Relativistic theory of neutron form factors

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We derive, for the first time, an expression for the generalized susceptibility $\chi(\mathbf{G}+\mathbf{q},\mathbf{q})$ of a metal by using a relativistic treatment based on the Dirac equation and linear response theory ($\mathbf{q}$ is the wave vector and $\mathbf{G}$ is a reciprocal-lattice vector). The induced-moment form factor is calculated in the $\mathbf{q}\rightarrow\mathbf{0}$ limit and is expressed as a sum of three terms, $\chi(\mathbf{G},\mathbf{0})=\chi_o(\mathbf{G},\mathbf{0})+\chi_s(\mathbf{G},\mathbf{0})+\chi_{so}(\mathbf{G},\mathbf{0})$. $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$, which also contain spin-orbit effects, reduce to the induced orbital and spin form factors obtained earlier in the nonrelativistic limit provided we use the same approximations. $\chi_{so}(\mathbf{G},\mathbf{0})$ is an explicit spin-orbit contribution which has no analog in the nonrelativistic limit. Our theory for neutron form factor is valid for $\mathbf{G}$ to be in any arbitrary direction while in the earlier (nonrelativistic) theories, $\mathbf{G}$ was restricted to be perpendicular to the magnetic field. Our expressions for $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_{so}(\mathbf{G},\mathbf{0})$ are also free from any divergences, while in the earlier theories each of these expressions contained divergent terms in the $\mathbf{q}\rightarrow\mathbf{0}$ limit which cancel only for a finite crystal. Our theory for induced magnetic form factor should be important in the analysis of the neutron scattering data of heavy transition metals in which spin-orbit interactions are important.

I. INTRODUCTION

Neutron diffraction is one of the most powerful microscopic probes used to study the response of metals to an applied magnetic field. By analyzing the measured magnetic form factor, it is possible to study the various contributions to the net magnetic moment, since each response mechanism such as spin, orbital, and core diamagnetism has different characteristic spatial distribution. In fact, in the past two decades the induced-moment form factor has been measured for a large number of transition metals. In analyzing the data, the total induced-moment form factor $\chi_T(\mathbf{G},\mathbf{0})$ for a reciprocal-lattice vector $\mathbf{G}$ is considered[1] to be the sum of a spin contribution $\chi_s(\mathbf{G},\mathbf{0})$ and an orbital contribution $\chi_o(\mathbf{G},\mathbf{0})$. It is well known[2] that the orbital contribution is large in transition metals which have nearly-half-filled d bands and arises from the Van Vleck paramagnetic susceptibility.

Hebborn and March[3] developed a linear-response formalism to obtain the orbital and spin contributions to the generalized wave-vector-dependent susceptibility. Oh *et al.*[4] used a tight-binding formalism and linear-response theory to calculate orbital and spin form factors for cubic transition metals. Recently, Liu *et al.*[5] have extended this theory to calculate the paramagnetic form factors of hcp transition metals. However, the limitation of these theories is that the reciprocal-lattice vector $\mathbf{G}$ and the wave vector $\mathbf{q}$ [defined through $\mathbf{B}(\mathbf{r})=\mathbf{B}e^{i\mathbf{q}\cdot\mathbf{r}}$, where $\mathbf{B}$ is the static magnetic field], are chosen to be parallel. This approximation is valid only so long as $\mathbf{G}$ is perpendicular to $\mathbf{B}$ and $\mathbf{M}$ and therefore puts a constraint on these theories. In addition, there are two divergent terms in the expression for the form factor ($\mathbf{q}\rightarrow\mathbf{0}$ limit) which cancel only for a finite crystal.

It may be noted that in all these derivations the entire effect of spin-orbit coupling has been ignored. In fact, it has been heretofore assumed that the effect of spin-orbit coupling can be accounted for in $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ through the modification of the Bloch functions. However, it is well known[6,7] that in the case of static magnetic susceptibility, in addition to the effects of modification of the Bloch functions in $\chi_o(\mathbf{0},\mathbf{0})$ and $\chi_s(\mathbf{0},\mathbf{0})$ and the replacement of the free-electron g factor by the effective g factor[8] in $\chi_s(\mathbf{0},\mathbf{0})$, there is an additional important contribution, $\chi_{so}(\mathbf{0},\mathbf{0})$ to the total magnetic susceptibility. It has been shown[6,7] that $\chi_{so}(\mathbf{0},\mathbf{0})$ arises due to the effect of spin-orbit coupling on the orbital motion of Bloch electrons. Recently, Yasui and Shimizu[9] have obtained a similar wave-vector-dependent spin-orbit susceptibility, $\chi_{so}(\mathbf{q},\mathbf{q})$ [in addition to $\chi_o(\mathbf{q},\mathbf{q})$ and $\chi_s(\mathbf{q},\mathbf{q})$] by using a relativistic treatment based on the Dirac equation. They have demonstrated the importance of relativistic effects in $4d$ and $5d$ transition metals. It may be noted that recently such additional contributions due to relativistic effects have also been obtained for Knight shift,[10] indirect nuclear interactions,[11] and chemical shift[12] in solids.

From the foregoing remarks, it is obvious that there remains a need for a theory of neutron form factors which properly accounts for relativistic effects. In this paper, we derive an expression for neutron form factors by using the Dirac equation and the linear-response theory. We consider $\mathbf{G}$ to be in an arbitrary direction and therefore our theory has no limitations. In addition, we formulate the theory such that there are no divergent terms in our expressions.

