Broken-symmetry-adapted Green function theory of condensed matter systems: Towards a vector spin-density-functional theory

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The group-theory framework developed by Fukutome for a systematic analysis of the various broken-symmetry types of Hartree-Fock solution exhibiting spin structures is here extended to the general many-body context using spinor Green function formalism for describing magnetic systems. Consequences of this theory are discussed for examining the magnetism of itinerant electrons in nanometric systems of current interest as well as bulk systems where a vector spin-density form is required, by specializing our work to spin-density-functional formalism. We also formulate the linear-response theory for such a system and compare and contrast our results with the recent results obtained for localized electron systems. The various phenomenological treatments of itinerant magnetic systems are here unified in this group-theoretical description. We apply this theory to the one-band Hubbard model to illustrate the usefulness of this approach.

I. INTRODUCTION

Irreducible representations of the symmetry group of a system that classify the eigenstates of its Hamiltonian have been discussed before.[1] However, many important physical phenomena such as superconductivity and many types of magnetic states of condensed matter display lower-symmetry characteristics, and are thus broken-symmetry states of the Hamiltonian.[1] These phenomena have been theoretically understood in terms of approximate solutions that break the full symmetry of the Schrödinger equation of the many-body system. For example, the celebrated Hartree-Fock(-Bogoliubov) self-consistent-field method has been used in this way. A clear description of this approach may be found in Ref. 1, where an enumeration of the various commonly found basic symmetries is also given. Fukutome[2] and his co-workers, based only on symmetry arguments, systematized the search for possible novel states of the system, which in the past depended on intuitive suggestions (viz., Bardeen, Overhauser, and Landau, for example). These authors developed a complete group-theoretical classification and characterization of all the possible magnetic symmetry structures arising from only the underlying symmetry group consisting of spin rotation (S), time-reversal (T), and spatial symmetry group (P) and its subgroups, within the Hartree-Fock (HF) approximation. Fukutome found that there are only eight subgroups of the symmetry group $S\times T$ consisting of spin rotations and time reversal. The Hamiltonian of the well-known electron gas, which is an important ingredient in the density-functional method, is invariant under $S\times T$. It is common knowledge that the electron gas exhibits several states of magnetic order when treated in HF and related mean-field approximations.[3] The eight different structures found correspond to those belonging to the eight subgroups. When the spatial symmetry group is combined with these, one gets many more varieties of structure. This theory has been more recently extended to include mean-field-type analysis of Hubbard-type models of one- and two-dimensional systems of great current interest.[4] In recent years, the spin-density-functional method[5] has become the method of choice, replacing the Hartree-Fock method both because it includes the important correlation effects not included in the HF scheme in describing the theory of magnetic systems and because of the present much improved computing techniques. There has been a suggestion to incorporate the Fukutome classification in the spin-density-functional formalism.[6] The Green function method for describing many-body systems is more general than the above schemes and broken-symmetry solutions can be incorporated in this framework as noted already in Ref. 1. A generalized version of the density-functional method that includes spin as well has been reformulated in the Green function language.[7] The various broken-symmetry states of the HF scheme will be more generally expressed here in terms of the symmetry of the Green function under the appropriate subgroups, for which we use the nomenclature ''broken-symmetry-adapted Green functions.'' The purpose of this paper is twofold; one, to incorporate the Fukutome classification into the Green function framework and, two, to focus attention on magnetic systems in general, by applying this formalism to the spin-density-functional method with an emphasis on the currently interesting findings of magnetic states in nanometric systems.[8] By this extension, we also provide a more complete vector spin-density-functional (VSDF) theory of magnetic systems, which goes beyond the currently used schemes for handling noncollinear magnetic materials.[9,10] The recent theoretical work on the magnetism of free atomic clusters exhibiting interesting geometric structures accompanying very large magnetic moments[11] provides another class of problem in magnetism requiring further investigation, particularly if the suggestion is true that these clusters can be formed on semiconductor interfaces.[12] In this case the possibilities of variety of geometric structures of cluster formation, each with its own magnetic features in

relation to the substrate, would provide some challenge in determining the appropriate broken-symmetry states of magnetism. The group-theoretical enumeration would make this search systematic and orderly.

In Sec. II, we first give a brief description of the magnetic system in terms of the spinor Green function[13] and the associated spinor self-energy operator.[14] We then develop the Fukutome classification of magnetic systems associated with this spinor Green function and the related spinor self-energy (or mass) operator, which is more general than the effective self-consistent potential of the HF theory. In Sec. III, the linear-response functions arising out of these Green functions[15] are examined to establish the stability aspects of the broken-symmetry structures. This approach will be shown to be related to the recent work of Ref. 16. In Sec. IV, the implications of the above developments for VSDF theory are spelled out. This is complementary to the work in Ref. 17. Section V, is a summary with concluding remarks in relation to the proposed work on magnetism of nanostructure systems, including magnetic atomic clusters.

II. BROKEN-SYMMETRY-ADAPTED GREEN FUNCTIONS: THE FUKUTOME CLASSIFICATION IN MAGNETIC SYSTEMS

A. Hamiltonian

A general spin-polarized system without spin-orbit interaction (for simplicity of presentation at this juncture) is described by the standard system Hamiltonian

$$H = T_e + V_{ii} + V_{ie} + V_{ee}. \tag{1}$$

Here, T_e is the kinetic energy operator of the electrons and V_{ii}, V_{ie}, and V_{ee} are operators representing the Coulomb interactions between the ions (i) and the electrons (e). We introduce $\psi_s(\mathbf{r})$, the usual field operator annihilating an electron of spin s at position $\mathbf{r}$, and $\psi_s^\dagger(\mathbf{r})$, the corresponding creation operator. Then we have the definitions of electron-density operator,

$$\hat{n}(\mathbf{r}) = \hat{s}_0(\mathbf{r}) = \sum_s \psi_s^\dagger(\mathbf{r})\psi_s(\mathbf{r}), \tag{2}$$

and vector spin-density operator,

$$\hat{\mathbf{s}} = \sum_{s,s'} \boldsymbol{\tau}_{ss'} \psi_{s'}^\dagger(\mathbf{r})\psi_s(\mathbf{r}), \tag{3}$$

where the Pauli spin matrix vector is $\boldsymbol{\tau}$. It is useful to consider the system as being subjected to an external, spin-dependent field described by

$$V_{\text{ext}} = \sum_{s,s'} \int d\mathbf{r}\, w_{ss'}(\mathbf{r}t)\psi_s^\dagger(\mathbf{r})\psi_{s'}(\mathbf{r}). \tag{4}$$

In the following we split $w_{ss'}$ into a scalar part $w_n \equiv f^0$, which acts on the electron density given by Eq. (2) and a traceless part w_S expressed in terms of the Pauli matrices, which acts on the spin density Eq. (3):

$$W_S(\mathbf{r}t) = \boldsymbol{\tau}\cdot\mathbf{f}(\mathbf{r}t). \tag{5}$$

We thus rewrite Eq. (4) in a physically transparent form,

$$V_{\text{ext}} = \int d\mathbf{r}[\hat{n}(\mathbf{r})w_n(\mathbf{r}t) + \hat{\mathbf{s}}(\mathbf{r})\cdot\mathbf{f}(\mathbf{r}t)]$$
$$= \sum_\alpha \int d\mathbf{r}\, \hat{s}_\alpha(\mathbf{r}) f^\alpha(\mathbf{r}t), \tag{6}$$

where we have introduced the four-vector notation

$$(f^\alpha) \equiv (w_n, \mathbf{f}), \quad (\tau_\alpha) \equiv (1, \boldsymbol{\tau}),$$

$$\hat{s}_\alpha(\mathbf{r}) \equiv \sum_{s,s'} \tau_{\alpha,ss'} \psi_{s'}^\dagger(\mathbf{r})\psi_s(\mathbf{r}). \tag{7}$$

In the above, greek indices run from 0 to 3. The Hamiltonian (1) is invariant under all spin rotations S and time reversal T.

