Spin-orbit interactions in the many-body theory of magnetic electron systems

A. K. Rajagopal
Naval Research Laboratory, Washington, D.C. 20375-5320

Mogus Mochena
Department of Physics, Florida A & M University, Tallahassee, Florida 32307
(Received 4 September 1997; revised manuscript received 9 December 1997)

We have developed here a many-body theory of magnetic electron systems including both the one- and two-particle spin-orbit interactions. Among the two-particle spin-orbit interactions, we focus attention on the spin-same orbit and spin-other orbit terms, which were considered recently in the literature for nonmagnetic systems. The spinor-Green function method employed here provides a clear self-consistent way of treating both the single-particle and the two-particle properties in the system. It enables us to express in an elegant fashion screening effects that appear in different forms with transparent physical significance to each type. We carry out in some detail these contributions in the random-phase approximation and point out their significance especially in the magnetic systems. This development is a contribution towards a new understanding of magnetism in a wide class of systems ranging from clusters to nanomagnets that possess very large spin moments. This should also be of importance in the new studies of spin transport and magnetoelectronics, specifically in magnetic systems in low dimensions. [S0163-1829(98)02117-1]

I. INTRODUCTION

The effects of spin-orbit coupling, including one- and two-particle contributions in atoms as well as in semiconductors have been discussed in the past.[1,2] In view of the recent experimental findings in spin transport,[3] suggestions of magnetoelectronics[4] in magnetic two-dimensional electron systems, and the enormous spin magnetic moments found in clusters of atoms such as manganese,[5] the understanding of the role of spin-orbit interactions in these systems becomes paramount. A many-body theory including these effects is thus called for in investigating magnetic systems mentioned here. Only recently Grimaldi and Fulde[6] investigated the many-body theory of screening of the phonon-modulated spin-orbit interaction in nonmagnetic metals. They did not consider magnetic systems and thus missed important effects that arise when these are included. They argue that the spin-orbit potential is unaffected by the electronic response and therefore introduce spin-other-orbit interaction to place the screening effects on the same footing. We find that this is true in the Hartree approximation used by them and for nonmagnetic systems. By considering spin polarized systems and by going beyond the Hartree approximation, we find interesting results, thus considerably enlarging the scope of the formalism to include the phenomena mentioned above. Only the changes in phonon spectrum due to spin-orbit effects in ferromagnetic metals were discussed some time back,[7] where the screening effects appear not only via density fluctuations but also due to spin-density fluctuations. For the nonmagnetic situation, the spin effects all reduce in such way as to lead to only the known density-fluctuation effects as in Ref. 6. The above investigations are all based on the leading-order contributions of the relativistic effects to the nonrelativistic description of atoms, molecules, and solids, as is described in detail in Slater's books.[1,2] The corresponding many-body theory in the relativistic formulation was developed only recently.[8,9] The purpose of this paper is to develop the many-body theory of magnetic electron systems including the one- and two-body spin-orbit interactions for two important reasons. First, for the experimental systems of the type discussed in Refs. 3–5, and for ''moderately heavy'' atom systems, such an approximation scheme, often called the Pauli approximation, [10] suffices, and second, the fully relativistic theory obscures the physical picture contained in the nonrelativistic-type description.

We employ a spinor-Green function method in this paper, originally developed for describing itinerant electron magnetic systems,[11] which exposes the physics of the system in a particularly transparent way. It provides a way to study both the single-particle and the two-particle properties of the system in an elegant self-consistent manner. A major result of this development is the appearance of new correlation functions (sixteen types) in this description besides the usual (three types) density-density and spin density-spin density and cross-correlations functions of magnetic systems. This is because the spin-orbit interactions involve the linear momentum density and spin-orbit density whose correlations with the other two enlarge the scope of the inherent correlations in the system. In this way, we are able to express the various contributions to screening in an elegant and physically meaningful fashion. In Sec. II, we describe the Hamiltonian of the system. In Sec. III, we develop the Green function theory and describe the physical meanings of various terms that appear at each stage of approximation. In Sec. IV, some approximation schemes such as Hartree mean field, exchange only, and random-phase approximation are derived. In Sec. V, we develop in detail the random-phase approximation and display the various contributions of the different types of correlations to the magnetic properties of the system. In Sec. VI, we give some concluding remarks. In particular, in the case of weak one-particle potentials considered in Ref. 6, we draw attention to the modified effective one-particle potential expressed in terms of the vertex functions introduced here, exhibiting clearly the nature of screening of the bare potentials.

II. HAMILTONIAN OF THE SYSTEM

The Hamiltonian operator of the system under consideration in the second quantized form may be written as

$$\hat{H}=\hat{H}_1+\hat{H}_2,\quad \hat{H}_1=\hat{T}_e+\hat{V}_{ei}+\hat{V}_{\mathrm{s.o}},$$
$$\hat{H}_2=\hat{V}_C+\hat{V}_{\mathrm{s.s.o}}+\hat{V}_{\mathrm{s.o.o}}. \tag{1}$$

The one-particle Hamiltonian operator $\hat{H}_1$ contains three parts: $\hat{T}_e$ is the usual kinetic energy operator of the electrons, $\hat{V}_{ei}$ is the (periodic) potential due to the ions in the system, and $\hat{V}_{\mathrm{s.o}}$ is the spin-orbit contribution. We have dropped two other contributions, one due to the magnetic field and another relativistic term that has no classical analog.[1] The two-particle Hamiltonian operator $\hat{H}_2$ also contains three parts: $\hat{V}_C$ is the usual two-particle Coulomb interaction between electrons, $\hat{V}_{\mathrm{s.s.o}}$ is the interaction between one electron and another electron under the influence of spin-orbit effect, termed here as spin-same-orbit interaction, and $\hat{V}_{\mathrm{s.o.o}}$ is a similar two-electron interaction except that the spin of one electron interacts with the orbital motion of the other, known as the spin-other-orbit interaction. We have dropped three other terms, representing orbit-orbit, spin-spin, and a relativistic term with no classical analog.[1] With this choice of the Hamiltonian, we believe we have captured the essential physical processes occurring in the systems under consideration. It may be remarked that Grimaldi and Fulde[6] choose to keep only two terms in $\hat{H}_2$ involving only spin-same-orbit interaction. (It may be noted that in Ref. 6 the term ''spin-other orbit'' is used but the expression for it is that for ''spin-same orbit'' interaction as given by Slater,[1] as we show later explicitly.) The introduction of the ion motion and hence the phonon modulated spin-orbit interaction is accomplished by adding the corresponding terms in $\hat{H}_1$. We display here the explicit forms of only those terms in $\hat{H}_1$ and $\hat{H}_2$ that may not be commonly known.

