilde{J}_0(r)\tilde{J}_0(r')+\int\int d^3r\,d^3r'\,K^{\mu\nu}(\vec{r}-\vec{r}')\tilde{J}_\mu(r)\tilde{J}_\nu(r')-\int\int d^3r\,d^3r'$$

$$\times[\mathcal{K}^{-1}(rr')]^{\mu\nu}\tilde{J}_\mu(r)\tilde{J}_\nu(r') \ . \quad (3.10)$$

Comparing (3.9) and (3.10) one obtains

$$K^{\mu\nu}(\vec{r}-\vec{r}')+\tfrac{1}{2}(e^2/|\vec{r}-\vec{r}'|)\delta_{\mu 0}\delta_{\nu 0}=\tfrac{1}{2}[\mathcal{K}^{-1}(rr')]^{\mu\nu} \ . \quad (3.11)$$

Thus the coefficient $K^{\mu\nu}$ in the functional expansion (3.5) is related to the corresponding element of the inverse matrix of the linear-response function $\mathcal{K}$. For the special case considered by HK, one has (in momentum space and in the nonrelativistic limit)

$$K_{00}(q)=\tfrac{1}{2}[\mathcal{K}_{00}^{-1}(q)-v(q)] \ ,$$

but $K_{00}(q)=[1/v(q)]\,[1-1/\epsilon(q)]$, where $\epsilon(q)$ is the usual dielectric function of the uniform system. Thus we obtain

$$K_{00}(q)=\tfrac{1}{2}v(q)[\epsilon(q)-1]^{-1},$$

in agreement with the result of HK.

When the orbital effects are neglected, one has only spin densities and, in fact, the $\mathcal{K}_{\mu\nu}$ then becomes just the various spin-correlation functions. Using the result of Ref. 15, one then obtains $K_{\mu\nu}$ derived by Pant and Rajagopal.[5] We may point out that the correlation functions $\mathcal{K}_{\mu\nu}$ of the uniform system are related to suitable vertex functions (Ref. 15) which in turn obey complicated integral equations. In effect, one can thus incorporate the effects of interaction in the uniform system as well as one could as, for instance, the variational solutions of the vertex equation (Ref. 16), and thus compute $\mathcal{K}_{\mu\nu}$ quite accurately.

IV. LOCAL EFFECTIVE POTENTIAL

Our further considerations will be based on the nonrelativistic limit of (2.20). It is clear that $\partial g/\partial t$ will be zero since the ground state is stationary. Further, we will ignore the ordinary current $\vec{j}(x)$ and thus discard diamagnetic effects. Our object is to study the spin dependence of the local effective potential. For this purpose, only the first two terms in (2.17) need be retained. All quantities are assumed to be independent of time. (See, however, Sec. III.)

It is desirable to extract from G the kinetic energy $T[J]$ of a system of noninteracting electrons. The remainder of G will be conventionally referred to as the exchange and correlation functional $E_{ex}(J)$:

$$G[J]=T[J]+E_{ex}[J]=T[n,\vec{s}]+E_{ex}[n,\vec{s}] \ . \quad (4.1)$$

We thus have for the total energy

$$E=T[n,\vec{s}]+\tfrac{1}{2}e^2\int\int d^3r\,d^3r'\,[n(r)n(r')/|\vec{r}-\vec{r}'|]$$
$$+e\int d^3r\,n(r)V(r)+(e/2m)\int\vec{s}(r)\cdot\vec{B}(r)d^3r$$
$$+E_{ex}[n,\vec{s}] \ . \quad (4.2)$$

In this expression we have dropped contributions from the transverse currents, since we are not interested in relativistic effect. The expressions (2.18a) and (2.18b) can be rewritten in terms of one-particle wave functions if we introduce a complete set of one-particle states in Fock space:

$$n(r)=\sum_{i\sigma}^{\text{occ}}\psi^*_{i\sigma}(r)\psi_{i\sigma}(r) \ ,$$
$$\vec{s}(r)=\sum_{i\sigma\sigma'}^{\text{occ}}\psi^*_{i\sigma}(r)\vec{\tau}_{\sigma\sigma'}\psi_{i\sigma'}(r) \ , \quad (4.3)$$

where $\vec{\tau}$ is the Pauli spinor.