B. Spinor Green function and spinor self-energy

The one-particle Green's function is written as a matrix in spin indices,[13]

$$G_{ss'}(\mathbf{r}t;\mathbf{r}'t') = -i\langle T(\psi_s(\mathbf{r}t)\psi_{s'}^\dagger(\mathbf{r}'t'))\rangle. \tag{8}$$

The equation of motion satisfied by this spinor Green function is often written in its most general form as

$$\left[i\frac{\partial}{\partial t_1} + \frac{\boldsymbol{\nabla}_1^2}{2m} - V_C(1) - w(1) \right] G(12)$$
$$- \int d(3)\Sigma(13)G(32) = \delta(12). \tag{9}$$

Here the spin-independent classical Coulomb potential V_C arising from the electron density $n(1) = \langle \hat{n}(1)\rangle = -i\,\mathrm{Tr}\,G(11^+)$ and the nuclei (V_{ion}) is given by

$$V_C(1) = \int (d2)v(12)n(2) + V_{\text{ion}}(1), \tag{10}$$

where the instantaneous Coulomb interaction between electrons is $v(12) = (1/|\mathbf{r}_1 - \mathbf{r}_2|)\delta(t_1 - t_2)$. Also, Tr stands for the trace over spin indices only. $w(1) = w_n(1) + \boldsymbol{\tau}\cdot\mathbf{f}(1)$ is the spinor representation of the external field. We have used 1 here to stand for the space-time point $(\mathbf{r}_1, t_1)$ and the other notations are standard usage, as in Ref. 13, for example. The last term on the left-hand side of Eq. (9) is the contribution due to interparticle interaction in its most general form, and we call it the ''exchange-correlation spinor self-energy'' contribution, in anticipation of later application to functional formalism. The general expression for this spinor self-energy matrix Σ is in general a functional of the spinor Green function G, and is given by

$$\Sigma(12) = i\int d(3) \int d(4) G(13)\Lambda_n(32;4)W(41), \tag{11}$$

where

$$\Lambda_n(12;3) = -\frac{\delta G^{-1}(12)}{\delta V_{\text{tot}}(3)} \tag{12}$$

is the screened charge-response vertex function, with $V_{\rm tot}=V_C+w_n$. W is the Coulomb interaction $v(12)$, screened by the dielectric function ϵ, both of which are spin scalars, defined by

$$\epsilon^{-1}(12)=\frac{\delta V_{\rm tot}(1)}{\delta w_n(2)}, \tag{13}$$

$$W(12)=\int d(3)\epsilon^{-1}(13)v(32). \tag{14}$$

Finally we write the Dyson equation (9) in the familiar form

$$G^{-1}(12)=\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}-V_C(1)-w(1)\right]\delta(12)-\Sigma(12)$$
$$\equiv G_0^{-1}-\Sigma. \tag{15}$$

In the usual HF approximation, Σ is the familiar unscreened exchange self-energy if we do not include the screening by the dielectric function of the medium: $\Sigma(12)\approx\Sigma_{\rm HF}(12)=iv(12)G_{\rm HF}(12)$. This exhibits the explicit dependence of the self-energy on the Green function and hence the self-consistency feature of Eq. (15). In Ref. 13, the spinor structure of G was used to construct a self-consistent solution to the general HF approximation in the Green function language, from which the general Overhauser spiral spin-density-wave solution was deduced. It was then recognized as a ''broken-symmetry'' solution of the HF equation because this solution breaks the spin-rotation and time-reversal symmetries of the interacting electron gas Hamiltonian. We should also point out that in constructing any approximation scheme for the self-energy Σ it is useful to have certain conservation principles as well as variational character. Baym[14] set up such a conserving scheme by introducing a functional $\Phi[G]$ whose first variational derivative with respect to G yields the exact Σ and constructed an expression for the grand potential

$$\Omega[G]=\mathrm{Tr\,tr}\{\ln(-G)\}-\mathrm{Tr\,tr}\,\Sigma G+\Phi[G] \tag{16}$$

that is stationary with respect to variations in G. Thus,

$$V_C+\Sigma=\frac{\delta\Phi}{\delta G}, \tag{17}$$

and the grand potential is constructed with $\Phi[G]$ as the building block such that it is stationary for variations of the spinor G that satisfies the exact matrix Dyson equation, Eq. (15). Here tr is the same notation as in Ref. 14, namely,

$$\mathrm{tr}\,AB=\int_0^{-i\beta}d1\int_0^{-i\beta}d2A(12)B(21^+), \tag{16'}$$

where β is the inverse temperature. Also, as in Ref. 14, the choice of the branch of the logarithm is such that the variation of the first term in Eq. (16) is taken to be of the form $\delta\{\mathrm{tr}\ln(-G)\}=-\mathrm{tr}\{(\delta G^{-1})G\}$. This formulation of the many-body theory is known in the literature as the Φ-derivable method and has recently been generalized to include the density-functional formalism in Ref. 7. With this introduction of the one-particle spinor Green function and the corresponding spinor self-energy of the system under consideration, we are now in a position to generalize the Fukutome symmetry considerations of the HF solutions and subsequent classification of the broken-symmetry solutions of a magnetic system.

Following Ref. 13, the most general forms of the spinor Green function and the spinor self-energy function with no spin-symmetry considerations are expressed in terms of the Pauli matrices:

$$G(12)=\tfrac{1}{2}\{g_n(12)+\boldsymbol{\tau}\cdot\mathbf{g}_S(12)\}, \tag{18}$$

$$\Sigma(12)=\{\sigma_n(12)+\boldsymbol{\tau}\cdot\boldsymbol{\sigma}_S(12)\}. \tag{19}$$

We first note that the physical electron density and the physical vector spin density are respectively given by

$$n(1)=\langle\hat{n}(1)\rangle=-i\,\mathrm{Tr}\,G(11^+)=-ig_n(11^+) \tag{20}$$

and

$$\mathbf{s}(1)=\langle\hat{\mathbf{s}}(1)\rangle=-i\,\mathrm{Tr}\{\boldsymbol{\tau}G(11^+)\}=-i\mathbf{g}_S(11^+). \tag{21}$$

The corresponding physical particle current vector and the physical spin current tensor respectively are given by

$$\mathbf{j}(1)=\langle\hat{\mathbf{j}}(1)\rangle$$
$$=-\frac{1}{2m}\mathrm{Tr}\{(\nabla_1-\nabla_{1'})G(11')\}_{1'=1^+}$$
$$=-\frac{1}{2m}\{(\nabla_1-\nabla_{1'})g_n(11')\}_{1'=1^+}, \tag{22}$$

$$\overleftrightarrow{j}_S(1)=\langle\hat{\overleftrightarrow{j}}(1)\rangle$$
$$=-\frac{1}{2m}\mathrm{Tr}\{\boldsymbol{\tau}(\nabla_1-\nabla_{1'})G(11')\}_{1'=1^+}$$
$$=-\frac{1}{2m}\{(\nabla_1-\nabla_{1'})\mathbf{g}_S(11')\}_{1'=1^+}. \tag{23}$$