We express the total induced-moment form factor $\chi_T(\mathbf{G},\mathbf{0})$ for a reciprocal-lattice vector $\mathbf{G}$ as

$$\chi_T(\mathbf{G},\mathbf{0})=\chi_o(\mathbf{G},\mathbf{0})+\chi_s(\mathbf{G},\mathbf{0})+\chi_{so}(\mathbf{G},\mathbf{0}) . \quad (1.1)$$

We show that in the nonrelativistic limit $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ are identical to the earlier results[4] if we use their approximations. $\chi_{so}(\mathbf{G},\mathbf{0})$ is an explicit spin-orbit contribution term due to relativistic effects. In addition, our $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ also include spin-orbit effects.

In Sec. II we derive an expression for generalized susceptibility by using linear-response theory from which both the neutron form factor $\chi(\mathbf{G},\mathbf{0})$ and bulk susceptibility $\chi(\mathbf{0},\mathbf{0})$ can be obtained. In Sec. III we use the Dirac equation to obtain an explicit expression for the generalized susceptibility $\chi(\mathbf{Q},\mathbf{q})$ which does not contain any divergent terms in the $\mathbf{q}\rightarrow\mathbf{0}$ limit. We calculate $\chi(\mathbf{Q},\mathbf{q})$ in the $\mathbf{q}\rightarrow\mathbf{0}$ limit to derive an expression for the induced-moment form factor. In Sec. IV we show that our results agree with the earlier results in the nonrelativistic limit. In Sec. V we summarize our results.

II. GENERALIZED SUSCEPTIBILITY

The magnetic moment density $\mathbf{M}(\mathbf{r})$ induced by a static magnetic field, with a sinusoidal spatial dependence $\mathbf{B}(\mathbf{r})=\mathbf{B}e^{i\mathbf{q}\cdot\mathbf{r}}$, has, in general, a complicated spatial dependence because the electron density in the metal is not uniform. However, for two points in the metal separated by a lattice vector $\mathbf{R}$, the local magnetizations are in the same ratio as the local fields. This implies the Bloch condition

$$\mathbf{M}(\mathbf{r}+\mathbf{R})=e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{M}(\mathbf{r}) . \quad (2.1)$$

One obtains, by Fourier transformation,

$$\mathbf{M}(\mathbf{r})=\sum_{\mathbf{Q}}\mathbf{M}(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{r}} , \quad (2.2)$$

where the allowed $\mathbf{Q}$ vectors are $\mathbf{Q}=\mathbf{G}+\mathbf{q}$ and $\mathbf{G}$ is an arbitrary reciprocal-lattice vector. The generalized susceptibility $\chi_{ij}(\mathbf{Q},\mathbf{q})$ is defined by the relation

$$M_i(\mathbf{Q})=\lim_{\mathbf{q}\rightarrow 0}\sum_j \chi_{ij}(\mathbf{Q},\mathbf{q})B_j . \quad (2.3)$$

If $\mathbf{B}$ is along a high-symmetry (z) direction of a cubic crystal, the induced moment would be also in the z direction. The induced-moment form factor is proportional to

$$\chi_{zz}(\mathbf{G},\mathbf{0})=\lim_{\mathbf{q}\rightarrow 0}\chi_{zz}(\mathbf{G}+\mathbf{q},\, \mathbf{q}) , \quad (2.4)$$

and the bulk static susceptibility is

$$\chi_{zz}(\mathbf{0})=\lim_{\mathbf{q}\rightarrow 0}\chi_{zz}(\mathbf{q},\mathbf{q}) . \quad (2.5)$$

The induced current due to the magnetic field, $\mathbf{j}(\mathbf{r})$, is related to the magnetic moment density $\mathbf{M}(\mathbf{r})$ by

$$\mathbf{j}(\mathbf{r})=c\nabla\times\mathbf{M}(\mathbf{r}) . \quad (2.6)$$

From Eqs. (2.2) and (2.6), we obtain

$$\mathbf{j}(\mathbf{Q})=ic\mathbf{Q}\times\mathbf{M}(\mathbf{Q}) , \quad (2.7)$$

which can be written in the alternate form

$$i\frac{\mathbf{Q}\times\mathbf{j}(\mathbf{Q})}{cQ^2}=\mathbf{M}(\mathbf{Q})-\frac{(\mathbf{Q}\cdot\mathbf{M})\mathbf{Q}}{Q^2} . \quad (2.8)$$

From Eqs. (2.3) and (2.8), we obtain

$$\chi_{ij}(\mathbf{Q},\mathbf{q})B_j(\mathbf{q})-\frac{Q_l\chi_{lj}B_jQ_i}{Q^2}=\frac{i\epsilon_{ijk}Q_jj_k(\mathbf{Q})}{cQ^2} , \quad (2.9)$$

where ϵ_{ijk} is the antisymmetric tensor of the third rank and we follow the Einstein summation convention. Since $\mathbf{B}$ is along the z direction and $\mathbf{M}$ is along the same direction, only $\chi_{zz}(\mathbf{Q},\mathbf{q})$ is nonzero and is given by

$$\chi_{zz}(\mathbf{Q},\mathbf{q})=\frac{i\epsilon_{ijk}\delta_{i3}Q_jj_k(\mathbf{Q})}{C(Q_x^2+Q_y^2)B(\mathbf{q})} , \quad (2.10)$$

where $z=3$. The vector potential $\mathbf{A}(\mathbf{r})$ is related to the magnetic field by