$$\hat{V}_{\mathrm{s.o}}=\mu_B^2\sum_{\sigma,\sigma'}\int d^3\mathbf{r}\,\psi_\sigma^\dagger(\mathbf{r})\{\mathbf{E}(\mathbf{r})\cdot(\hat{\mathbf{p}}_r\times\boldsymbol{\tau}_{\sigma\sigma'})\}\psi_{\sigma'}(\mathbf{r}), \tag{2}$$

$$\hat{V}_{\mathrm{s.s.o}}=\mu_B^2\sum_{\sigma_1,\sigma_2,\sigma_3}\int d^3\mathbf{r}\int d^3\mathbf{r}'\,\psi_{\sigma_1}^\dagger(\mathbf{r})\psi_{\sigma_2}^\dagger(\mathbf{r}')\{\boldsymbol{\nabla}_r\nu_C(\mathbf{r},\mathbf{r}')\cdot(\hat{\mathbf{p}}_r\times\boldsymbol{\tau}_{\sigma_1\sigma_3})\}\psi_{\sigma_2}(\mathbf{r}')\psi_{\sigma_3}(\mathbf{r}), \tag{3}$$

$$\hat{V}_{\mathrm{s.o.o}}=-2\mu_B^2\sum_{\sigma_1,\sigma_2,\sigma_3}\int d^3\mathbf{r}\int d^3\mathbf{r}'\,\psi_{\sigma_1}^\dagger(\mathbf{r})\psi_{\sigma_2}^\dagger(\mathbf{r}')\{\boldsymbol{\nabla}_r\nu_C(\mathbf{r},\mathbf{r}')\cdot(\hat{\mathbf{p}}_{r'}\times\boldsymbol{\tau}_{\sigma_1\sigma_3})\}\psi_{\sigma_2}(\mathbf{r}')\psi_{\sigma_3}(\mathbf{r}), \tag{4}$$

where

$$\mu_B=\frac{e\hbar}{2mc}=\text{Bohr magneton},$$
$$\hat{\mathbf{p}}_r=-i\boldsymbol{\nabla}_r \text{ is the linear momentum operator,}$$
$$\mathbf{E}(\mathbf{r})=-\boldsymbol{\nabla}_r V_{ei}(\mathbf{r}) \text{ and } \nu_C(\mathbf{r},\mathbf{r}')=|\mathbf{r}-\mathbf{r}'|^{-1}.$$

Here and elsewhere we denote the vector-cross-product by $\times$. We have chosen the notations to make the meaning of the terms self-evident. In all subsequent development, we use units with $\hbar=1$. By expressing the total Hamiltonian in terms of the two coupling constants, e^2 and μ_B^2, we hope to have exhibited the relative orders of magnitude of the two interactions. We should point out that all of magnetism is of order μ_B^2, and the Coulomb interactions in general get screened by the other electrons while the magnetic terms are (Pauli) enhanced by the interactions, we have here a subtle interplay of interactions and correlations among the electrons. The purpose of this paper is to address this point in some detail, which, to the best of our knowledge, has not been explicitly discussed in the literature. For ease of comparison of our Hamiltonian with that considered in Ref. 6, we express Eqs. (3) and (4) in the plane-wave representation as is done in Ref. 6:

$$\hat{V}_{\mathrm{s.s.o}}=i\mu_B^2\sum_{kk'q,\alpha\beta\gamma}\nu_C(q)[(\mathbf{q}\times\mathbf{k})\cdot\boldsymbol{\tau}_{\beta\alpha}]C_{k\beta}^\dagger C_{k'\gamma}^\dagger C_{k'+q\gamma}C_{k-q\alpha}, \tag{3'}$$

$$\hat{V}_{\mathrm{s.o.o}}=-2i\mu_B^2\sum_{kk'q,\alpha\beta\gamma}\nu_C(q)[(\mathbf{q}\times\mathbf{k}')\cdot\boldsymbol{\tau}_{\beta\alpha}]C_{k\beta}^\dagger C_{k'\gamma}^\dagger C_{k'+q\gamma}C_{k-q\alpha}. \tag{4'}$$

Here we have written $\nu_C(q)=4\pi/q^2$, which is the Fourier transform of $\nu_C(\mathbf{r},\mathbf{r}')$ given above. From this it is clear by comparing with Eq. (34) given in Ref. 6, the authors misrepresented what they called spin-other-orbit interaction (see Yafet, Ref. 6).

III. SPINOR-GREEN FUNCTION THEORY

We generalize here the method of spinor-Green function used in the theory of magnetic electron systems[11] by introducing external space- and time-dependent scalar potential $U_{\mathrm{ext}}(\mathbf{r},t)$, divergenceless vector potential $\mathbf{A}_{\mathrm{ext}}(\mathbf{r},t)$, magnetic field $\mathbf{B}_{\mathrm{ext}}(\mathbf{r},t)$, and electric field $\mathbf{E}_{\mathrm{ext}}(\mathbf{r},t)$. These generate, respectively, the electron density $\hat{n}(\mathbf{r})=\Sigma_\sigma\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r})$, the linear

momentum density $\Sigma_\sigma \psi^\dagger_\sigma(\mathbf{r})[\hat{\mathbf{p}}_r \psi_\sigma(\mathbf{r})]$, the spin density $\Sigma_{\sigma,\sigma'} \psi^\dagger_\sigma(\mathbf{r})\boldsymbol{\tau}_{\sigma\sigma'}\psi_{\sigma'}(\mathbf{r})$, and the spin-orbit vector density $\Sigma_{\sigma\sigma'}\psi^\dagger_\sigma(\mathbf{r})\boldsymbol{\tau}_{\sigma\sigma'}\times[\hat{\mathbf{p}}_r\psi_{\sigma'}(\mathbf{r})]$, and facilitate the calculation of the effects of interaction Hamiltonian on the many-electron properties of the system. Here $\boldsymbol{\tau}$ is the well-known Pauli spin-matrix vector. The one-particle spinor-Green function has the form [henceforth, $1 \equiv (\mathbf{r}_1, t_1)$]

$$G^{-1}(1,2) = G_0^{-1}(1,2) - \Sigma_{xc}(1,2), \tag{5}$$

with

$$G_0^{-1}(1,2) = \begin{bmatrix} i\dfrac{\partial}{\partial t_1} - \dfrac{\hat{\vec{p}}^2_{r_1}}{2m} - V_{ei}(\vec{r}_1) - \mu_B^2 \vec{E}(\vec{r}_1)\cdot(\hat{\vec{p}}_{r_1}\times\vec{\tau}) \\ -U_{ext}(1) - \vec{B}_{ext}(1)\cdot\vec{\tau} - \vec{A}_{ext}(1)\cdot\vec{p}_{r_1} - \vec{E}_{ext}(1)\cdot(\hat{\vec{p}}_{r_1}\times\vec{\tau}) \\ -\Sigma_H(1) \end{bmatrix} \delta(1-2). \tag{6}$$

Here $\Sigma_H(1)$ is the Hartree-like mean-field contribution to the self-energy from all the interactions and $\Sigma_{xc}(12)$ is the corresponding nonlocal exchange and correlation contribution to the self-energy. Thus,

$$\begin{aligned} \Sigma_H(1) = &-ie^2\int d\bar{2}\nu_C(1\bar{2})\mathrm{tr}G(\bar{2}\bar{2}^+) - i\mu_B^2\int d\bar{2}\{\mathrm{tr}G(\bar{2}\bar{2}^+)\}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau}) \\ &+ i\mu_B^2\int d\bar{2}\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\cdot\{\mathrm{tr}[\hat{\mathbf{p}}_{r_2}\times\boldsymbol{\tau}G(\bar{2}\bar{2}')]\}_{\bar{2}'=\bar{2}^+} + 2i\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\mathrm{tr}\{\hat{\mathbf{p}}_{r_2}G(\bar{2}\bar{2}')\}_{\bar{2}'=\bar{2}^+}]\cdot\boldsymbol{\tau} \\ &+ 2i\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\mathrm{tr}\{\boldsymbol{\tau}G(\bar{2}\bar{2}^+)\}]\cdot\hat{\mathbf{p}}_{r_1}. \end{aligned} \tag{7}$$