Here we have expressed these quantities of interest in terms of the corresponding spin-scalar and spin-vector components of the full spinor Green function, Eq. (18). From Eq. (9), we have

$$\left\{\frac{\partial}{\partial t_1}+\frac{1}{2mi}\nabla_1\cdot(\nabla_1-\nabla_{1'})\right\}G^<(11')|_{1'=1^+}$$
$$-\frac{1}{2i}\{[\boldsymbol{\tau}\cdot\mathbf{f}(1)]G^<(11^+)-G^<(11^+)[\boldsymbol{\tau}\cdot\mathbf{f}(1)]\}$$
$$=\frac{1}{i}\int d(2)\{\Sigma^>(12)G^<(21^+)+G^<(12)\Sigma^>(21^+)$$
$$-\Sigma^<(12)G^>(21^+)-G^>(12)\Sigma^<(21^+)\}. \tag{24}$$

From this, using Eqs. (18) and (19), we deduce the following general continuity equations relating the densities and currents given in Eqs. (20)–(23):

$$\frac{\partial n(1)}{\partial t_1}+\boldsymbol{\nabla}_1\cdot\mathbf{j}(1)=-\int d(2)\{\sigma_n^{>}(12)g_n^{<}(21^+)+\cdots + \boldsymbol{\sigma}_S^{>}(12)\cdot\mathbf{g}_S^{<}(21^+)+\cdots\}, \tag{25}$$

$$\frac{\partial \mathbf{s}(1)}{\partial t_1}+\boldsymbol{\nabla}_1\cdot\overleftrightarrow{j}_S(1)-[\mathbf{f}(1)\times\mathbf{s}(1)] =-\int d(2)\{\boldsymbol{\sigma}_S^{>}(12)g_n^{<}(21^+)+\cdots+i\boldsymbol{\sigma}_S^{>}(12) \times\mathbf{g}_S^{<}(21^+)+\cdots\}. \tag{26}$$

The ellipses in the above denote other terms arising from the indicated manipulations required to express Eq. (24) in terms of the particle and spin densities. Equation (25) is the usual continuity equation for the particle density while Eq. (26) is the corresponding one for the vector spin density. The third term on the left-hand side of Eq. (26) is the torque term due to external field acting on the spin vector while the right-hand side involves interaction contributions, which are of two kinds. The first is due to the spin vector modified by the particle density, while the second is the cross product of the spin vector with the field due to interactions. The difference between the itinerant and the localized spin cases thus becomes clear. In the itinerant case the divergence terms and the others on the right side contribute to give rise to spin-wave dispersion while in the localized case the divergence term is absent (no spin current) and only the cross product of spins contributes on the right-hand side. We will return to this in the next section.

C. Fukutome's classification of the broken-symmetry-adapted Green functions and the corresponding self-energies

Consider the Dyson equation in the absence of external fields obtained by dropping w in Eq. (15). It transforms under any unitary transformation U to the form

$$G'^{-1}=G_0'^{-1}-\Sigma', \tag{27}$$

where

$$G_0'^{-1}=U\left[i\frac{\partial}{\partial t_1}+\frac{\boldsymbol{\nabla}_1^2}{2m}-V_C(1)\right]\delta(12)U^\dagger,$$

$$G'=UGU^\dagger,$$

and

$$\Sigma'=U\Sigma U^\dagger=\Sigma[G'].$$

The Hamiltonian H given by Eq. (1) leads to the self-energy as well as the first term on the right-hand side of Eq. (27). Now $G_0'^{-1}=G_0^{-1}$ because it is the noninteracting part; the self-energy, on the other hand, reflects the contributions due to interactions, and is a therefore a functional of G, and has the form given in Eq. (11). Two cases arise as with the HF theory:[1] (a) $G'=G$, i.e., G commutes with U and thus is invariant under the transformation U and $\Sigma'=\Sigma$. In this case, U represents the self-consistent symmetry of the corresponding Σ scheme (compare the HF scheme[1]). (b) G is not invariant under U but leads to G' and Σ' obeying the same form of the equation as G. Then U represents a *broken* symmetry. Fukutome[2] pointed out in the context of the HF scheme that if U_1 belongs to a subgroup of the group of transformations U, then G'_{HF} and the corresponding self-consistent Σ'_{HF} form broken-symmetry-adapted solutions. From this it is clear that such a scheme holds for the general self-energy that appears in the equation for the Green function as in Eq. (15), which we explore in detail in this work. We will now present this generalized version of the Fukutome[2] analysis and describe these broken-symmetry possibilities.

TABLE I. The eight subgroups.

$S\times T$		S
$A(\hat{e})\times T$	$A(\hat{e})\times M(\hat{e}')\ (\hat{e}\cdot\hat{e}'=0)$	$A(\hat{e})$
T	$M(\hat{e}')$	$\mathbf{I}\times I$

We first consider only the group S of all spin rotations $\{\mathbf{I},\mathbf{U}\}$, being the unit operator in the rotation group, and the group T of time-reversal operation $\{I,\mathbf{T}\}$ which is of order 2, I is the unit operator and $\mathbf{T}=i\tau_2\mathbf{C}$ [$\mathbf{C}$ is the complex conjugation operator, under which the Hamiltonian (1) is invariant]. As in Ref. 2, the inclusion of spatial symmetry has to be dealt with individually depending on the type of spatial symmetry one wants to consider. A general consideration involving only S and T is sufficient for the present and indeed, as will be discussed in Sec. IV, the results obtained here form the basis for vector spin-density-functional theory of magnetic systems, where the interacting electron gas system provides the underlying functional for investigating the properties of many important inhomogeneous systems (see, for example, Refs. 9 and 10). Since S commutes with T, the group of all S and T is the direct product group $D\equiv S\times T=\{\mathbf{I}\times I,\mathbf{T},\mathbf{U},\mathbf{UT}\}$. There are eight different subgroups of D, which we will now enumerate. We note at once that $\mathbf{I}\times I$, S, and T individually are three subgroups of D. The spin rotation $A(\hat{e})$, about a fixed axis denoted by the unit vector $\hat{e}$, is a subgroup of S: $A(\hat{e})=\{\mathbf{U}(\hat{e},\theta)\}$, where $\{\mathbf{U}(\hat{e},\theta)\}$ is given by

$$\mathbf{U}(\hat{e},\theta)=\exp[-i\theta/2(\boldsymbol{\tau}\cdot\hat{e})] =\cos\frac{\theta}{2}-i(\boldsymbol{\tau}\cdot\hat{e})\sin\frac{\theta}{2}. \tag{28}$$

The fifth subgroup $M(\hat{e}')$ is of order 2, consisting of the unit operator and the combined operation of $\mathbf{T}$ with a spin rotation through an angle π around an axis $\hat{e}'$: $M(\hat{e}')=\{I,\mathbf{TU}(\hat{e}',\pi)\}$. There are two more subgroups that arise from the product of the elements $A(\hat{e})$ and $M(\hat{e}')$:

$$A(\hat{e})\times M(\hat{e}')=\{\mathbf{U}(\hat{e},\theta),\mathbf{U}(\hat{e},\theta)\mathbf{U}(\hat{e}',\pi)\mathbf{T}\}. \tag{29}$$

This gives rise to two groups, one when the unit vectors are orthogonal, $\hat{e}\cdot\hat{e}'=0$, and second when $\hat{e}=\pm\hat{e}'$, which is the group $A(\hat{e})\times T$. Collecting them all together, we have the eight subgroups listed in Table I.