$$\mathbf{B}(\mathbf{r})=\nabla\times\mathbf{A}(\mathbf{r}) . \quad (2.11)$$

In a transverse gauge ($\nabla\cdot\mathbf{A}=0$), it is easy to show that

$$\mathbf{A}(\mathbf{q})=\mathbf{A}(\mathbf{r})e^{-i\mathbf{q}\cdot\mathbf{r}} =\frac{i\mathbf{q}\times\mathbf{B}(\mathbf{q})}{q^2} , \quad (2.12)$$

where $\mathbf{q}$ is a wave vector such that $\mathbf{q}\cdot\mathbf{B}=0$. We note that Eq. (2.10) is the expression for generalized susceptibility obtained by using linear-response theory from which both the neutron form factor $\chi(\mathbf{G},\mathbf{0})$ and bulk susceptibility $\chi(\mathbf{0},\mathbf{0})$ can be obtained.

III. RELATIVISTIC FORMULATION

We start with the Dirac equation for an electron in a periodic potential V,

$$(c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2+IV)\phi_i=\varepsilon_i\phi_i , \quad (3.1)$$

where

$$\boldsymbol{\alpha}=\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix},\quad \beta=\begin{bmatrix}E & 0\\ 0 & -E\end{bmatrix},\quad I=\begin{bmatrix}E & 0\\ 0 & E\end{bmatrix} ,$$

$\boldsymbol{\sigma}$ is the Pauli spin matrix vector, E is a 2×2 unit matrix, $\mathbf{p}$ is the momentum operator, m is the rest mass of the electron, and ϕ_i is a four-component Bloch function with an energy ε_i. The suffix i signifies a set of the wave vector, band index, and spin direction and is hereafter limited to positive energy states.

When an external magnetic field is applied, ϕ_i and ε_i change to Φ_i and E_i, which are solutions of the Dirac equation

$$(c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2+IV+e\boldsymbol{\alpha}\cdot\mathbf{A})\Phi_i=E_i\Phi_i , \quad (3.2)$$

where $\mathbf{A}$ is the vector potential. If the external field is weak, one obtains, by using perturbation theory,

$$\Phi_i=\phi_i+\sum_j{}'\frac{\langle j\,|\,e\boldsymbol{\alpha}\cdot\mathbf{A}\,|\,i\,\rangle\phi_j}{\varepsilon_i-\varepsilon_j}=\phi_i+\sum_j{}' a_{ji}\phi_j \tag{3.3}$$

and

$$E_i=\varepsilon_i+\langle i\,|\,e\boldsymbol{\alpha}\cdot\mathbf{A}\,|\,i\,\rangle\ . \tag{3.4}$$

In Eq. (3.3) the summation is over both the positive and negative energy states of the unperturbed system. Further, the matrix element in Eq. (3.4) vanishes for $\mathbf{q}\neq\mathbf{0}$ since $\mathbf{A}(\mathbf{r})$ varies as $e^{i\mathbf{q}\cdot\mathbf{r}}$ in space. Hence $E_i=\varepsilon_i$ in the first order of $\mathbf{A}$ and the Fermi level E_F of the perturbed system is the same as that of the unperturbed system. The current density in the perturbed system is given by

$$\mathbf{J}(\mathbf{Q})=-e\sum_i\Theta(E_F-E_i)\int\Phi_i^\dagger c\boldsymbol{\alpha}e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i d\tau\ , \tag{3.5}$$

where $\Theta(x)$ is a step function; $\Theta(x)=1$ if $x\geq 0$ and $\Theta(x)=0$ if $x<0$. The summation is carried over the positive energy states of the perturbed system. We shall now use Gordon-like decomposition.[13] Multiplying Eq. (3.2) by β and replacing E_i by $i\hbar(\partial\Phi_i/\partial t)$, we obtain

$$i\hbar\beta\frac{\partial\Phi_i}{\partial t}=c\beta\alpha_j p_j\Phi_i+\beta^2mc^2\Phi_i+IV\beta\Phi_i+e\beta\alpha_j A_j\Phi_i\ . \tag{3.6}$$

From Eq. (3.6), we have

$$\Phi_i=\frac{1}{mc^2}\left[\beta\left[i\hbar\frac{\partial\Phi_i}{\partial t}\right]-c\beta\alpha_j p_j\Phi_i-IV\beta\Phi_i-e\beta\alpha_j A_j\Phi_i\right]\ , \tag{3.7}$$

and

$$\Phi_i^\dagger=\frac{1}{mc^2}\left[-\left[\frac{i\hbar\partial}{\partial t}\right]\Phi_j^\dagger\beta-c(p_j\Phi_i)^\dagger\alpha_j\beta-IV\Phi_i^\dagger\beta-\Phi_i^\dagger e\alpha_j A_j\beta\right]\ . \tag{3.8}$$

Multiplying Eq. (3.7) by $\frac{1}{2}\Phi_i^\dagger c\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}$ on the left and Eq. (3.8) by $\frac{1}{2}c\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i$ on the right and adding, we obtain

$$\Phi_i^\dagger c\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i=\frac{i\hbar}{2mc}\left[\Phi_i^\dagger\alpha_k\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\frac{\partial\Phi_i}{\partial t}-\frac{\partial\Phi_i^\dagger}{\partial t}e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_k\Phi_i\right]-\frac{1}{2m}(\Phi_i^\dagger\alpha_k\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\alpha_j p_j\Phi_i+\Phi_i^\dagger p_j\alpha_j\beta\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)$$
$$-\frac{e}{2mc}(\Phi_i^\dagger\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_j A_j\Phi_i+\Phi_i^\dagger\alpha_j A_j\beta\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)\ . \tag{3.9}$$