Here tr denotes trace over spin indices. As in Ref. 11, we may express the spinor-Green function G quite generally in terms of the Pauli matrices containing a scalar and a vector component as follows:

$$\begin{aligned} G(12) = \tfrac{1}{2}\{g(12) + \boldsymbol{\tau}\cdot\mathbf{s}(12)\} \text{ so that } -iG(22^+) = \tfrac{1}{2}\{n(2) + \boldsymbol{\tau}\cdot\mathbf{s}(2)\}, \\ \text{where } n(2) = \text{number density, } \mathbf{s}(2) = \text{vector spin density.} \end{aligned} \tag{8}$$

Then Eq. (7) takes an elegant form:

$$\begin{aligned} \Sigma_H(1) = &e^2\int d\bar{2}\nu_C(1\bar{2})n(\bar{2}) + \mu_B^2\int d\bar{2}n(\bar{2})\{[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\times\hat{\mathbf{p}}_{r_1}\}\cdot\boldsymbol{\tau} - \mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot\{\hat{\mathbf{p}}_{r_2}\times\mathbf{s}(\bar{2}\bar{2}')\}_{\bar{2}'=\bar{2}^+} \\ &- 2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\times\{\hat{\mathbf{p}}_{r_2}n(\bar{2}\bar{2}')\}_{\bar{2}'=\bar{2}^+}\cdot\boldsymbol{\tau} - 2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot[\mathbf{s}(\bar{2})\times\hat{\mathbf{p}}_{r_1}]. \end{aligned} \tag{9}$$

The first term is the well-known spin-independent scalar Hartree potential due to all other electrons that is partly canceled by the positive ion contribution not explicitly displayed here; the second term is the spin-orbit contribution due to the mean electric field of all the other electrons and is a spin-dependent operator; the third term is a scalar, spin-independent mean spin-orbit potential due to all other electrons of the system; the fourth term is the self-energy due to the mean magnetic field created by the mean linear momentum of the moving electrons interacting with the electric field of the Coulomb interaction, giving rise to a spin-dependent contribution; and finally, the last term is a spin-independent operator contribution due to the mean spin-magnetic moment interacting with the electric field. Equation (9) is valid quite generally.

The exchange-correlation contribution, on the other hand, is a spinor, nonlocal contribution, and involves four types of vertex functions, reflecting the various types of interactions arising out of the electric and magnetic fields generated by the moving charges and spins in the system. Thus, we have,

$$\begin{aligned} \Sigma_{xc}(12) = &-ie^2\int d\bar{2}\int d\bar{3}\nu_C(1\bar{2})G(1\bar{3})\Gamma_0(\bar{3}\bar{2};\bar{2}) - i\mu_B^2\int d\bar{2}\int d\bar{3}\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\cdot[(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})G(1\bar{3})\Gamma_0(\bar{3}\bar{2};\bar{2})] \\ &+ i\mu_B^2\int d\bar{2}\int d\bar{3}\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\cdot G(1\bar{3})\Gamma_{SO}(\bar{3}\bar{2};\bar{2}) + 2i\mu_B^2\int d\bar{2}\int d\bar{3}\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\cdot[\boldsymbol{\tau}\times G(1\bar{3})\boldsymbol{\Gamma}_p(\bar{3}\bar{2};\bar{2})] \\ &- 2i\mu_B^2\int d\bar{2}\int d\bar{3}\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\cdot[\hat{\mathbf{p}}_{r_1}\times G(1\bar{3})\boldsymbol{\Gamma}_s(\bar{3}\bar{2};\bar{2})]. \end{aligned} \tag{10}$$

The four vertex functions appearing here are defined as follows:

$$\Gamma_0(12;3)=\frac{\delta G^{-1}(12)}{\delta U_{\rm ext}(3)};\quad \mathbf{\Gamma}_{SO}(12;3)=\frac{\delta G^{-1}(12)}{\delta \mathbf{E}_{\rm ext}(3)};\quad \mathbf{\Gamma}_p(12;3)=\frac{\delta G^{-1}(12)}{\delta \mathbf{A}_{\rm ext}(3)};\quad \mathbf{\Gamma}_s(12;3)=\frac{\delta G^{-1}(12)}{\delta \mathbf{B}_{\rm ext}(3)}. \tag{11}$$

The subscripts on the vertex functions are chosen to indicate clearly their physical meaning. Thus, Γ_0, indicating the vertex associated with particle-density, $\mathbf{\Gamma}_{SO}$, with spin-orbit density, $\mathbf{\Gamma}_p$, with particle-momentum density, and $\mathbf{\Gamma}_s$, with the spin density. The latter three are vector vertex functions. The equations obeyed by these vertex functions are deduced by taking the appropriate functional derivatives of Eq. (5), which we will not display here in its full glory. In the next section however, we will outline some commonly employed approximation schemes.

IV. APPROXIMATION SCHEMES: GENERAL

The following approximation schemes and their consequences are worth noting:

(a) Mean-field approximation: This is the lowest order scheme where all the vertex functions are set equal to zero. Even at this level, the single-particle Green function is a spinor, due to the various spin-orbit contributions in the Hartree-like scheme given by Eq. (9), and must be solved self-consistently. This Green function gives us the spectrum of single-particle energies. We may point out that in Ref. 6, third and fifth terms in their Hartree approximation are missing because they did not consider spin polarization of the magnetic system. Also missing is the fourth term due to their neglect of spin-same orbit contribution.

(b) Exchange only approximation: This is the leading order approximation to the equations obeyed by the vertex functions. They are

$$\begin{aligned}
\Gamma_0(12;3)&\approx-\delta(12)\,\delta(13)=\gamma_0(12;3),\\
\mathbf{\Gamma}_{SO}(12;3)&\approx-\delta(13)(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})\,\delta(12)=\boldsymbol{\gamma}_{SO}(12;3),\\
\mathbf{\Gamma}_p(12;3)&\approx-\delta(13)\hat{\mathbf{p}}_{r_1}\delta(12)=\boldsymbol{\gamma}_p(12;3),\ \text{and}\\
\mathbf{\Gamma}_s(12;3)&\approx-\boldsymbol{\tau}\delta(12)\,\delta(13)=\boldsymbol{\gamma}_s(12;3),
\end{aligned}\tag{12}$$

and the exchange only self-energy is then given by

$$\begin{aligned}
\Sigma_x(12)=&\,ie^2\nu_C(12)G^<(12)\\
&+i\mu_B^2[\nabla_{r_1}\nu_C(12)]\times[\hat{\mathbf{p}}_{r_1}\cdot\boldsymbol{\tau}G^<(12)]\\
&+2i\mu_B^2[\nabla_{r_1}\nu_C(12)]\times[\hat{\mathbf{p}}_{r_2}\cdot\boldsymbol{\tau}G^<(12)]\\
&+i\mu_B^2\{[\nabla_{r_1}\nu_C(12)]\times[\hat{\mathbf{p}}_{r_2}G^<(12)]\}\cdot\boldsymbol{\tau}\\
&-2i\mu_B^2\{[\nabla_{r_1}\nu_C(12)]\times[\hat{\mathbf{p}}_{r_1}G^<(12)]\}\cdot\boldsymbol{\tau}.
\end{aligned}\tag{13}$$

In obtaining this result we have integrated by parts whenever needed in the manipulation of δ functions and some well-known vector identities. As with the Hartree approximation, the various terms have similar significance: the first term is the well-known exchange contribution due to Coulomb interactions between electrons, while the last four terms are due to the two types of spin-orbit interactions among the electrons. These contributions were not considered in Ref. 6.