In Table II, we have used the invariance of the continuity equations, Eqs. (25) and (26), under time-reversal operation, which in turn leads to the respective transformation properties of particle, particle-current, spin, and spin-current densities:

TABLE II. Broken-symmetry-adapted Green function solutions of the Dyson equation.

Invariance involving spin	Group T of time reversal	Invariance involving time: Group $M(\hat{e}')$ consisting of T and π rotations about $\hat{e}'$ axis	**I**
Group S of all spin rotations		Paramagnetic system $G_1=(1/2)(g_n)$ with $\mathbf{j}=0$ $\Sigma_1=\sigma_n$ Nonmagnetic insulator	Charge-current-wave system $G_2=(1/2)(g_n)$ with $\mathbf{j}\neq\mathbf{0}$ $\Sigma_2=\sigma_n$ Nonmagnetic metal or semiconductor
Group $A(\hat{e})$ of spin rotations about $\hat{e}$ axis (axial)	Axial spin-current-wave system $G_3=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}=\mathbf{0}$ and $\overleftrightarrow{J}_S\neq 0$ $\Sigma_3=\sigma_n+(\vec{\boldsymbol{\tau}}\cdot\hat{\vec{e}})\sigma_S^{\parallel}$ Insulating $\hat{e}$ axis antiferromagnet	Axial spin-density-wave system $G_4=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}=\mathbf{0}$ and $\overleftrightarrow{J}_S=0$ $\Sigma_4=\sigma_n+(\boldsymbol{\tau}\cdot\hat{e})\sigma_S^{\parallel}$ Insulating axial antiferromagnet $(\hat{e}'\cdot\hat{e}=0)$	Axial spin-wave system $G_5=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}\neq\mathbf{0}$ and $\overleftrightarrow{J}_S\neq 0$ $\Sigma_5=\sigma_n+(\boldsymbol{\tau}\cdot\hat{e})\sigma_S^{\parallel}$ Itinerant-electron axial ferromagnet
I	General spin-current-wave system $G_6=(1/2)(g_n+\boldsymbol{\tau}\cdot\mathbf{g}_S)$ such that $\mathbf{j}=\mathbf{0}$, $\mathbf{s}=\mathbf{0}$, but $\overleftrightarrow{j}_S\neq 0$, div $\overleftrightarrow{j}_S=0$ $\Sigma_6=(\sigma_n+\boldsymbol{\tau}\cdot\boldsymbol{\sigma}_S)$ Insulating spin-current-density state (antiferromagnet)	General spin-density-wave system $G_7=(1/2)\{g_n+(\boldsymbol{\tau}\cdot\hat{e}')g_S^{\parallel}+[\boldsymbol{\tau}-\hat{e}(\boldsymbol{\tau}\cdot\hat{e}')]\cdot\mathbf{g}_S^{\perp}\}$ $\Sigma_7=\{\sigma_n+(\boldsymbol{\tau}\cdot\hat{e}')\sigma_S^{\parallel}+[\boldsymbol{\tau}-\hat{e}(\boldsymbol{\tau}\cdot\hat{e}')]\cdot\boldsymbol{\sigma}_S^{\perp}\}$ Itinerant-electron helical SDW state (e.g., Overhauser)	General spin-wave system (with no constraint on spin-density vector) $G_8=(1/2)(g_n+\boldsymbol{\tau}\cdot\mathbf{g}_S)$ $\Sigma_8=(\sigma_n+\boldsymbol{\tau}\cdot\boldsymbol{\sigma}_S)$ Most general itinerant-electron SDW state

$$n\rightarrow n,\quad \mathbf{j}\rightarrow-\mathbf{j},\quad \mathbf{s}\rightarrow-\mathbf{s},\quad \mathbf{j}_S\rightarrow\mathbf{j}_S\,. \tag{30}$$

This representation is equivalent to but more physical than the one given by Fukutome,[2] who expresses his results in terms of the real and imaginary parts of the density matrix. It may be worth pointing out that several types of itinerant spin-density-wave states occurring in rare-earth systems were discussed before in a phenomenological way.[18]

D. Classification of broken-symmetry states of the one-band Hubbard model

One of the popular models to study the various magnetic states is described by the one- or two-band Hubbard Hamiltonian. Most recently, Singh[19] has examined the various possible states of a one-band Hubbard model in a decoupling scheme that goes beyond the Hartree-Fock approximation. Arita *et al.*[20] have examined the relationship between the three-dimensional lattice structure and magnetism of the system using Baym's[14] formalism, alluded to by us earlier. In this section, we use our group-theoretical analysis to enumerate the various possible states of this system. The one-band Hubbard model in localized representation is given by

$$H=\sum_{ij}\ t_{ij}a_{i\sigma}^{\dagger}a_{j\sigma}+U\sum_{i}\ a_{i\uparrow}^{\dagger}a_{i\uparrow}a_{i\downarrow}^{\dagger}a_{i\downarrow}\,, \tag{31}$$

which is equivalently written in the ''band'' representation as

$$H=\sum_{\mathbf{k}}\ \epsilon(\mathbf{k})a_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}^{\dagger}a_{\mathbf{k}\sigma}+U\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\ a_{\mathbf{k}+\mathbf{q}\uparrow}^{\dagger}a_{\mathbf{k}\uparrow}a_{\mathbf{k}'-\mathbf{q}\downarrow}^{\dagger}a_{\mathbf{k}'\downarrow}\,. \tag{32}$$

The spinor matrix Green function for the system is

$$\underline{G}(ij;t)=G_{\sigma\sigma'}(it;j0)=-i\langle T(a_{i\sigma}(t)a_{j\sigma'}^{\dagger}(0))\rangle \tag{33}$$

in localized representation. An important consequence of this is that the physical quantities, the total particle number at site i, $\Sigma_{\sigma}\langle a_{i\sigma}^{\dagger}(t)a_{i\sigma}(t)\rangle$ and spin-density vector $\Sigma_{\sigma\sigma'}\boldsymbol{\tau}_{\sigma\sigma'}\langle a_{i\sigma}^{\dagger}(t)a_{i\sigma}(t)\rangle$, may be expressed as traces over the product of unit and Pauli matrices as in Eqs. (7), (20), and (21):

$$n_{i\uparrow}+n_{i\downarrow}=n=-i\ \mathrm{tr}\ \underline{G}(ii,t=0^{-}),$$
$$\mathbf{s}_i=i\ \mathrm{tr}\ \boldsymbol{\tau}\underline{G}(ii;t=0^{-}). \tag{34}$$

In HF theory, the self-energy is found to be of the form

$$\underline{\Sigma}=-iU\underline{G}(ii,t=0^{-}), \tag{35}$$

from which we can deduce the eight different forms dictated by the group-theory considerations. Localized representation is used to obtain the self-energies for systems with no current while the ''band'' representation is employed when the current is nonzero as indicated in Table I. A mixed representation is applied when one kind of current is zero and the other is not, as is the case in two of the eight cases in Table I.