Since $\alpha_k\beta=-\beta\alpha_k$, we can write the first term in Eq. (3.9) as

$$\frac{i\hbar}{2mc}\left[\Phi_i^\dagger\alpha_k\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\frac{\partial\Phi_i}{\partial t}-\frac{\partial\Phi_i^\dagger}{\partial t}e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_k\Phi_i\right]=-\frac{i\hbar}{2mc}\frac{\partial}{\partial t}(\Phi_i^\dagger e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_k\Phi_i)\ . \tag{3.10}$$

By using partial integration, we can write the second term in Eq. (3.9) as

$$-\frac{1}{2m}(\Phi_i^\dagger\alpha_k\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\alpha_j p_j\Phi_i+\Phi_i^\dagger p_j\alpha_j\beta\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)=-\frac{i\hbar}{2m}[\Phi_i^\dagger\beta\alpha_k\alpha_j e^{-i\mathbf{Q}\cdot\mathbf{r}}\nabla_j\Phi_i-(\nabla_j\Phi_i^\dagger)\beta\alpha_j\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i]\ . \tag{3.11}$$

The α matrices have the property

$$\alpha_k\alpha_j=I\delta_{kj}+i\epsilon_{kjl}\Sigma_l\ , \tag{3.12}$$

where $\boldsymbol{\Sigma}$ is a 4×4 matrix defined as $\boldsymbol{\Sigma}=\mathbf{E}\times\boldsymbol{\sigma}$. From Eqs. (3.11) and (3.12), we obtain, after some straightforward algebra,

$$-\frac{1}{2m}(\Phi_i^\dagger\alpha_k\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\alpha_j p_j\Phi_i+\Phi_i^\dagger p_j\alpha_j\beta\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)$$
$$=\frac{i\hbar}{2m}\nabla_k(\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)-\frac{\hbar}{2m}Q_k\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i-\frac{i\hbar}{m}\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\nabla_k\Phi_i+\frac{\hbar}{2m}[\nabla\times(\Phi_i^\dagger\beta\boldsymbol{\Sigma}e^{-i\mathbf{Q}\cdot\mathbf{r}})]_k$$
$$+\frac{i\hbar}{2m}\Phi_i^\dagger\beta(\mathbf{Q}\times\boldsymbol{\Sigma})_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i\ . \tag{3.13}$$

Using Eq. (3.12) in the last term of Eq. (3.9), we obtain

$$-\frac{e}{2mc}(\Phi_i^\dagger\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_j A_j\Phi_i+\Phi_i^\dagger\alpha_j A_j\beta\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)=\frac{e}{mc}\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}A_k\Phi_i\ . \tag{3.14}$$

From Eqs. (3.9), (3.10), (3.13), and (3.14), we obtain

$$\Phi_i^\dagger c\alpha_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i = -\frac{i\hbar}{2mc}\frac{\partial}{\partial t}(\Phi_i^\dagger e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\alpha_k\Phi_i)+\frac{i\hbar}{2m}\nabla_k(\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i)$$
$$-\frac{\hbar}{2m}Q_k\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i-\frac{i\hbar}{2m}\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\nabla_k\Phi_i+\frac{\hbar}{2m}[\nabla\times(\Phi_i^\dagger\beta\mathbf{\Sigma}e^{-i\mathbf{Q}\cdot\mathbf{r}})]_k$$
$$+\frac{i\hbar}{2m}\Phi_i^\dagger\beta(\mathbf{Q}\times\mathbf{\Sigma})_k e^{-i\mathbf{Q}\cdot\mathbf{r}}\Phi_i+\frac{e}{mc}\Phi_i^\dagger\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}A_k\Phi_i \ . \tag{3.15}$$

From Eqs. (2.12), (3.3), (3.5), and (3.15), we obtain

$$J_k(\mathbf{Q})=J_k^0(\mathbf{Q})-\frac{e^2}{mc}\sum_i\Theta_i\langle i\,|\,\beta e^{-i(\mathbf{Q}-\mathbf{q})\cdot\mathbf{r}}\,|\,i\rangle A_k(\mathbf{q})$$
$$+\frac{ie^2\hbar}{mc}\sum_{i,j}{}'\frac{\Theta_i}{\varepsilon_i-\varepsilon_j}\left[\langle j\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}c\alpha_l\,|\,i\rangle A_l\left[\left\langle i\left|e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\frac{\partial}{\partial x_k}\right|j\right\rangle-\frac{i}{2}Q_k\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\,|\,j\rangle\right.\right.$$
$$\left.\left.-\tfrac{1}{2}\epsilon_{mlk}Q_m\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta\Sigma_l\,|\,j\rangle\right]+(i\leftrightarrow j)\right] \ . \tag{3.16}$$

Here and hereafter, $\Theta_i=\Theta(\varepsilon_F-\varepsilon_i)$ and $(i\leftrightarrow j)$ represents a term obtained from the preceding one by interchanging the suffices i and j. In Eq. (3.16), $J_k^0(\mathbf{Q})$ is the current density for the unperturbed system,

$$J_k^0(\mathbf{Q})=-e\sum_i\Theta_i\int\Phi_i^\dagger c\alpha e^{-i\mathbf{Q}\cdot\mathbf{r}}\phi_i d\tau \ . \tag{3.17}$$