(c) Random-phase approximation: Here the vertex functions are derived by considering the Hartree contributions in Eq. (6) and so the various vertex functions in Eq. (7) take on additional contributions. These equations can be solved as they are algebraic in structure, as in the conventional case. It suffices here to note that this approximation leads to ''screening'' of the interactions in Eq. (13), thus leading to a generalized ''screened exchange scheme.'' This generalization includes terms arising not only from the density fluctuations but also from the spin density, momentum density due to orbital motion, as well as spin-momentum density fluctuations in addition to cross correlations between them, which have not been considered in the literature before, it appears. Many of these contributions are zero if we consider nonmagnetic systems and systems with center of symmetry. These aspects will be discussed in a subsequent, more detailed paper.

(d) Random-phase approximation with exchange corrections: Here the exchange terms are included in setting up the equations for the various vertex functions, which then obey integral equations, which have to be solved in conjunction with the Green function equations. We will relegate discussion of these to another paper.

The inclusion of phonon mediated spin-orbit interaction proceeds by considering ion displacements in the electron ion and the single-particle spin-orbit interaction arising from the ions as considered in Ref. 6. Our technique for dealing with these contributions proceeds by adopting the Green function technique to include these contributions in a generalization of the self-consistent perturbation method given in Ref. 12. We not only derive the results given in Ref. 6 but also find the appropriate screening of the spin-orbit contribution when spin polarization is included, even when only the Coulomb interaction between electrons is taken into account, showing that there is a screening contribution without invoking spin-other-orbit interaction. This was already seen in a discussion of the phonon spectrum of magnetic systems in Ref. 7.

In a fully relativistic formulation, it may be remarked, the effects considered here would appear in a simple looking elegant form, in terms of the four-current correlations, and the corresponding vertex functions. When resolved in terms of a nonrelativistic scheme, these become expanded in terms of particle current, particle density, spin density, spin-current density with corresponding external four potential taking the form of electric and magnetic fields, and the scalar and vector potentials. For our present purposes, our development suffices and is transparent. In the next section, we examine in detail the random-phase approximation and its implications.

V. RESULTS BASED ON RANDOM-PHASE APPROXIMATION

Using Eq. (7) for the Hartree self-energy and the definitions of the four vertex functions in Eq. (11), we see that the

equation for each of them leads to four correlation functions corresponding to the four densities contained therein as explained in Eq. (9). These equations, being algebraic, can all be solved as in the magnetic case.[11] In this paper, we will illustrate these solutions for metallic magnetic systems where plane-wave solutions are pertinent. In a separate paper, we will present the solutions in terms of the orbitals that take account of the one-particle spin-orbit potential so that the solutions are applicable more generally. By using the plane-wave scheme, we may be able to understand the physical meaning of the various contributions, which are here derived for the first time. We will present the details of the calculation for the vertex associated with the density Γ_0 and give the final results for the rest of the vertex functions. This involves four types of correlation functions defined in a manner similar to the ones in Ref. 11:

$$\chi_{o,o}(12)=-i\,\frac{\delta}{\delta U_{\rm ext}(2)}\,{\rm tr}G(11^+)=i\int d\bar{1}d\bar{2}\,{\rm tr}[G(1\bar{1})\Gamma_0(\bar{1}\bar{2};2)G(\bar{2}\bar{1}^+)],$$

$$\boldsymbol{\chi}_{so,o}(12)=-i\,\frac{\delta}{\delta U_{\rm ext}(2)}\,{\rm tr}[(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})G(11'^+)]_{1'=1}=i\int d\bar{1}d\bar{2}\,{\rm tr}[(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})G(1\bar{1})\Gamma_0(\bar{1}\bar{2};2)G(\bar{2}\bar{1}'^+)]_{1'=1},$$

$$\boldsymbol{\chi}_{p,o}(12)=-i\,\frac{\delta}{\delta U_{\rm ext}(2)}\,{\rm tr}[(\hat{\mathbf{p}}_{r_1})G(11'^+)]_{1'=1}=i\int d\bar{1}d\bar{2}\,{\rm tr}[(\hat{\mathbf{p}}_{r_1})G(1\bar{1})\Gamma_0(\bar{1}\bar{2};2)G(\bar{2}\bar{1}'^+)]_{1'=1},$$

and

$$\boldsymbol{\chi}_{s,o}(12)=-i\,\frac{\delta}{\delta U_{\rm ext}(2)}\,{\rm tr}[(\boldsymbol{\tau})G(11^+)]=i\int d\bar{1}d\bar{2}\,{\rm tr}[(\boldsymbol{\tau})G(1\bar{1})\Gamma_0(\bar{1}\bar{2};2)G(\bar{2}\bar{1}^+)]. \tag{14}$$

The first one is the particle density-particle density, the second, the spin-orbit density-particle density, the third, the momentum density-particle density, and the last one is the spin density-particle density correlation functions. The first and the last ones were introduced earlier in the study of the magnetic problem without spin-orbit effects.[11] The vertex function Γ_0 obeys the equation, from the definition in Eqs. (11) and (5), and those in Eq. (14):

$$\begin{aligned}\Gamma_0(12;3)=\gamma_0(12;3)-e^2\int d\bar{2}\chi_{o,o}(\bar{2}\bar{3})\nu_C(1\bar{2})\delta(1-2)-\mu_B^2\int d\bar{2}\chi_{o,o}(\bar{2}\bar{3})[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})\delta(1-2)\\ +\mu_b^2\int d\bar{2}\boldsymbol{\chi}_{so,o}(\bar{2}\bar{3})\cdot[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\delta(1-2)+2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\boldsymbol{\chi}_{p,o}(\bar{2}\bar{3})]\cdot\boldsymbol{\tau}\delta(1-2)\\ +2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\boldsymbol{\chi}_{s,o}(\bar{2}\bar{3})]\cdot\hat{\mathbf{p}}_{r_1}\delta(1-2).\end{aligned} \tag{15}$$

Further analysis of this equation and its solution is now presented in the plane-wave representation appropriate for metallic systems as in Ref. 11. Thus we define, using the standard four-dimensional notation

$$G(12)=\int G(k)e^{ik(1-2)}\,\frac{d^4k}{(2\pi)^4},\quad \Gamma(12;3)=\int\Gamma(k,q)e^{ik(1-2)+iq(1-3)}\,\frac{d^4k}{(2\pi)^4}\,\frac{d^4q}{(2\pi)^4}, \tag{16}$$

and obtain the following expressions for the correlation functions defined in Eq. (15):

$$\chi_{o,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,{\rm tr}[G(k+q)\Gamma_0(k,q)G(k)],$$

$$\boldsymbol{\chi}_{so,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,{\rm tr}\{[(\mathbf{k}+\mathbf{q})\times\boldsymbol{\tau}]G(k+q)\Gamma_0(k,q)G(k)\},$$

$$\boldsymbol{\chi}_{p,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,{\rm tr}[(\mathbf{k}+\mathbf{q})G(k+q)\Gamma_0(k,q)G(k)],$$

and

$$\boldsymbol{\chi}_{s,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,{\rm tr}[(\boldsymbol{\tau})G(k+q)\Gamma_0(k,q)G(k)], \tag{17}$$