For a system invariant under translation and spin rotation, we get

$$\underline{\Sigma}_{\sigma\sigma'}=-iU\underline{G}_{\overline{\sigma}\overline{\sigma}}(ii,t=0^{-})\delta_{\sigma\sigma'},\quad \overline{\sigma}=-\sigma, \tag{36}$$

which for $n_{i\uparrow}=n_{i\downarrow}$ is the self-energy of a paramagnetic system. A similar expression is obtained in band representation for the nonmagnetic metal or semiconductor with $n_{\bar{\sigma}}=\Sigma_{\mathbf{k}}\langle a^{\dagger}_{\mathbf{k}\bar{\sigma}}(t)a_{\mathbf{k}\bar{\sigma}}(t)\rangle$. If the spin rotations are restricted to axial ones, the off-diagonal terms in $\underline{\underline{\Sigma}}$ appear in both representations. In the localized case, this leads to an insulating axial antiferromagnet and to an itinerant-electron ferromagnet for ''band'' representation. The self-energies in either case have a similar structure and can be written as

$$\underline{\underline{\Sigma}}=U\begin{pmatrix} n^{l,b}_{\downarrow} & -s^{l,b}_{-} \\ -s^{l,b}_{+} & n^{l,b}_{\uparrow} \end{pmatrix}, \tag{37}$$

where l, b stand for localized and band representations respectively, $n^{l}_{\sigma}=n_{i\sigma}$, $n^{b}_{\sigma}=n_{\sigma}$, $s^{l}_{+}=\langle a^{\dagger}_{i\uparrow}a_{i\downarrow}\rangle$, $s^{l}_{-}=\langle a^{\dagger}_{i\downarrow}a_{i\uparrow}\rangle$, $s^{b}_{+}=\Sigma_{q}\langle a^{\dagger}_{\mathbf{k+q}\uparrow}(t)a_{\mathbf{k+q}\downarrow}(t)\rangle$, and $s^{b}_{-}=\Sigma_{\mathbf{q}}\langle a^{\dagger}_{\mathbf{k-q}\downarrow}(t)\times a_{\mathbf{k-q}\uparrow}(t)\rangle$. One can equally express the interaction terms in mixed representation in such a way that one gets the localized results for the diagonal terms in spin indices of the self-energy such that $\mathbf{j}=\mathbf{0}$ and delocalized ones for the off-diagonal terms in spin indices such that $\mathbf{j}_s\neq 0$ to get the insulating $\hat{e}$ axis antiferromagnet.

For systems with broken translational symmetry, a plane wave of the form $\exp(i\mathbf{k}\cdot\mathbf{r})$ with up spin and $\exp[i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}]$ with down spin are assigned to derive the self-energy.[3] Here the vector $\mathbf{Q}$ is a measure of the spiral nature of the spin density and points in an arbirary direction for the most general itinerant-electron SDW state, and the self-energy is given by

$$\underline{\underline{\Sigma}}=U\begin{pmatrix} n^{Q}_{\downarrow} & -s^{Q}_{-} \\ -s^{Q}_{+} & n_{\uparrow} \end{pmatrix} \tag{38}$$

where $n^{Q}_{\downarrow}=\Sigma_{\mathbf{k}}\langle a^{\dagger}_{\mathbf{k+Q}\downarrow}(t)a_{\mathbf{k+Q}\downarrow}(t)\rangle$, $n_{\uparrow}=\Sigma_{\mathbf{k}}\langle a^{\dagger}_{\mathbf{k}\uparrow}(t)a_{\mathbf{k}\uparrow}(t)\rangle$, $s^{Q}_{+}=\Sigma_{\mathbf{q}}\langle a^{\dagger}_{\mathbf{k+q}\uparrow}(t)a_{\mathbf{k+Q+q}\downarrow}(t)\rangle$, and $s^{Q}_{-}=\Sigma_{\mathbf{q}}\langle a^{\dagger}_{\mathbf{k+Q-q}\downarrow}(t)a_{\mathbf{k-q}\uparrow}(t)\rangle$. The itinerant-electron helical SDW state is a special case of the general SDW state with spin vectors having projections along specific axes $\hat{e}$ and $\hat{e}'$, and the general spin-current-wave system can be obtained in mixed representation as discussed above.

We have thus demonstrated here the use of the general group-theoretical method in a special model system. In the next section, we address the important question of the linear response of these systems in an equally comprehensive manner.

III. LINEAR RESPONSE FUNCTIONS: SYMMETRY CONSIDERATIONS

The well-known theory of linear-response functions in itinerant magnetic systems may be expressed in terms of the functional derivatives of the inverse Green function, Eq. (15), with respect to the external fields f^{α} of Eqs. (6) and (7). From these one examines the possible collective excitations in the system (see, for example, Refs. 13 and 15). Additionally these response functions allow us to test the stability of the state (for example, in Refs. 13 and 15) that is obtained as the solution of Eq. (9) or equivalently Eq. (15). Alternately, the stability question may be reformulated as the criterion of minimum free energy, as was originally done in Ref. 14 and in a more physical way recently in Ref. 16 where a localized site representation was used. Such a version is not applicable to itinerant-electron systems, where one has contribution from the mobile electrons as is evident from the work of Refs. 13 and 15. One way to realize this is to note that in Eq. (26) there is a contribution from the divergence of the spin current which is absent when there are no itinerant electrons. To bring out this feature, instead of repeating the work in Refs. 13 and 15, we give here a brief outline of linear-response theory. The various types of response function $\chi_{\alpha\beta}$ can be expressed as appropriate variational derivatives, which in turn are expressed in terms of the corresponding appropriate variational derivatives of the self-energy:

$$\begin{aligned}\chi_{\alpha\beta}(12)&=-i\{\langle T(\hat{s}_{\alpha}(1)\hat{s}_{\beta}(2))\rangle-s_{\alpha}(1)s_{\beta}(2)\}\\&=\frac{\delta s_{\alpha}(1)}{\delta f^{\beta}(2)}=-i\,\mathrm{Tr}\,\mathrm{tr}\,\tau_{\alpha}\frac{\delta G(11^{+})}{\delta f^{\beta}(2)}\\&=-i\,\mathrm{Tr}\,\mathrm{tr}\int\tau_{\alpha}G\Lambda_{\beta}G,\end{aligned}$$

$$\Lambda_{\beta}(12;3)=-\frac{\delta G^{-1}(12)}{\delta f^{\beta}(3)}=\delta(12)\delta(13)\tau_{\beta}+\frac{\delta\Sigma(12)}{\delta f^{\beta}(3)}.$$

Recalling the definitions given in Eqs. (7), (20), and (21), we have 16 response functions, involving the particle density and the three components of the spin vector density. In the localized-electron scheme, the cross terms involving the density and spin vector will not appear. This is another important difference between the localized- and itinerant-electron systems. From such a linear-response theory, one often deduces the low-energy collective excitations in the system, such as spin waves in ferromagnetic, antiferromagnetic, and SDW systems. Such a discussion may be found, for example, in Ref. 15.

The objective in Ref. 16 was to derive expressions for the energy of the known localized effective spin models of magnetic systems. From this one can also deduce the low-energy collective excitations in the system. In the itinerant-electron system, it should be pointed out that there are important contributions not found in the localized spin systems, as is evident from Ref. 15, for example. We adopt the alternate formulation in this section to obtain a generalization of the ''local force theorem'' in Ref. 16 that is applicable to both the localized and itinerant systems.