The induced current density $j(\mathbf{Q})$ is obtained from the relation

$$j_k(\mathbf{Q})=J_k(\mathbf{Q})-J_k^0(\mathbf{Q}) \ . \tag{3.18}$$

From Eqs. (2.10), (2.12), (3.16), and (3.18), after some algebra, we obtain the expression for the generalized susceptibility,

$$\chi_{zz}(\mathbf{Q},\mathbf{q})=-\frac{e^2(Q_xq_x+Q_yq_y)}{mc^2(Q_x^2+Q_y^2)q^2}\sum_i\Theta_i\langle i\,|\,\beta e^{-i(\mathbf{Q}-\mathbf{q})\cdot\mathbf{r}}\,|\,i\rangle$$
$$+\frac{ie^2\hbar}{mc^2(Q_x^2+Q_y^2)q^2}\sum_{i,j}{}'\frac{\Theta_i}{\varepsilon_i-\varepsilon_j}\{\langle j\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}c(q_x\alpha_y-q_y\alpha_x)\,|\,i\rangle$$
$$\times\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta[(Q_x\partial/\partial y-Q_y\partial/\partial x)+\tfrac{1}{2}(Q_x^2+Q_y^2)\Sigma_z$$
$$-\tfrac{1}{2}(Q_x\Sigma_x+Q_y\Sigma_y)Q_z]\,|\,j\rangle]+(i\leftrightarrow j)\} \ . \tag{3.19}$$

In order to simplify Eq. (3.19), we use the results of Gordon decomposition obtained in Eq. (3.15), except that we replace the perturbed functions Φ_i by the unperturbed functions ϕ_i. In this limit, $i\hbar(\partial\phi_i/\partial t)=\varepsilon_i\phi_i$, $A_k=0$, and one can show, after some algebra,

$$\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}c(Q_x\alpha_y-Q_y\alpha_x)\,|\,j\rangle=\frac{1}{2mc}(\varepsilon_i-\varepsilon_j)\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta(Q_x\alpha_y-Q_y\alpha_x)\,|\,j\rangle-\frac{i\hbar}{m}\langle i\,|\,\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\partial/\partial y-Q_y\partial/\partial x)\,|\,j\rangle$$
$$-\frac{i\hbar}{2m}\langle i\,|\,\beta e^{-i\mathbf{Q}\cdot\mathbf{r}}[(Q_x^2+Q_y^2)\Sigma_z-(Q_x\Sigma_x+Q_y\Sigma_y)Q_z]\,|\,j\rangle \ . \tag{3.20}$$

From Eqs. (3.12), (3.19), and (3.20), we obtain

$$\chi_{zz}(\mathbf{Q},\mathbf{q})=-\frac{e^2}{(Q_x^2+Q_y^2)q^2}\sum_{i,j}{}'\Theta_{ij}\langle j\,|\,e^{i\mathbf{q}\cdot\mathbf{r}}(q_x\alpha_y-q_y\alpha_x)\,|\,i\rangle\langle i\,|\,e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\alpha_y-Q_y\alpha_x)\,|\,j\rangle \ , \tag{3.21}$$

where

$$\Theta_{ij}=\frac{\Theta_i-\Theta_j}{\varepsilon_i-\varepsilon_j} \ , \tag{3.22}$$

and we have used the completeness of the wave functions to simplify the expression for generalized susceptibility. However, it is not possible to obtain either the induced-moment form factor or the bulk susceptibility directly from

Eq. (3.21) since it appears to diverge in the limit $\mathbf{q}\to 0$. Therefore, we use the Gordon decomposition to obtain

$$\langle i \mid e^{i\mathbf{q}\cdot\mathbf{r}} c(q_x\alpha_y - q_y\alpha_x) \mid j\rangle = \frac{1}{2mc}(\varepsilon_i - \varepsilon_j)\langle i \mid e^{i\mathbf{q}\cdot\mathbf{r}}\beta(q_x\alpha_y - q_y\alpha_x)\mid j\rangle - \frac{i\hbar}{m}\langle i \mid \beta e^{i\mathbf{q}\cdot\mathbf{r}}(q_x\partial/\partial y - q_y\partial/\partial x)\mid j\rangle + \frac{i\hbar}{2m}\langle i \mid \beta e^{i\mathbf{q}\cdot\mathbf{r}}[(q_x^2+q_y^2)\Sigma_z - (q_x\Sigma_x + q_y\Sigma_y)q_z] \ . \tag{3.23}$$

From Eqs. (3.21) and (3.23), we obtain, by using the completeness property of the wave functions,

$$\chi_{zz}(\mathbf{Q},\mathbf{q}) = -\frac{e^2(Q_xq_x+Q_yq_y)}{mc^2(Q_x^2+Q_y^2)q^2}\sum_i \Theta_i\langle i \mid \beta e^{-i(\mathbf{Q}-\mathbf{q})\cdot\mathbf{r}}\mid i\rangle + \frac{ie^2\hbar}{mc(Q_x^2+Q_y^2)q^2}\sum_{i,j}{}'\Theta_{ij}\langle j \mid \beta e^{i\mathbf{q}\cdot\mathbf{r}}(q_x\partial/\partial y - q_y\partial/\partial x)\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\alpha_y - Q_y\alpha_x)\mid j\rangle - \frac{ie^2\hbar}{2mc(Q_x^2+Q_y^2)}\sum_{i,j}{}'\Theta_{ij}\{\langle j \mid \beta e^{i\mathbf{q}\cdot\mathbf{r}}[(q_x^2+q_y^2)\Sigma_z - (q_x\Sigma_x+q_y\Sigma_y)q_z]\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\alpha_y - Q_y\alpha_x)\mid j\rangle\} \ . \tag{3.24}$$