We then use the variational principle on the density functional to derive the equations for these wave functions. (The density variation is equally achieved by varying the one-particle wave function.) Thus, the wave function $\psi_{\sigma i}(r)$ obeys the equation

$$\left(-\frac{\nabla^2}{2m}+V(r)+e^2\int\frac{n(\mathbf{r}')}{|\vec{r}-\vec{r}'|}\,d^3r'\right)\psi_{\sigma i}(r)+\mu_{ex\,\sigma,\sigma}[n(r),\vec{s}(r)]\psi_{\sigma i}(r)+\mu_{ex\,\sigma,-\sigma}[n(r),\vec{s}(r)]\psi_{-\sigma i}(r)=\epsilon_i\psi_{\sigma i}(r),$$
$$\sigma=\uparrow,\downarrow \quad (4.4)$$

where

$$\mu_{ex\,\sigma,\sigma}[n(r),\vec{s}(r)]=\frac{\delta E_{ex}[n,\vec{s}]}{\delta n_\sigma(r)} \ ,$$
$$\mu_{ex\,\sigma,-\sigma}[n(r),\vec{s}(r)]=\frac{\delta E_{ex}[n,\vec{s}]}{\delta\rho_{\sigma,-\sigma}(r)} \quad \text{for } \sigma=\uparrow,\ \sigma=\downarrow; \quad (4.5)$$

$\rho_{\sigma,-\sigma}(r)$ here means s_+, s_-, the spherical transverse components of $\vec{s}(r)$. This generalizes the equation derived by Kohn and Sham.[2,3]

A. Ferromagnetic System

From Refs. 15–17 we have for the Coulomb gas the result, neglecting correlation contributions,

$$E_{ex}[n, \vec{s}] \equiv E_{ex}[n_\uparrow, n_\downarrow] = -\tfrac{3}{4}(e^2/\pi)\int d^3r\{n_\uparrow(r)[6\pi^2 n_\uparrow(r)]^{1/3} + n_\downarrow(r)[6\pi^2 n_\downarrow(r)]^{1/3}\} . \quad (4.6)$$

Here the magnetization is specified as $\vec{s} = (0, 0, s_z)$, where $s_z(r) = n_\uparrow(r) - n_\downarrow(r)$ and $n(r) = n_\uparrow(r) + n_\downarrow(r)$. Then the wave functions for the $\uparrow$, $\downarrow$ spins are, from (4.5), (4.6), and (4.4),

$$\left(-\frac{1}{2m}\nabla^2 + V(r) + e^2\int d^3r' \frac{n(r')}{|\vec{r}-\vec{r}'|} - \frac{e^2}{\pi}[6\pi^2 n_\uparrow(r)]^{1/3}\right)\psi_{\uparrow i}(r) = \epsilon_i \psi_{\uparrow i}(r) , \quad (4.7a)$$

$$\left(-\frac{1}{2m}\nabla^2 + V(r) + e^2\int d^3r' \frac{n(r')}{|\vec{r}-\vec{r}'|} - \frac{e^2}{\pi}[6\pi^2 n_\downarrow(r)]^{1/3}\right)\psi_{\downarrow i}(r) = \epsilon_i \psi_{\downarrow i}(r) , \quad (4.7b)$$

$$n_{\uparrow,\downarrow}(r) = \sum_i^{occ} |\psi_{\uparrow,\downarrow i}(r)|^2 . \quad (4.8)$$

In the paramagnetic limit, $n_\uparrow = n_\downarrow = \frac{1}{2}n$ and the distinction between $\uparrow$, $\downarrow$ disappears.