Unlike in the general linear-response theory described above, we now consider the effect of an infinitesimal rotation of the spin about a general direction denoted by a unit vector $\hat{e}$, $\delta\boldsymbol{\theta}=\hat{e}\,\delta\theta$, obtained from Eq. (28): $\delta U=(1-i\,\delta\boldsymbol{\theta}\cdot\boldsymbol{\tau}/2)$, on the free energy, Eq. (16), in the same fashion as in Ref. 16, holding G fixed:

$$\delta\Omega=-\,\mathrm{Tr}\,\mathrm{tr}\,G(\delta\Sigma),$$

$$\begin{aligned}\delta\Sigma&=i\frac{\delta\boldsymbol{\theta}}{2}\cdot(\boldsymbol{\tau}\Sigma-\Sigma\boldsymbol{\tau})\\&=i\frac{\delta\boldsymbol{\theta}}{2}\cdot[\boldsymbol{\tau}(\boldsymbol{\tau}\cdot\boldsymbol{\sigma}_s)-(\boldsymbol{\tau}\cdot\boldsymbol{\sigma}_s)\boldsymbol{\tau}]\\&=-\boldsymbol{\tau}\cdot(\delta\boldsymbol{\theta}\times\boldsymbol{\sigma}_s),\end{aligned}$$

and so

$$\delta\Omega = \delta\boldsymbol{\theta}\cdot \mathrm{tr}(\boldsymbol{\sigma}_s \times \mathbf{g}_s) \equiv \delta\boldsymbol{\theta}\cdot \mathbf{V}. \tag{39}$$

Here we used the representations given in Eqs. (18) and (19) and some well-known identities to arrive at the expression for the torque $\mathbf{V}$ due to the rotation. This expression differs from the one given in Ref. 16 because of a factor of one-half in our definition of the spinor Green function in contrast to theirs. As in Ref. 16, the Dyson equation gives us the sum rules on the components of the spinor Green function, after using Eq. (15):

$$\begin{aligned} GG^{-1} &= 1 = G(G_0^{-1} - \Sigma) \\ &= \tfrac{1}{2}(g_n + \boldsymbol{\tau}\cdot\mathbf{g}_S)(G_0^{-1} - \sigma_n - \boldsymbol{\tau}\cdot\boldsymbol{\sigma}_S), \\ G^{-1}G &= 1 = (G_0^{-1} - \Sigma)G \\ &= (G_0^{-1} - \sigma_n - \boldsymbol{\tau}\cdot\boldsymbol{\sigma}_S)\tfrac{1}{2}(g_n + \boldsymbol{\tau}\cdot\mathbf{g}_S). \end{aligned} \tag{40}$$

From this we get the relations

$$(G_0^{-1} - \sigma_n)g_n - \boldsymbol{\sigma}_S\cdot\mathbf{g}_S = 2, \tag{41a}$$

$$(G_0^{-1} - \sigma_n)\mathbf{g}_S - \boldsymbol{\sigma}_S g_n - i\boldsymbol{\sigma}_S\times\mathbf{g}_S = \mathbf{0}, \tag{41b}$$

$$g_n(G_0^{-1} - \sigma_n) - \mathbf{g}_S\cdot\boldsymbol{\sigma}_S = 2, \tag{42a}$$

$$\mathbf{g}_S(G_0^{-1} - \sigma_n) - g_n\boldsymbol{\sigma}_S - i\mathbf{g}_S\times\boldsymbol{\sigma}_S = \mathbf{0}. \tag{42b}$$

From these we derive the following sum rules corresponding to those given in Ref. 16 but in a coordinate representation valid for both itinerant- and localized-electron systems. Multiplying (41a) by g_n on the left and (42a) on the right we obtain

$$\begin{aligned} 2g_n &= g_n(G_0^{-1} - \sigma_n)g_n - g_n(\boldsymbol{\sigma}_S\cdot\mathbf{g}_S) \\ &= g_n(G_0^{-1} - \sigma_n)g_n - (\mathbf{g}_S\cdot\boldsymbol{\sigma}_S)g_n. \end{aligned} \tag{43}$$

Multiplying (41a) by $\mathbf{g}_S$ on the left and using (42b) we obtain

$$\begin{aligned} 2\mathbf{g}_S &= g_n\boldsymbol{\sigma}_S g_n - \mathbf{g}_S(\boldsymbol{\sigma}_S\cdot\mathbf{g}_S) + i(\mathbf{g}_S\times\boldsymbol{\sigma}_S)g_n \\ &= g_n\boldsymbol{\sigma}_S g_n - (\mathbf{g}_S\cdot\boldsymbol{\sigma}_S)\mathbf{g}_S + ig_n(\boldsymbol{\sigma}_S\times\mathbf{g}_S). \end{aligned} \tag{44}$$

The second expression is obtained by multiplying (42a) by $\mathbf{g}_S$ on the right and using (41b). From Eqs. (39) and (44), we obtain the general expression for the torque vector,

$$\begin{aligned} \mathbf{V} &= \mathrm{tr}(\boldsymbol{\sigma}_S\times\mathbf{g}_S) \\ &= -\tfrac{1}{2}\mathrm{tr}\{\boldsymbol{\sigma}_S\times[-g_n\boldsymbol{\sigma}_S g_n + (\mathbf{g}_S\cdot\boldsymbol{\sigma}_S)\mathbf{g}_S \\ &\quad - ig_n(\boldsymbol{\sigma}_S\times\mathbf{g}_S)]\}. \end{aligned} \tag{45}$$

By integrating back the expression given by Eq. (39), effectively the spin-only part of the free energy may be rewritten as

$$\begin{aligned} \Omega_{\mathrm{SP}} &\cong \mathrm{tr}\,\mathrm{Tr}(G\Sigma) \cong \mathrm{tr}(\mathbf{g}_S\cdot\boldsymbol{\sigma}_S) \\ &= -\tfrac{1}{2}\mathrm{tr}\{(\mathbf{g}_S\cdot\boldsymbol{\sigma}_S)(\mathbf{g}_S\cdot\boldsymbol{\sigma}_S) - (\boldsymbol{\sigma}_S g_n)\cdot(\boldsymbol{\sigma}_S g_n) \\ &\quad - i[(\boldsymbol{\sigma}_S\times g_n\boldsymbol{\sigma}_S)\cdot\mathbf{g}_S]\}. \end{aligned} \tag{46}$$

Here Eq. (44) was used in further simplification. The second approximation symbol is because we have dropped the spin-independent contribution $\mathrm{tr}\,g_n\sigma_n$ arising in the first expression. Note, however, that from Eq. (43) g_n, σ_n depend on the spin vector. Had we kept this contribution, we would have additional contributions due to particle-density-density, particle-density, and spin-density vectors mentioned in the linear-response theory at the beginning of this section. For completeness, we give this here:

$$\Omega_{ns} \cong \mathrm{tr}\,g_n\sigma_n \cong \tfrac{1}{2}\mathrm{tr}\{\sigma_n g_n(G_0^{-1} - \sigma_n)g_n - \sigma_n g_n(\boldsymbol{\sigma}_S\cdot\mathbf{g}_S)\}.$$

Here Eq. (43) was used in further simplification. It should be noted that the notation tr used here is as defined before in Eq. (16′). In the site local representation used in Ref. 16, Eq. (46) transforms to that given there.

Using Table II, we have eight types of Green function and their corresponding self-energies associated with the allowed broken-symmetry solutions. Using these in the general expressions for the spin-spin interaction energies obtained above, one can deduce the structure of the corresponding spin-spin contribution to the free energy of the system.