Using the commutation relation $[\alpha_i,\Sigma_j]=2i\epsilon_{ijk}\alpha_k$, substituting the expression for $\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\alpha_y - Q_y\alpha_x)\mid j\rangle$ from Eq. (3.20) in the second term in Eq. (3.24), noting that $q_z=0$, and rearranging the terms, we obtain

$$\begin{aligned}\chi_{zz}(\mathbf{Q},\mathbf{q}) = &-\frac{4\mu_B^2 m(Q_xq_x+Q_yq_y)}{\hbar^2(Q_x^2+Q_y^2)q^2}\sum_i\Theta_i\langle i \mid \beta e^{i(\mathbf{q}-\mathbf{Q})\cdot\mathbf{r}}\mid i\rangle \\ &-\frac{4i\mu_B^2}{c\hbar(Q_x^2+Q_y^2)q^2}\sum_i\Theta_i\langle i \mid e^{i(\mathbf{q}-\mathbf{Q})\cdot\mathbf{r}}\Big[(Q_x\alpha_y - Q_y\alpha_x)(q_x\partial/\partial y - q_y\partial/\partial x) + \frac{i}{2}q^2(\alpha_xQ_x+\alpha_yQ_y) \\ &\qquad - \frac{i}{2}(q_xQ_y - q_yQ_x)(Q_x\alpha_y - Q_y\alpha_x) + \tfrac{1}{2}(\alpha_xQ_y - \alpha_yQ_x)q^2\Sigma_z\Big]\mid i\rangle \\ &+\frac{4\mu_B^2}{(Q_x^2+Q_y^2)q^2}\sum_{i,j}{}'\Theta_{ij}\{\langle j \mid e^{i\mathbf{q}\cdot\mathbf{r}}\beta(q_x\partial/\partial y - q_y\partial/\partial x)\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta(Q_x\partial/\partial y - Q_y\partial/\partial x)\mid j\rangle \\ &\qquad + \tfrac{1}{2}\langle j \mid e^{i\mathbf{q}\cdot\mathbf{r}}\beta(q_x\partial/\partial y - q_y\partial/\partial x)\mid i\rangle \\ &\qquad \times\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta[(Q_x^2+Q_y^2)\Sigma_z - Q_z(Q_x\Sigma_x+Q_y\Sigma_y)]\mid j\rangle \\ &\qquad - \tfrac{1}{2}\langle j \mid e^{i\mathbf{q}\cdot\mathbf{r}}\beta q^2\Sigma_z\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta(Q_x\partial/\partial y - Q_y\partial/\partial x)\mid j\rangle \\ &\qquad - \tfrac{1}{4}\langle j \mid e^{i\mathbf{q}\cdot\mathbf{r}}\beta q^2\Sigma_z\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta[(Q_x^2+Q_y^2)\Sigma_z - (Q_x\Sigma_x+Q_y\Sigma_y)Q_z]\mid j\rangle\} \ .\end{aligned} \tag{3.25}$$

Using Eq. (3.20) and Gordon decomposition, it can be shown that

$$\begin{aligned}&\frac{4\mu_B^2}{(Q_x^2+Q_y^2)q^2}\Theta_{ij}\langle j \mid \beta(q_x\partial/\partial y - q_y\partial/\partial x)\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta(Q_x\partial/\partial y - Q_y\partial/\partial x)\mid j\rangle \\ &= \frac{4i\mu_B^2}{\hbar c(Q_x^2+Q_y^2)q^2}\Bigg\{\sum_i\Theta_i\Bigg[\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\Big[(Q_x\alpha_y - Q_y\alpha_x)(q_x\partial/\partial y - q_y\partial/\partial x) \\ &\qquad - \frac{i}{2}(q_xQ_y - q_yQ_x)(Q_x\alpha_y - Q_y\alpha_x)\Big]\mid i\rangle - \frac{imc}{\hbar}(Q_xq_x+Q_yq_y)\langle i \mid \beta e^{-i\mathbf{Q}\cdot\mathbf{r}}\mid i\rangle\Bigg] \\ &\qquad + \frac{ic\hbar}{2}\sum_{i,j}{}'\Theta_{ij}\Bigg[\langle j \mid \beta(q_x\partial/\partial y - q_y\partial/\partial x)\mid i\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}\beta[(Q_x^2+Q_y^2)\Sigma_z - Q_z(Q_x\Sigma_x+Q_y\Sigma_y)]\mid j\rangle \\ &\qquad + \frac{2m^2c^2}{\hbar^2}\langle j \mid (q_x\alpha_y - q_y\alpha_x)\mid \iota\rangle\langle i \mid e^{-i\mathbf{Q}\cdot\mathbf{r}}(Q_x\alpha_y - Q_y\alpha_x)\mid j\rangle\Bigg]\Bigg\} \ .\end{aligned} \tag{3.26}$$

We have shown in the Appendix that, for $i \neq j$,

$$\langle j \,|\, (q_x \alpha_y - q_y \alpha_x) \,|\, i \rangle = 0 \; . \tag{3.27}$$