Equation (15) then reads

$$\Gamma_0(k,q)=-1-e^2\nu_C(q)\chi_{o,o}(q)-i\mu_B^2\nu_C(q)\chi_{o,o}(q)[(\mathbf{k}\times\boldsymbol{\tau})\cdot\mathbf{q}]+i\mu_B^2\nu_C(q)\mathbf{q}\cdot\boldsymbol{\chi}_{so,o}(q)$$
$$+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\boldsymbol{\chi}_{p,o}(q)]\cdot\boldsymbol{\tau}+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\boldsymbol{\chi}_{s,o}(q)]\cdot\mathbf{k}. \tag{18}$$

This expression in Eq. (17) leads to the determination of the four correlation functions in terms of 16 types of correlation functions of the Lindhard type:

$$\Pi_{o,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[G(k+q)G(k)],\quad \boldsymbol{\Pi}_{o,so}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[G(k+q)(\mathbf{k}\times\boldsymbol{\tau})G(k)],$$

$$\boldsymbol{\Pi}_{o,s}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[G(k+q)\boldsymbol{\tau}G(k)],\quad \boldsymbol{\Pi}_{o,p}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[G(k+q)\mathbf{k}G(k)], \tag{19a}$$

going with the equation for $\chi_{0,0}$:

$$\chi_{o,o}(q)=-\Pi_{o,o}(q)-\nu_C(q)[e^2\Pi_{o,o}(q)+i\mu_B^2\mathbf{q}\cdot\boldsymbol{\Pi}_{o,so}(q)]\chi_{o,o}(q)+i\mu_B^2\nu_C(q)\Pi_{o,o}(q)\mathbf{q}\cdot\boldsymbol{\chi}_{so,o}(q)$$
$$+2i\mu_B^2\nu_C(q)\boldsymbol{\Pi}_{o,s}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{p,o}(q)]+2i\mu_B^2\nu_C(q)\boldsymbol{\Pi}_{o,p}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{s,o}(q)]. \tag{19b}$$

Similarly,

$$\boldsymbol{\Pi}_{so,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}\{[(\mathbf{k}+\mathbf{q})\times\boldsymbol{\tau}]G(k+q)G(k)\},\quad \overleftrightarrow{\Pi}_{so,so}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}\{[(\mathbf{k}+\mathbf{q})\times\boldsymbol{\tau}]G(k+q)(\mathbf{k}\times\boldsymbol{\tau})G(k)\},$$

$$\overleftrightarrow{\Pi}_{so,s}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}\{[(\mathbf{k}+\mathbf{q})\times\boldsymbol{\tau}]G(k+q)\boldsymbol{\tau}G(k)\},\quad \overleftrightarrow{\Pi}_{so,p}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}\{[(\mathbf{k}+\mathbf{q})\times\boldsymbol{\tau}]G(k+q)\mathbf{k}G(k)\}, \tag{20a}$$

going with

$$\boldsymbol{\chi}_{so,o}(q)=-\boldsymbol{\Pi}_{so,o}(q)-\nu_C(q)[e^2\boldsymbol{\Pi}_{so,o}(q)+i\mu_B^2\mathbf{q}\cdot\overleftrightarrow{\Pi}_{so,so}(q)]\chi_{o,o}(q)+i\mu_B^2\nu_C(q)\boldsymbol{\Pi}_{so,o}(q)[\mathbf{q}\cdot\boldsymbol{\chi}_{so,o}(q)]$$
$$+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{so,s}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{p,o}(q)]+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{so,p}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{s,o}(q)]. \tag{20b}$$

$$\boldsymbol{\Pi}_{p,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[(\mathbf{k}+\mathbf{q})G(k+q)G(k)],\quad \overleftrightarrow{\Pi}_{p,so}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[(\mathbf{k}+\mathbf{q})G(k+q)(\mathbf{k}\times\boldsymbol{\tau})G(k)],$$

$$\overleftrightarrow{\Pi}_{p,s}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[(\mathbf{k}+\mathbf{q})G(k+q)\boldsymbol{\tau}G(k)],\quad \overleftrightarrow{\Pi}_{p,p}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[(\mathbf{k}+\mathbf{q})G(k+q)\mathbf{k}G(k)], \tag{21a}$$

going with

$$\boldsymbol{\chi}_{p,o}(q)=-\boldsymbol{\Pi}_{p,o}(q)-\nu_C(q)[e^2\boldsymbol{\Pi}_{p,o}(q)+i\mu_B^2\mathbf{q}\cdot\overleftrightarrow{\Pi}_{p,so}(q)]\chi_{o,o}(q)+i\mu_B^2\nu_C(q)\boldsymbol{\Pi}_{p,o}(q)[\mathbf{q}\cdot\boldsymbol{\chi}_{so,o}(q)]$$
$$+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{p,s}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{p,o}(q)]+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{p,p}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{s,o}(q)]. \tag{21b}$$

$$\boldsymbol{\Pi}_{s,o}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[\boldsymbol{\tau}G(k+q)G(k)],\quad \overleftrightarrow{\Pi}_{s,so}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[\boldsymbol{\tau}G(k+q)(\mathbf{k}\times\boldsymbol{\tau})G(k)],$$

$$\overleftrightarrow{\Pi}_{s,s}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[\boldsymbol{\tau}G(k+q)\boldsymbol{\tau}G(k)],\quad \overleftrightarrow{\Pi}_{s,p}(q)=i\int\frac{d^4k}{(2\pi)^4}\,\mathrm{tr}[\boldsymbol{\tau}G(k+q)\mathbf{k}G(k)], \tag{22a}$$

going with

$$\boldsymbol{\chi}_{s,o}(q)=-\boldsymbol{\Pi}_{s,o}(q)-\nu_C(q)[e^2\boldsymbol{\Pi}_{s,o}(q)+i\mu_B^2\mathbf{q}\cdot\overleftrightarrow{\Pi}_{s,so}(q)]\chi_{o,o}(q)+i\mu_B^2\nu_C(q)\boldsymbol{\Pi}_{s,o}(q)[\mathbf{q}\cdot\boldsymbol{\chi}_{so,o}(q)]$$
$$+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{s,s}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{p,o}(q)]+2i\mu_B^2\nu_C(q)\overleftrightarrow{\Pi}_{s,p}(q)\cdot[\mathbf{q}\times\boldsymbol{\chi}_{s,o}(q)]. \tag{22b}$$

These simultaneous linear equations for the four correlation functions can be solved in terms of the generalized Lindhard-like functions introduced above and, in their turn, they determine the vertex function Γ_0. To give an indication of the type of result we would obtain, we here give an approximate solution of this problem, by observing for the present that the Coulomb term is the most dominant while those appearing with the Bohr magneton are smaller in magnitude. This is strictly for purposes of illustration only and more detailed examination of these equations will be relegated to another paper. Here we want to establish that this study has important implications to magnetic properties of systems.