We may caution the reader at this stage that, apart from the assumption of slow spatial variation, the result (4.6) yields in the uniform case only either the fully saturated or the paramagnetic phase and so (4.7a) and (4.7b) may not perhaps be meaningful for application to the case of unsaturated ferromagnets. Equations (4.7a) and (4.7b) have, however, frequently been used in the literature in constructing the band structure of metals. To rectify this situation, one could perhaps argue that the Coulomb potential is always screened by the electron motions and one should use an expression more like that given in Stoner's theory in place of (4.6). If this is done, we have[15]

$$E_{ex}[n, \vec{s}] = -\tfrac{1}{2}\bar{V}\int d^3r\,[n_\uparrow^2(r) + n_\downarrow^2(r)] , \quad (4.9)$$

where $\bar{V}$ is a strength parameter either assumed, given experimentally, or related to the T matrix.[18] It is related to the Stoner parameter (Ref. 15) via the relationship

$$m\bar{V}k_F/3\pi^2 = K\theta'/\epsilon_F . \quad (4.10)$$

In (4.7a) and (4.7b) one must replace

$$-(e^2/\pi)[6\pi^2 n_\uparrow(r)]^{1/3}, \quad -(e^2/\pi)[6\pi^2 n_\downarrow(r)]^{1/3} ,$$

respectively, by

$$-\bar{V}n_\uparrow(r), \quad -\bar{V}n_\downarrow(r) . \quad (4.11)$$

In this manner one would at least have applied the principle of HK properly. One could make more sophisticated models by using a Yukawa interaction instead of the Coulomb repulsion (Ref. 15) but this, while retaining the structure of (4.7a) and (4.7b), in fact makes their appearance more complex.

As with Kohn–Sham,[2] the analog of the usual Hartree–Fock theory can be set up. This turns out to yield the equations [compare (4.4) and (4.5) with the foregoing equations]

$$\left(-\frac{1}{2m}\nabla^2 + V(r) + e^2\int \frac{n(r')}{|\vec{r}-\vec{r}'|}\,d^3r'\right)\psi_{\sigma i}(r) - e^2\int \frac{\rho_{\sigma\sigma}(r, r')}{|\vec{r}-\vec{r}'|}\,\psi_{\sigma i}(r')\,d^3r' - e^2\int \frac{\rho_{\sigma-\sigma}(r, r')}{|\vec{r}-\vec{r}'|}\,\psi_{-\sigma i}(r')\,d^3r' = \epsilon_i\psi_{\sigma i}(r) ,$$

$$\sigma = \uparrow, \downarrow . \quad (4.12)$$

Here

$$\rho_{\sigma\sigma'}(r, r') = \sum_j^{occ} \psi_{\sigma j}(r)\psi^*_{\sigma', j}(r'), \quad \sigma, \sigma' = \uparrow, \downarrow \quad (4.13)$$

are the usual density matrices and

$$\rho_{\uparrow\uparrow}(r, r) = n_\uparrow(r) , \quad \rho_{\uparrow\downarrow}(r, r) = s_+(r),$$

etc.

In the ferromagnetic case then, the KS procedure is simply to replace the local operators in (4.7a) and (4.7b) by the nonlocal operator in (4.12) but with $\rho_{\uparrow\downarrow}$ and $\rho_{\downarrow\uparrow}$ set equal to zero. The nonlocal forms (4.12) will now be employed to set up the "local potentials" for the spin-density-wave (SDW) case.