IV. IMPLICATIONS FOR VECTOR SPIN-DENSITY-FUNCTIONAL THEORY

The development of the vector spin-density-functional theory, especially the local (LSD) approximation, has in recent years produced a much better theoretical understanding of itinerant magnetism. (See, for example, Refs. 5, 9, and 10.) In particular, in Ref. 15, a spinor Green function version of the LSD theory was developed where the self-energy in Eqs. (9) or (15) is taken to be of the form, local in space and time,

$$\Sigma_{\mathrm{LSD}}(12) \cong \{V_{\mathrm{xc}}[n,\mathbf{s};\mathbf{r}_1] + \boldsymbol{\tau}\cdot\mathbf{W}_{\mathrm{xc}}[n,\mathbf{s};\mathbf{r}_1]\}\delta(12), \tag{47}$$

where V_{xc} is the spin-scalar part of the self-energy, which is in general a local functional of particle density n and spin-density vector $\mathbf{s}$, whereas $\mathbf{W}_{\mathrm{xc}}$ is its spin-vector counterpart, for describing itinerant magnetic systems. The approximate forms for these functionals arise as the respective functional derivatives of the exchange-correlation energy, $E_{\mathrm{xc}}[n,\mathbf{s},] \equiv E_{\mathrm{xc}}[s_\alpha]$ [using the notation of Eq. (7)] of a spin-polarized homogeneous electron gas (see references in Ref. 5, for example). In fact, $V_{\mathrm{xc}} = \delta E_{\mathrm{xc}}/\delta n$, $\mathbf{W}_{\mathrm{xc}} = \delta E_{\mathrm{xc}}/\delta\mathbf{s}$, or, more generically, $V_{\mathrm{xc}}^{(\alpha)} = \delta E_{\mathrm{xc}}/\delta s_\alpha$, so that $\Sigma_{\mathrm{LSD}} = \tau_\alpha V_{\mathrm{xc}}^{(\alpha)}$. The resulting equation is the LSD equation,

$$\begin{aligned} &\left[i\frac{\partial}{\partial t_1} + \frac{\boldsymbol{\nabla}_1^2}{2m} - V_C(1) - w_n(1) - \boldsymbol{\tau}\cdot\mathbf{f}(1) \right] \\ &\qquad \times G(12) - \{V_{\mathrm{xc}}[n,\mathbf{s};1] + \boldsymbol{\tau}\cdot\mathbf{W}_{\mathrm{xc}}[n,\mathbf{s};1]\}G(12) \\ &\qquad = \delta(12). \end{aligned} \tag{48}$$

This is solved self-consistently by numerical methods.

The continuity equations for the particle and spin density derived from this LSD equation (48) now take the forms

$$\frac{\partial n(1)}{\partial t_1} + \boldsymbol{\nabla}_1\cdot\mathbf{j}(1) = 0,$$

TABLE III. Broken-symmetry-adapted Green function solutions of the LDS equation.

Invariance involving spin	Invariance involving time: Group T of time reversal	Group $M(\hat{e}')$ consisting of T and π rotation about $\hat{e}'$ axis	**I**
	Paramagnetic system		
Group S of all spin rotations	$G_1=(1/2)(g_n)$ with $\mathbf{j}=\mathbf{0}$. $\Sigma_1=\delta(12)V_{\rm xc}$ Nonmagnetic insulator		Charge-current-wave system $G_2=(1/2)(g_n)$ with $\mathbf{j}\neq 0$ $\Sigma_2=\delta(12)V_{\rm xc}$ Nonmagnetic metal or semiconductor
Group $A(\hat{e})$ of spin rotations about $\hat{e}$ axis (axial)	Axial spin-current-wave system $G_3=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}=\mathbf{0}$ and $\overleftrightarrow{j}_S\neq 0$ $\Sigma_3=\delta(12)[V_{\rm xc}+(\boldsymbol{\tau}\cdot\hat{e})\mathbf{W}_{\rm xc}^{\parallel}]$ Insulating $\hat{e}$ axis antiferromagnet	Axial spin-density-wave system $G_4=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}=\mathbf{0}$ and $\overleftrightarrow{j}_S=0$ $\Sigma_4=\delta(12)[V_{\rm xc}+(\boldsymbol{\tau}\cdot\hat{e})\mathbf{W}_{\rm xc}^{\parallel}]$ Insulating axial antiferromagnet $(\hat{e}'\cdot\hat{e}=0)$	Axial spin-wave system $G_5=(1/2)[g_n+(\boldsymbol{\tau}\cdot\hat{e})g_S^{\parallel}]$ with $\mathbf{j}\neq\mathbf{0}$ and $\overleftrightarrow{j}_S\neq 0$ $\Sigma_5=\delta(12)[V_{\rm xc}+(\boldsymbol{\tau}\cdot\hat{e})]\mathbf{W}_{\rm xc}^{\parallel}$ Itinerant-electron axial ferromagnet
I	General spin-current-wave system $G_6=(1/2)(g_n+\boldsymbol{\tau}\cdot\mathbf{g}_s)$ such that $\mathbf{j}=\mathbf{0}$, $\mathbf{s}=0$, but $\overleftrightarrow{j}_S\neq 0$, div $\overleftrightarrow{j}_S=0$ $\Sigma_6=\delta(12)(V_{\rm xc}+\boldsymbol{\tau}\cdot\mathbf{W}_{\rm xc})$ Insulating spin-current-density state (antiferromagnet)	General spin-density-wave system $G_7=(1/2)\{g_n+(\boldsymbol{\tau}\cdot\hat{e}')g_S^{\parallel}+[\boldsymbol{\tau}-\hat{e}(\boldsymbol{\tau}\cdot\hat{e}')]\cdot\mathbf{g}_S^{\perp}\}$ $\Sigma_7=\delta(12)\{V_{\rm xc}+(\boldsymbol{\tau}\cdot\hat{e}')\mathbf{W}_{\rm xc}^{\parallel}+[\boldsymbol{\tau}-\hat{e}(\boldsymbol{\tau}\cdot\hat{e}')]\cdot\mathbf{W}_{\rm xc}^{\perp}\}$ Itinerant-electron helical SDW state (e.g., Overhauser)	General spin-wave system (with no constraint on spin-density vector) $G_8=(1/2)(g_n+\boldsymbol{\tau}\cdot\mathbf{g}_S)$ $\Sigma_8=\delta(12)(V_{\rm xc}+\boldsymbol{\tau}\cdot\mathbf{W}_{\rm xc})$ Most general itinerant-electron SDW state

$$\frac{\partial\mathbf{s}(1)}{\partial t_1}+\boldsymbol{\nabla}_1\cdot\overleftrightarrow{j}_S(1)=\mathbf{W}_{\rm xc}\times\mathbf{s}(1). \tag{49}$$

The second equation for the spin-density vector has a contribution from the torque due to the spin polarization of the spin system, besides having a contribution from the divergence of the moving spins producing a spin-current density.