Thus we have the following approximate results:

$$\chi_{o,o}(q)\cong-\varepsilon^{-1}(q)\Pi_{o,o}(q),\ \ \boldsymbol{\chi}_{so,o}(q)\cong-\varepsilon^{-1}(q)\boldsymbol{\Pi}_{so,o}(q),$$

$$\boldsymbol{\chi}_{p,o}(q)\cong-\varepsilon^{-1}(q)\boldsymbol{\Pi}_{p,o}(q),\ \text{ and }\ \boldsymbol{\chi}_{s,o}(q)\cong-\varepsilon^{-1}(q)\boldsymbol{\Pi}_{s,o}(q),$$

$$\text{where }\ \varepsilon(q)=1+e^2\nu_C(q)\Pi_{o,o}(q)=\text{RPA dielectric function.} \tag{23}$$

This in turn gives the vertex function Γ_0 from Eq. (18) to be

$$\Gamma_0(k,q)\equiv\varepsilon^{-1}(q)\left\{-1+i\mu_B^2\nu_C(q)\begin{bmatrix}\Pi_{0,0}(q)(\vec{q}\times\vec{k})\cdot\vec{\tau}\\ -\vec{q}\cdot\vec{\Pi}_{s0,0}(q)-2(\vec{q}\times\vec{\Pi}_{p,0}(q))\cdot\vec{\tau}\\ -2(\vec{q}\times\vec{\pi}_{s,0}(q))\cdot\vec{k}\end{bmatrix}\right\}. \tag{24}$$

We should remark here that in a more complete theory, the random-phase approximation (RPA) dielectric function would be replaced by a more complete and complicated screening function and the expressions (23) and (24) would be much different from those given here. These will be discussed in another paper. A similar calculation gives the other three vertex functions of interest and we give them here without exhibiting their derivation as they are obtained in the same manner as was described above.

$$\begin{aligned}\boldsymbol{\Gamma}_{so}(12;3)=\boldsymbol{\gamma}_{so}(12;3)&-e^2\int d\overline{2}\,\boldsymbol{\chi}_{o,so}(\overline{23})\nu_C(1\overline{2})\delta(1-2)-\mu_B^2\int d\overline{2}\,\boldsymbol{\chi}_{o,so}(\overline{23})[\boldsymbol{\nabla}_{r_1}\nu_C(1\overline{2})]\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})\delta(1-2)\\&+\mu_B^2\int d\overline{2}\,\overleftrightarrow{\chi}_{so,so}(\overline{23})\cdot[\boldsymbol{\nabla}_{r_1}\nu_C(1\overline{2})]\delta(1-2)+2\mu_B^2\int d\overline{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\overline{2})\times\overleftrightarrow{\chi}_{p,so}(\overline{23})]\cdot\boldsymbol{\tau}\delta(1-2)\\&+2\mu_B^2\int d\overline{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\overline{2})\times\overleftrightarrow{\chi}_{s,so}(\overline{23})]\cdot\hat{\mathbf{p}}_{r_1}\delta(1-2).\end{aligned} \tag{25a}$$

In the plane-wave representation, this is

$$\begin{aligned}\boldsymbol{\Gamma}_{so}(k,q)=&-(\mathbf{k}\times\boldsymbol{\tau})-e^2\nu_C(q)\boldsymbol{\chi}_{o,so}(q)-i\mu_B^2\nu_C(q)\boldsymbol{\chi}_{o,so}(q)[(\mathbf{k}\times\boldsymbol{\tau})\cdot\mathbf{q}]+i\mu_B^2\nu_C(q)\mathbf{q}\cdot\overleftrightarrow{\chi}_{so,so}(q)\\&+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{p,so}(q)]\cdot\boldsymbol{\tau}+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{s,so}(q)]\cdot\mathbf{k}.\end{aligned} \tag{25b}$$

The approximate results corresponding to Eqs. (23) and (24) are then

$$\boldsymbol{\chi}_{o,so}(q)\cong-\varepsilon^{-1}(q)\boldsymbol{\Pi}_{o,so}(q),$$

$$\overleftrightarrow{\chi}_{so,so}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{so,so}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{so,so}\Pi_{o,o}-\boldsymbol{\Pi}_{so,o}\boldsymbol{\Pi}_{o,so})\},$$

$$\overleftrightarrow{\chi}_{p,so}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{p,so}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{p,so}\Pi_{o,o}-\boldsymbol{\Pi}_{p,o}\boldsymbol{\Pi}_{o,so})\},$$

$$\text{and }\ \overleftrightarrow{\chi}_{s,so}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{s,so}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{s,so}\Pi_{o,o}-\boldsymbol{\Pi}_{s,o}\boldsymbol{\Pi}_{o,so})\},$$

$$\text{where }\ \varepsilon(q)=1+e^2\nu_C(q)\Pi_{o,o}(q)=\text{RPA dielectric function.} \tag{25c}$$

This gives to leading order in the interaction strengths e^2,μ_B^2,

$$\vec{\Gamma}_{s0}(k,q)\cong\varepsilon^{-1}(q)\left\{\begin{array}{l}-(\vec{k}\times\vec{\tau})(1+e^2\nu_C(q)\Pi_{0,0}(q))+e^2\nu_C(q)\vec{\boldsymbol{\Pi}}_{0,s0}(q)\\ +i\mu_B^2\nu_C(q)\begin{bmatrix}\vec{\boldsymbol{\Pi}}_{0,s0}(q)(\vec{q}\times\vec{k})\cdot\vec{\tau}\\ -\vec{q}\cdot\vec{\Pi}_{s0,s}(q)-2(\vec{q}\times\vec{\overleftrightarrow{\Pi}}_{p,s0}(q))\cdot\vec{\tau}\\ -2(\vec{q}\times\vec{\overleftrightarrow{\Pi}}_{s,s0}(q))\cdot\vec{k}\end{bmatrix}\end{array}\right\} \tag{25d}$$

Similarly, we have

$$\mathbf{\Gamma}_p(12;3)=\boldsymbol{\gamma}_p(12;3)-e^2\int d\bar{2}\,\boldsymbol{\chi}_{o,p}(\bar{2}\bar{3})\,\nu_C(1\bar{2})\,\delta(1-2)-\mu_B^2\int d\bar{2}\,\boldsymbol{\chi}_{o,p}(\bar{2}\bar{3})[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})\,\delta(1-2)$$
$$+\mu_B^2\int d\bar{2}\,\overleftrightarrow{\chi}_{so,p}(\bar{2}\bar{3})\cdot[\boldsymbol{\nabla}_{r_1}\nu_c(1\bar{2})]\delta(1-2)+2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\overleftrightarrow{\chi}_{p,p}(\bar{2}\bar{3})]\cdot\boldsymbol{\tau}\delta(1-2)$$
$$+2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\overleftrightarrow{\chi}_{s,p}(\bar{2}\bar{3})]\cdot\hat{\mathbf{p}}_{r_1}\delta(1-2). \tag{26a}$$

In the plane-wave representation, this is

$$\mathbf{\Gamma}_p(k,q)=-\mathbf{k}-e^2\nu_C(q)\boldsymbol{\chi}_{o,p}(q)-i\mu_B^2\nu_C(q)\boldsymbol{\chi}_{o,p}(q)[(\mathbf{k}\times\boldsymbol{\tau})\cdot\mathbf{q}]+i\mu_B^2\nu_C(q)\mathbf{q}\cdot\overleftrightarrow{\chi}_{so,p}(q)$$
$$+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{p,p}(q)]\cdot\boldsymbol{\tau}+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{s,p}(q)]\cdot\mathbf{k}. \tag{26b}$$

The approximate results corresponding to Eqs. (23) and (24) are then

$$\boldsymbol{\chi}_{o,p}(q)\cong-\varepsilon^{-1}(q)\mathbf{\Pi}_{o,p}(q),$$
$$\overleftrightarrow{\boldsymbol{\chi}}_{so,p}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{so,p}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{so,p}\Pi_{o,o}-\mathbf{\Pi}_{so,o}\mathbf{\Pi}_{o,p})\},$$
$$\overleftrightarrow{\chi}_{p,p}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{p,p}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{p,p}\Pi_{o,o}-\mathbf{\Pi}_{p,o}\mathbf{\Pi}_{o,p})\},$$
$$\text{and}\quad\overleftrightarrow{\chi}_{s,p}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{s,p}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{s,p}\Pi_{o,o}-\mathbf{\Pi}_{s,o}\mathbf{\Pi}_{o,p})\},$$
$$\text{where}\quad\varepsilon(q)=1+e^2\nu_C(q)\Pi_{o,o}(q)=\text{RPA dielectric function}. \tag{26c}$$