B. SDW System

For systems such as chromium, it seems fairly well established that the ground state is a spiral-spin-density-wave state of Overhauser. Since no closed expression can be written down even for the uniform system, it seems $E_{ex}[n, s]$ cannot be put in a neat form. From the work of Ref. 17, however, one may suggest the following replacements:

$$-e^2\int \frac{\rho_{\sigma\sigma}(rr')}{|\vec{r}-\vec{r}'|}\,\psi_{\sigma i}(r')\,d^3r' \to -\frac{e^2}{\pi}[3\pi^2 n(r)]^{1/3}\psi_{\sigma i}(r) ,$$

$$-e^2\int \frac{\rho_{\sigma-\sigma}(\mathbf{r}\mathbf{r}')}{|\vec{\mathbf{r}}-\vec{\mathbf{r}}'|}\psi_{-\sigma i}(\mathbf{r}')d^3\mathbf{r}' \rightarrow -\frac{e^2}{\pi}[6\pi^2 s_{\sigma-\sigma}(\mathbf{r})]^{1/3}\psi_{-\sigma i}(\mathbf{r}). \tag{4.14}$$

This has the feature that $s_{\uparrow\downarrow} \rightarrow 0$ leads to the correct paramagnetic system and connects the ↑, ↓ spins. One then finds

$$s_{\sigma-\sigma}(\mathbf{r}) = \sum_j^{\text{occ}} \psi_{\sigma j}(\mathbf{r})\,\psi^*_{-\sigma j}(\mathbf{r}) = e^{-i\vec{\mathbf{Q}}\cdot\vec{\mathbf{r}}}\,\tilde{s}_{\sigma-\sigma}(\mathbf{r})$$

and

$$s_{-\sigma\sigma}(\mathbf{r}) = e^{i\vec{\mathbf{Q}}\cdot\vec{\mathbf{r}}}\,\tilde{s}^*_{\sigma-\sigma}(\mathbf{r}),$$

where Q is the pitch of the spin spiral. This corresponds to E_{ex}:

$$\begin{aligned} E_{\text{ex}}[n,\vec{s}\,] = &-\tfrac{3}{4}(e^2/\pi)\int d^3\mathbf{r}\, n(\mathbf{r})[6\pi^2 n(\mathbf{r})]^{1/3} \\ &-\tfrac{3}{4}(e^2/\pi)\int d^3\mathbf{r}\{s_{\uparrow\downarrow}(\mathbf{r})[6\pi^2 s_{\uparrow\downarrow}(\mathbf{r})]^{1/3} \\ &+ s_{\downarrow\uparrow}(\mathbf{r})[6\pi^2 s_{\downarrow\uparrow}(\mathbf{r})]^{1/3}\}. \end{aligned} \tag{4.15}$$

Equations (4.14) in (4.12a) and (4.12b) would then be the local equations for determining the band structure of chromium.

V. SPIN SPLITTING OF ENERGY BANDS IN FERROMAGNETS

The insensitivity of the ferromagnetic splitting of the one-electron energies will now be shown by an explicit calculation. This is actually another aspect of the cancellation of the vertex corrections and the one-particle renormalizations since the criterion of the ferromagnetic state may be thought of as the instability of the static-long-wavelength paramagnetic susceptibility.[15,16] The latter involves only quantities evaluated at the Fermi surface. The point to note is that $n_\sigma(\mathbf{r})$ does not differ greatly from $\frac{1}{2}n(\mathbf{r})$ in actual practice. It is then legitimate to write

$$n_\sigma(\mathbf{r}) = \tfrac{1}{2}n(\mathbf{r}) + \delta n_\sigma(\mathbf{r}). \tag{5.1}$$

All the relevant quantities may be expanded to leading order in $\delta n_\sigma(\mathbf{r})$; $n(\mathbf{r})$ here is the number density. In the Stoner model, the one-electron potential is

$$V_\sigma^{\text{Stoner}}(\mathbf{r}) = -\bar{V}n_\sigma(\mathbf{r}) = -\tfrac{1}{2}\bar{V}n(\mathbf{r}) - \bar{V}\delta n_\sigma(\mathbf{r}). \tag{5.2}$$