We substitute Eqs. (3.26) and (3.27) in Eq. (3.25), use the result $\alpha_i \Sigma_j = i\epsilon_{ijk}\alpha_k$, and rearrange the terms to obtain the expression for generalized susceptibility in the form

$$\begin{aligned} \chi_{zz}(\mathbf{Q},\mathbf{q}) = &-\frac{4\mu_B^2 m\,(Q_x q_x + Q_y q_y)}{\hbar^2 (Q_x^2+Q_y^2) q^2} \sum_i \Theta_i \langle i \,|\, \beta (e^{i\mathbf{q}\cdot\mathbf{r}}-1) e^{-i\mathbf{Q}\cdot\mathbf{r}} \,|\, i \rangle \\ &+ \frac{4\mu_B^2}{(Q_x^2+Q_y^2)q^2} \sum_{i,j}{}' \Theta_{ij} \{ \langle j \,|\, (e^{i\mathbf{q}\cdot\mathbf{r}}-1)\beta(q_x \partial/\partial y - q_y \partial/\partial x) \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{Q}\cdot\mathbf{r}} \beta (Q_x \partial/\partial y - Q_y \partial/\partial x) \,|\, j \rangle \\ &\qquad + \tfrac{1}{2} \langle j \,|\, (e^{i\mathbf{q}\cdot\mathbf{r}}-1)\beta(q_x \partial/\partial y - q_y \partial/\partial x) \,|\, i \rangle \\ &\qquad \times \langle i \,|\, e^{-i\mathbf{Q}\cdot\mathbf{r}} \beta [(Q_x^2+Q_y^2)\Sigma_z - Q_z(Q_x\Sigma_x + Q_y\Sigma_y)] \,|\, j \rangle \\ &\qquad - \tfrac{1}{2} \langle j \,|\, e^{i\mathbf{q}\cdot\mathbf{r}} \beta q^2 \Sigma_z \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{Q}\cdot\mathbf{r}} \beta (Q_x \partial/\partial y - Q_y \partial/\partial x) \,|\, j \rangle \\ &\qquad - \tfrac{1}{4} \langle j \,|\, e^{i\mathbf{q}\cdot\mathbf{r}} \beta q^2 \Sigma_z \,|\, i \rangle \langle \,|\, e^{-i\mathbf{Q}\cdot\mathbf{r}} \beta [(Q_x^2+Q_y^2)\Sigma_z - (Q_x\Sigma_x + Q_y\Sigma_y) Q_z] \,|\, j \rangle \} \; . \end{aligned} \tag{3.28}$$

We have now obtained the generalized susceptibility in a form which does not diverge in the limit $\mathbf{q} \to \mathbf{0}$. It is easy to show that, in the limit $\mathbf{q} \to \mathbf{0}$,

$$\frac{1}{q^2}(e^{i\mathbf{q}\cdot\mathbf{r}}-1)(q_x \partial/\partial y - q_y \partial/\partial x) = -\frac{1}{2\hbar} L_z \tag{3.29}$$

and

$$\frac{Q_x q_x + Q_y q_y}{q^2}(e^{i\mathbf{q}\cdot\mathbf{r}}-1) = \frac{i}{2}(G_x x + G_y y) \; . \tag{3.30}$$

Substituting Eqs. (3.29) and (3.30) in Eq. (3.28), we write the induced-moment form factors in the form

$$\chi(\mathbf{G},\mathbf{0}) = \lim_{\mathbf{q}\to\mathbf{0}} \chi(\mathbf{Q},\mathbf{q}) = \chi_o(\mathbf{G},\mathbf{0}) + \chi_s(\mathbf{G},\mathbf{0}) + \chi_{so}(\mathbf{G},\mathbf{0}) \; , \tag{3.31}$$

where

$$\begin{aligned} \chi_o(\mathbf{G},\mathbf{0}) = &-\frac{2im\mu_B^2}{\hbar^2(G_x^2+G_y^2)} \sum_i \Theta_i \langle i \,|\, e^{-i\mathbf{G}\cdot\mathbf{r}} \beta (G_x x + G_y y) \,|\, i \rangle \\ &- \frac{2i\mu_B^2}{\hbar^2(G_x^2+G_y^2)} \sum_{i,j}{}' \Theta_{ij} \langle j \,|\, \beta L_z \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{G}\cdot\mathbf{r}} \beta (G_x p_y - G_y p_x) \,|\, j \rangle \; , \end{aligned} \tag{3.32}$$

$$\chi_s(\mathbf{G},\mathbf{0}) = -\frac{\mu_B^2}{G_x^2+G_y^2} \sum_{i,j}{}' \Theta_{ij} \langle j \,|\, \beta \Sigma_z \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{G}\cdot\mathbf{r}} \beta [(G_x^2+G_y^2)\Sigma_z - G_z(G_x\Sigma_x + G_y\Sigma_y)] \,|\, j \rangle \tag{3.33}$$

and

$$\begin{aligned} \chi_{so}(\mathbf{G},\mathbf{0}) = &-\frac{\mu_B^2}{\hbar(G_x^2+G_y^2)} \sum_{i,j}{}' \Theta_{ij} \{ \langle j \,|\, \beta L_z \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{G}\cdot\mathbf{r}} \beta [(G_x^2+G_y^2)\Sigma_z - G_z(G_x\Sigma_x + G_y\Sigma_y)] \,|\, j \rangle \\ &\qquad + 2i \langle j \,|\, \beta \Sigma_z \,|\, i \rangle \langle i \,|\, e^{-i\mathbf{G}\cdot\mathbf{r}} \beta (G_x p_y - G_y p_x) \,|\, j \rangle \} \; , \end{aligned} \tag{3.34}$$