To leading order in the interaction strengths, as before,

$$\vec{\Gamma}_p(k,q)\cong\varepsilon^{-1}(q)\left\{\begin{array}{l}-(\vec{k})(1+e^2\nu_C(q)\Pi_{0,0}(q))+e^2\nu_C(q)\vec{\Pi}_{0,p}(q)\\ +i\mu_B^2\nu_C(q)\left[\begin{array}{l}\vec{\pi}_{0,p}(q)(\vec{q}\times\vec{k})\cdot\vec{\tau}\\ -\vec{q}\cdot\overleftrightarrow{\Pi}_{s0,p}(q)-2(\vec{q}\times\overleftrightarrow{\pi}_{p,p}(q))\cdot\vec{\tau}\\ -2(\vec{q}\times\overleftrightarrow{\Pi}_{s,p}(q))\cdot\vec{k}\end{array}\right]\end{array}\right\} \tag{26d}$$

And finally,

$$\mathbf{\Gamma}_s(12;3)=\boldsymbol{\gamma}_s(12;3)-e^2\int d\bar{2}\,\boldsymbol{\chi}_{o,s}(\bar{2}\bar{3})\,\nu_C(1\bar{2})\,\delta(1-2)-\mu_B^2\int d\bar{2}\,\boldsymbol{\chi}_{o,s}(\bar{2}\bar{3})[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})\,\delta(1-2)$$
$$+\mu_B^2\int d\bar{2}\,\overleftrightarrow{\chi}_{so,s}(\bar{2}\bar{3})\cdot[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})]\delta(1-2)+2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\overleftrightarrow{\chi}_{p,s}(\bar{2}\bar{3})]\cdot\boldsymbol{\tau}\delta(1-2)$$
$$+2\mu_B^2\int d\bar{2}[\boldsymbol{\nabla}_{r_1}\nu_C(1\bar{2})\times\overleftrightarrow{\chi}_{s,s}(\bar{2}\bar{3})]\cdot\hat{\mathbf{p}}_{r_1}\delta(1-2). \tag{27a}$$

In the plane-wave representation, this is

$$\mathbf{\Gamma}_s(k,q)=-\boldsymbol{\tau}-e^2\nu_C(q)\boldsymbol{\chi}_{o,s}(q)-i\mu_B^2\nu_C(q)\boldsymbol{\chi}_{o,s}(q)[(\mathbf{k}\times\boldsymbol{\tau})\cdot\mathbf{q}]+i\mu_B^2\nu_C(q)\mathbf{q}\cdot\overleftrightarrow{\chi}_{so,s}(q)$$
$$+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{p,s}(q)]\cdot\boldsymbol{\tau}+2i\mu_B^2\nu_C(q)[\mathbf{q}\times\overleftrightarrow{\chi}_{s,s}(q)]\cdot\mathbf{k}. \tag{27b}$$

The approximate results corresponding to Eqs. (23) and (24) are then

$$\boldsymbol{\chi}_{o,s}(q)\cong-\varepsilon^{-1}(q)\mathbf{\Pi}_{o,s}(q),$$
$$\overleftrightarrow{\chi}_{so,s}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{so,s}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{so,s}\Pi_{o,o}-\mathbf{\Pi}_{so,o}\mathbf{\Pi}_{o,s})\},$$
$$\overleftrightarrow{\chi}_{p,s}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{p,s}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{p,s}\Pi_{o,o}-\mathbf{\Pi}_{p,o}\mathbf{\Pi}_{o,s})\},$$
$$\text{and}\quad\overleftrightarrow{\chi}_{s,s}(q)\cong-\varepsilon^{-1}(q)\{\overleftrightarrow{\Pi}_{s,s}(q)+e^2\nu_C(\overleftrightarrow{\Pi}_{s,s}\Pi_{o,o}-\mathbf{\Pi}_{s,o}\mathbf{\Pi}_{o,s})\},$$
$$\text{where}\quad\varepsilon(q)=1+e^2\nu_C(q)\Pi_{o,o}(q)=\text{RPA dielectric function}. \tag{27c}$$

And, again to leading order in the interaction strengths,

$$\vec{\Gamma}(k,q)\equiv\varepsilon^{-1}(q)\left\{\begin{array}{c}-(\vec{\tau})(1+e^2\nu_C(q)\Pi_{0,0}(q))+e^2\nu_C(q)\mathbf{\Pi}_{0,s}(q)\\ +i\mu_B^2\nu_C(q)\left[\begin{array}{l}\mathbf{\Pi}_{0,s}(q)(\vec{q}\times\vec{k})\cdot\vec{\tau}\\ -\vec{q}\cdot\vec{\vec{\Pi}}_{s0,s}(q)-2(\vec{q}\times\vec{\vec{\Pi}}_{p,s}(q))\cdot\vec{\tau}\\ -2(\vec{q}\times\vec{\vec{\Pi}}_{s,s}(q)\cdot\vec{k}\end{array}\right]\end{array}\right\} \tag{27d}$$

This derivation of the various vertex functions even within a simple RPA is significant because it gives us important insights into the many-body contributions to ''screening'' of the various interactions and into the nature of the various response functions that arise in this system. To bring the first point out, we now write the exchange-correlation self-energy, Eq. (10), in the plane-wave representation:

$$\begin{aligned}\Sigma_{xc}(k)=&-ie^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')\Gamma_o(k,k')+i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')(\mathbf{k}'\times\mathbf{k})\cdot\boldsymbol{\tau}G(k+k')\Gamma_0(k,k')\\&-i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')\mathbf{k}'\cdot\mathbf{\Gamma}_{so}(k,k')-2i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')\mathbf{k}'\cdot[\boldsymbol{\tau}\times G(k+k')\mathbf{\Gamma}_p(k,k')]\\&-2i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')(\mathbf{k}'\times\mathbf{k})\cdot\mathbf{\Gamma}_s(k,k').\end{aligned} \tag{28}$$

This expression clearly shows that the screenings of the various interactions are determined by the four vertex functions. As in Sec. IV, we can now discuss several levels of approximations. Neglecting the vertex functions entirely is the ''mean-field'' approximation discussed in Ref. 6 that we have commented upon already. The next level is to take the leading-order approximations to these vertex functions as in Eq. (12). We thus obtain

$$\begin{aligned}\Sigma_x(k)=&+ie^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')-i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')(\mathbf{k}'\times\mathbf{k})\cdot\boldsymbol{\tau}G(k+k')\\&+i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')(\mathbf{k}'\times\mathbf{k})\cdot\boldsymbol{\tau}+2i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')(\mathbf{k}'\times\mathbf{k})\cdot\boldsymbol{\tau}G(k+k')\\&+2i^2\mu_B^2\int\frac{d^4k'}{(2\pi)^4}\,\nu_C(k')G(k+k')(\mathbf{k}'\times\mathbf{k})\cdot\boldsymbol{\tau}.\end{aligned} \tag{29}$$

It is important to note the orders of the spinor Green function and the Pauli matrix appearing in the above expressions. In the nonmagnetic case, with a scalar Green function, the second and third terms cancel out leaving behind the last two combining into a single term.