From Ref. 15, $\bar{V}$ can be related to the parameters of a highly screened Coulomb gas:

$$\bar{V} = 4\pi e^2/\xi^2 k_F^2$$

and

$$\xi^2 = 4\alpha r_s/\pi \tag{5.3}$$

in the Thomas–Fermi scheme; αr_s and k_F have their usual significance. The Stoner parameter introduced in (4.10) then has the form

$$\frac{K\theta'}{\epsilon_F} = \frac{4}{3}\frac{\alpha r_s}{\xi^2}. \tag{5.4}$$

Hence the energy splitting of the ↑, ↓ spin bands in this theory is

$$\delta V_\sigma^{\text{Stoner}}(\mathbf{r}) = -\frac{2}{3\pi}\,e^2 k_F\left(\frac{2}{\xi^2}\right)\left(\frac{\delta n_\sigma(\mathbf{r})}{n(\mathbf{r})}\right). \tag{5.5}$$

The corresponding result for the Coulomb system obtained from (4.7a) and (4.7b) will now be obtained. We will call the local potential in this scheme the "Slater" potential:

$$V_\sigma^{\text{Slater}}(\mathbf{r}) = \lambda(e^2/\pi)[6\pi^2 n_\sigma(\mathbf{r})]^{1/3}, \tag{5.6}$$

where $\lambda = \frac{2}{3}$ for the Kohn–Sham-like theory derived above and $\lambda = 1$ for the Slater theory. So,

$$V_\sigma^{\text{Slater}}(\mathbf{r}) = -\frac{\lambda e^2 k_F}{\pi} - \lambda\frac{2}{3}\frac{e^2 k_F}{\pi}\left(\frac{\delta n_\sigma(\mathbf{r})}{n(\mathbf{r})}\right), \tag{5.7}$$

where we have employed the relation that $n(\mathbf{r}) = k_F^3/3\pi^2$ and (5.1) for $n_\sigma(\mathbf{r})$, and expanded (5.6) to leading order in $\delta n_\sigma(\mathbf{r})$. Incidentally, the KS theory gives better results—magneton number and the like—for nickel. Thus,

$$\delta V_\sigma^{\text{Slater}}(\mathbf{r}) = -\frac{2}{3\pi}\,e^2 k_F\lambda\left(\frac{\delta n_\sigma(\mathbf{r})}{n(\mathbf{r})}\right). \tag{5.8}$$

Comparison of (5.5) and (5.8) yields that δV_σ will be of the same order if $\lambda \simeq 2/\xi^2$, and in practice λ lies between 1 and $\frac{2}{3}$ corresponding to $r_s \approx 2$ or so, a density range quite close to that found in transition metals. The argument then is that the splitting potential is of the form

$$\delta V_\sigma(\mathbf{r}) \simeq A\,\frac{\delta n_\sigma(\mathbf{r})}{n(\mathbf{r})}. \tag{5.9}$$

The constant A does not vary greatly between different theories. This demonstrates in a succinct way the insensitivity of $\delta V_\sigma(\mathbf{r})$ to the nature of approximations made in the literature in computing it.

VI. SUMMARY

The arguments based on quantum electrodynamics are used to generalize the Hohenberg–Kohn–Sham theory of the inhomogeneous electron gas for the purpose of incorporating spin effects. It is shown that, for a fixed external vector potential, the ground-state energy is a unique functional of the four-current density provided that the current density obeys the equation of continuity. From this, we pass on to the nonrelativistic limit using the Gordon decomposition and derive the corresponding energy functional. This enables us to set up local equations for the spin functions in a magnetic system. Applications of this to ferromagnetic and SDW antiferromagnetic systems are given.

Note added in proof. Recently Booth and Hedin [J. Phys. C 5, 1629 (1972)] have also developed local exchange and correlation potentials for spin-polarized systems in the same spirit as in Sec. IV of the present paper.

*Supported in part by the U. S. Air Force Office of Scientific Research under Grant No. AFOSR 71-2020.

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