Proceeding as in Eqs. (41) and (42), we have the equations

$$(G_0^{-1}-V_{\rm xc})g_n-(\mathbf{W}_{\rm xc})\cdot\mathbf{g}_S=2, \tag{50a}$$

$$(G_0^{-1}-V_{\rm xc})\mathbf{g}_S-(\mathbf{W}_{\rm xc})g_n-i(\mathbf{W}_{\rm xc})\times\mathbf{g}_S=0, \tag{50b}$$

$$g_n(G_0^{-1}-V_{\rm xc})-\mathbf{g}_S\cdot(\mathbf{W}_{\rm xc})=2, \tag{51a}$$

$$\mathbf{g}_S(G_0^{-1}-V_{\rm xc})-g_n(\mathbf{W}_{\rm xc})-i\mathbf{g}_S\times(\mathbf{W}_{\rm xc})=0. \tag{51b}$$

From these we obtain the expressions

$$2g_n=g_n(G_0^{-1}-V_{\rm xc})g_n-g_n(\mathbf{W}_{\rm xc}\cdot\mathbf{g}_S) \tag{52a}$$

$$=g_n(G_0^{-1}-V_{\rm xc})g_n-(\mathbf{g}_S\cdot\mathbf{W}_{\rm xc})g_n, \tag{52b}$$

$$2\mathbf{g}_S=g_n(\mathbf{W}_{\rm xc})g_n+i(\mathbf{g}_S\times\mathbf{W}_{\rm xc})g_n-\mathbf{g}_S(\mathbf{W}_{\rm xc}\cdot\mathbf{g}_S) \tag{53a}$$

$$=g_n(\mathbf{W}_{\rm xc})g_n+ig_n(\mathbf{W}_{\rm xc}\times\mathbf{g}_S)-(\mathbf{g}_S\cdot\mathbf{W}_{\rm xc})\mathbf{g}_S. \tag{53b}$$

Finally the expression for the spin-only contribution to the free energy in the LSD case is obtained in a manner similar to that given in Sec. III, Eq. (46):

$$\Omega_{\rm sp}^{\rm LSD}=-\tfrac{1}{2}{\rm tr}\{(\mathbf{g}_S\cdot\mathbf{W}_{\rm xc})(\mathbf{g}_S\cdot\mathbf{W}_{\rm xc})-(g_n\mathbf{W}_{\rm xc})\cdot(g_n\mathbf{W}_{\rm xc})-ig_n(\mathbf{W}_{\rm xc}\times\mathbf{g}_S)\cdot\mathbf{W}_{\rm xc}\}. \tag{54}$$

The corresponding particle-density and spin-density contributions to the free energy are given by

$$\Omega_{ns}^{\rm LSD}\cong{\rm tr}\,g_nV_{\rm xc}=\tfrac{1}{2}{\rm tr}\{V_{\rm xc}g_n(G_0^{-1}-V_{xc})g_n-V_{\rm xc}g_n(\mathbf{W}_{\rm xc}\cdot\mathbf{g}_S)\}.$$

In Eq. (54), as in Eq. (46), the first term represents a multispin interaction energy involving four spins or more, the middle term is like the spin-spin interaction involving two spins or more, whereas the last term is a Dzialoshinskii-Moriya-type interaction, involving three or more spins. In Ref. 15, a spatially slowly varying approximation was considered in an approximate way and only the middle term resembling an effective Heisenberg spin-spin interaction energy was derived along with the cross terms containing particle density and spin density. The higher-order spin terms and the Dzialoshinskii-Moriya terms did not appear in that derivation because self-consistent relations as in Eqs. (52) and (53) were not invoked. The above remark arises from the observation that the vector part of the self-energy functional $\mathbf{W}_{\rm xc}$ is an odd functional of the spin vector beginning with a linear functional of the spin vector.

In Table III, the eight types of Green function and the corresponding self-energies are given associated with the various broken-symmetry types for the case of LSD theory. From the above general expressions for the free energy, one may then deduce the structure of the spin-dependent energies

that follow for each of these cases. The phenomenological description[20] is here supported by the considerations of group theory.

Applying the linear-response theory outlined in Sec. III to the LSD scheme, one obtains a tensor

$$\frac{\delta\Sigma}{\delta f^{\beta}} = \mathrm{tr}\frac{\delta\Sigma}{\delta s^{\gamma}}\frac{\delta s_{\gamma}}{\delta f^{\beta}} \quad \text{(chain rule)}$$

$$= \tau_{\alpha}\mathrm{tr}\frac{\delta^2 E_{\mathrm{xc}}}{\delta s^{\alpha}\delta s^{\gamma}}\frac{\delta s_{\gamma}}{\delta f^{\beta}},$$

as was shown in Ref. 15. The broken-symmetry considerations leading to Table III may be applied to this tensor to deduce the corresponding eight structures. As shown in Ref. 15 and more recently in Ref. 10, the use of homogeneous electron gas results in LSD theory requires a subtle and important modification in incorporating the vector nature of the spin density when studying the spin-wave properties of itinerant magnets. Another way of expressing this point is that the traditional electron gas theory leads to an Ising-like treatment of the spins, which is converted into a Heisenberg-like treatment (see, for example, Ref. 9) by a spin rotation. This does not lead to correct answers, as was shown in Ref. 10, and this is due to the subtle nature of the treatment of the spin vector in the theory. In Ref. 10, a perturbation theory approach was presented to include this feature, thus making a significant difference.

V. SUMMARY AND CONCLUDING REMARKS

In summary, the structures of the Green functions and their associated self-energies arising from group-theoretical considerations of the spin rotation and time-reversal invariance are given in Table II for general magnetic many-electron systems and in Table III for the vector spin-density-functional formalism of itinerant-electron systems. This is expected to systematize the procedure of analysis of magnetic structures that may appear in magnetic nanometric systems and in magnetic atomic clusters, just as the earlier similar work of Fukutome systematized the Hartree-Fock solutions of magnetic states of molecular systems. We also consider consequences of this by setting up the linear-response theory and an alternative version of it in the form of an ''effective spin Hamiltonian,'' to exhibit the differences between localized-electron systems and those where the electrons are itinerant. We hope that the search for various types of magnetic structures in nanometric[8] and atomic cluster[11] systems, particularly when the clusters are deposited on semiconductor substrates,[12] will be systematized by the procedure given here. In these systems, as seen from the work in Ref. 11, magnetic properties are correlated with the geometric structures of the clusters; the group-theoretical analysis presented here is expected to make the search for this feature systematic. In this context, the work presented here incorporated into that in Ref. 17 may be expected to lead to efficient procedures for computation of magnetic properties in nanometric systems and in atomic clusters. We applied this theory to the one-band Hubbard model to illustrate the usefulness of this approach.

We have here pointed out the significance of incorporating the vector nature of spin density in LSD theory, particularly in the modification needed in the traditional use of the homogeneous electron gas results. In this context, the recent work in Ref. 10 should be mentioned as an important step in a proper treatment of the vector spin. In Ref. 10, the transverse part of the vector spin was incorporated in a perturbative way and was shown to lead to a better understanding of the magnetism of iron than previously.[9] The localized treatment of spin interactions deduced in Ref. 16 is here generalized to itinerant-electron magnetic systems and the differences arising from this are spelled out. It may also be pointed out that the phenomenology of the various types of SDW structure given in Ref. 18 may be deduced from Table III.

In this paper, we have not included the gauge group needed to incorporate superconducting phases nor have we included the lattice translation group. The addition of the translation group into the considerations given here brings in the irreducible representation characterized by the q vector associated with the Brillouin zone and the little group of the q vector. The gauge group is also useful particularly because the high-T_C superconductors involving d- and s-wave pairing possess interesting vortex structures. Inclusion of these within the mean-field (HF) theory has been reported in some special cases.[2,4] The generalization of all these features in the Green function framework will be addressed in a future article.

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