In the next level of approximation, we use the approximate RPA vertex functions derived above in Eq. (26), which clearly shows the screening of the various terms in a clear fashion. To leading order in the interaction strengths, only the first term in Eq. (29), the Coulomb interaction is screened by the RPA dielectric function, while in the rest of the terms it is not. But, a more sophisticated approximation, beyond the simplified version of RPA presented here and not in terms of orders of interaction strengths, immediately shows that screening occurs in different forms for each of the terms in Eq. (29) according to the form of the interaction, as for example, the spin-susceptibility enhancement due to interactions familiar in other contexts. This will be taken up for study in another paper.

The second point of interest in this development is the sixteen types of correlation functions that appear in this system. This reflects the varied nature of physical mechanisms underlying the two-particle interactions when the spin-orbit effects are included in our considerations. In physical terms, they arise because the linear momentum and spin momentum vectors can now be independently specified, and therefore the system acquires chirality. This is specially important in the magnetic systems where such anisotropy is evident in the domain structure, optical dichroism, etc. This also indicates another important feature of a possible vector-spin density-functional theory in contrast to the magnetic electron-gas spin-density-functional theory where one can only specify one component of the spin density, as in an Ising model of magnetism. These features will be explored in a future paper.

VI. CONCLUDING REMARKS

In conclusion, we have here presented a theoretical framework for incorporating spin-orbit effects in a many-body

theory of itinerant magnetic systems. We have shown here a variety of contributions, not present in nonmagnetic systems, that arise due to spin polarization and the spin-orbit interaction already within a simplified approximation of the RPA. More sophisticated integral equations for the vertex functions appear when we take the nonlocal exchange self-energy in their construction. Much work needs to be done in the analysis of these equations along with their physical implications. These considerations are expected to be of importance not only in the development of the vector-spin density-functional theory of itinerant electron magnetism, but also in many of the new investigations of magnetic phenomena particularly in low-dimensional nanometric systems and in magnetic cluster materials. The development given here brings out the spin and spatial anisotropies in the system in an elegant way. Among the sixteen types of correlation functions that appear in this system, the ones corresponding to purely particle density, spin density, and linear momentum density are familiar in separate physical contexts of dielectric, magnetic, and electromagnetic response, respectively. But in the present discussion, these, along with the new spin-orbit density, add to the structure of the theory of itinerant electron magnetism. To make this point explicit, consider as in Ref. 6 the one-particle terms $\hat{V}_{ei}$, the (periodic) potential due to the ions in the system, and $\hat{V}_{\mathrm{s.o}}$, the spin-orbit contribution in Eq. (1) to be weak so that a perturbation treatment would suffice. When the two-particle interactions are brought into consideration, these contributions are modified. The vertex function method[12] provides a clear way of developing this perturbation scheme including the nonlocal contributions. For purposes of illustration, we here follow Ref. 6, and exhibit the result in the Hartree approximation. Observing that the (periodic) potential $\hat{V}_{ei}$ then takes the place of the external potential $U_{\mathrm{ext}}(\mathbf{r},t)$, and the spin-orbit potential $\hat{V}_{\mathrm{s.o}}$ takes the place of the external electric field $\mathbf{E}_{\mathrm{ext}}(\mathbf{r},t)$ without their time dependence, we obtain the modified effective one-particle potential in the form

$$V_{\mathrm{eff}}(\mathbf{r}_1)\cong\left[V_{ei}(\mathbf{r}_1)+\int d2\,\frac{-\delta\Sigma_H(1)}{\delta V_{ei}(\mathbf{r}_2)}\,V_{ei}(\mathbf{r}_2)\right]+\left[\mu_B^2\mathbf{E}(\mathbf{r}_1)\cdot(\hat{\mathbf{p}}_{r_1}\times\boldsymbol{\tau})+\int d2\,\frac{-\delta\Sigma_H(1)}{\delta\mathbf{E}(\mathbf{r}_2)}\cdot\mathbf{E}(\mathbf{r}_2)\right]. \tag{30}$$

Here we have used the form appearing in Eq. (6). From Eq. (7) we see that the vertex functions Γ_0, associated with particle-density $\mathbf{\Gamma}_{SO}$, with spin-orbit density, appear upon performing the indicated functional derivatives. We may then use the plane-wave expressions given in Eqs. (18) and (25b) to work out the effective potential in detail. Even with simplified approximations subsequently given in Eqs. (24) and (25c) we see the different forms of the screening effects for the two terms. A detailed discussion of these will be given in another paper. It suffices here to draw attention to these important features of the effects of interaction on both the effective one-particle potential the electron experiences as well as the two-particle correlations. We should also remark that the nonlocal exchange correlation effects also contribute to these in important ways, just as in the itinerant electron systems.[11]

ACKNOWLEDGMENTS

We thank Dr. Kristl Hathaway for drawing attention to the problem considered here. Dr. P. Jena stressed the importance of these considerations in the physics of magnetic clusters. A.K.R. thanks Professor Walter Kohn for drawing his attention to the works of Awschalom and co-workers. M.M.'s visit to NRL, where this work was begun, was sponsored by the Navy/ASEE Summer Faculty Program, which is gratefully acknowledged. He also acknowledges support from NSF Grant No. HDR-9707076 and NASA Grant No. NAGW-2930. This work is supported in part by the Office of Naval Research.

[1] J. C. Slater, *Quantum Theory of Atomic Structure, Vol. II* (McGraw-Hill, New York, 1961).

[2] J. C. Slater, *Quantum Theory of Molecules and Solids, Vol. II* (McGraw-Hill, New York, 1965).

[3] I. P. Smorchkova, N. Samarth, J. M. Kikkawa, and D. D. Awschalom, Phys. Rev. Lett. **78**, 3571 (1997); see also D. D. Awschalom and D. P. Di Vincenzo, Phys. Today **48**, 43 (1995).

[4] G. A. Prinz, Phys. Today **48**, 58 (1995).

[5] J. R. Friedman, M. P. Sarachik, J. Tejada, and R. Ziolo, Phys. Rev. Lett. **76**, 3830 (1996); L. Thomas, F. Lionti, R. Ballou, D. Gatteschi, R. Sassoli, and B. Barabara, Nature (London) **383**, 145 (1996); see also a preprint by S. K. Nayak and P. Jena (1997) for a theoretical account of magnetism in clusters of atoms.

[6] C. Grimaldi and P. Fulde, Phys. Rev. B **55**, 15 523 (1997); see also Y. Yafet, Solid State Phys. **14**, 1 (1963).

[7] A. K. Rajagopal and S. K. Joshi, Phys. Lett. **24A**, 95 (1967).

[8] M. V. Ramana and A. K. Rajagopal, Adv. Chem. Phys. **54**, 231 (1983).

[9] E. Engel, B. Müller, C. Speicher, and R. M. Dreizler, in *Density Functional Theory*, edited by E. K. U. Gross and R. M. Dreizler (Plenum, New York, 1994); see also H. J. F. Jansen, Phys. Today **48**, 50 (1995).

[10] H. A. Bethe and E. E. Salpeter, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, New York, 1957).

[11] A. K. Rajagopal, H. Brooks, and N. R. Ranganathan, Nuovo Cimento Suppl. **(I)5**, 807 (1967).

[12] A. K. Rajagopal, Nuovo Cimento Suppl. **(I)5**, 794 (1967).