where $\mathbf{p}$ and $\mathbf{L}$ are linear- and angular-momentum operators. In the next section we shall show that in the nonrelativistic limit $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ reduce to the orbital and spin contributions to the induced-moment form factor, while χ_{so} reduces to zero. Hence, we denote $\chi_o(\mathbf{G},\mathbf{0})$ the orbital form factor, $\chi_s(\mathbf{G},\mathbf{0})$ spin form factor, and $\chi_{so}(\mathbf{G},\mathbf{0})$ the spin-orbit form factor. However, we would like to emphasize that relativistic effects are included in each of these terms. We note that $\chi_{so}(\mathbf{G},\mathbf{0})$ is an entirely new contribution to the induced-moment form factor, which has been heretofore neglected. This new contribution should be important for analysis of neutron form factors of heavier transition metals. We further note that in the earlier theories $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ have been obtained nonrelativistically only in the special case where $\mathbf{G}$ is parallel to $\mathbf{q}$, i.e., $G_z=0$ (since $q_z=0$). Our results are valid for any arbitrary $\mathbf{G}$. Finally we note that our expressions do not contain any divergent terms, unlike the earlier results.

IV. NONRELATIVISTIC LIMIT

We shall derive expressions for $\chi_o(\mathbf{G},\mathbf{0})$, $\chi_s(\mathbf{G},\mathbf{0})$, and $\chi_{so}(\mathbf{G},\mathbf{0})$ in the nonrelativistic limit in order to compare our results with the earlier results. In this limit, $\beta=1$, $\Sigma=\sigma$, i and j are the two-component functions in the Bloch representation, and $\Theta_i=f_{n\mathbf{k}}$, the Fermi factor. In this limit, Eq. (3.33) reduces to

$$\chi_s(\mathbf{G},\mathbf{0})=-\frac{\mu_B^2}{G_x^2+G_y^2}\sum_{n,n',\mathbf{k},\mathbf{k}'}\frac{f_{n\mathbf{k}}-f_{n'\mathbf{k}'}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\langle n\mathbf{k}\,|\,\sigma_z\,|\,n'\mathbf{k}'\rangle\langle n'\mathbf{k}'\,|\,e^{-i\mathbf{G}\cdot\mathbf{r}}[(G_x^2+G_y^2)\sigma_z-G_z(G_x\sigma_x+G_y\sigma_y)]\,|\,n\mathbf{k}\rangle\ , \tag{4.1}$$

where $E_{n\mathbf{k}}$ is the energy of the eigenstate $|n\mathbf{k}\rangle$ of the electron in band n with crystal momentum $\mathbf{k}$. In the absence of spin-orbit interaction, $|n\mathbf{k}\rangle$ is an eigenfunction of σ_z and Eq. (4.1) reduces to

$$\chi_s(\mathbf{G},\mathbf{0})=-\mu_B^2\sum_{n,n',\mathbf{k},\mathbf{k}'}\frac{f_{n\mathbf{k}}-f_{n'\mathbf{k}'}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}'}}\langle n\mathbf{k}\,|\,e^{-i\mathbf{G}\cdot\mathbf{r}}\,|\,n'\mathbf{k}'\rangle \times\delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'}\ , \tag{4.2}$$

which can be written in the familiar form

$$\chi_s(\mathbf{G},\mathbf{0})=\int\rho(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}d^3r\ , \tag{4.3}$$

where

$$\rho(\mathbf{r})=2\mu_B^2\sum_n\oint_{\varepsilon=\varepsilon_F}\frac{ds(\mathbf{k})}{|\nabla_k\varepsilon(\mathbf{k})|}\,|\psi_{n\mathbf{k}}(\mathbf{r})|^2 \tag{4.4}$$

is the spin density due to the conduction electrons at the Fermi surface, and we have included a factor of 2 for band spin degeneracy. We note that in deriving the nonrelativistic spin-polarized term in Eq. (4.3) from the relativistic expression for $\chi_s(\mathbf{G},\mathbf{0})$ in Eq. (3.33), we have made approximations which are equivalent to neglecting the spin-orbit interaction, the relativistic correction to the kinetic energy, as well as the Darwin term. Therefore the relativistic expression for $\chi_s(\mathbf{G},\mathbf{0})$ includes spin-orbit effects in addition to $\chi_{so}(\mathbf{G},\mathbf{0})$, which is an explicit spin-orbit contribution to the induced-momentum form factor. One can find an analogy in the case of static magnetic susceptibility,[6,7] where the spin-orbit effects in $\chi_s(\mathbf{0},\mathbf{0})$ are included in the effective g factor, while $\chi_{so}(\mathbf{0},\mathbf{0})$ is an additional contribution due to the effect of spin-orbit coupling on orbital motion of Bloch electrons. In the present case, since we have used Dirac equations, the relativistic correction to kinetic energy and the Darwin term are also included.

Using the same approximations, the orbital form factor in Eq. (3.32) can be written as

$$\chi_o(\mathbf{G},\mathbf{0})=-\frac{4im\mu_B^2N}{\hbar^2(G_x^2+G_y^2)}\sum_{n,\mathbf{k}}f_{n\mathbf{k}}\langle n\mathbf{k}\,|\,e^{-i\mathbf{G}\cdot\mathbf{r}}(xG_x-yG_y)\,|\,n\mathbf{k}\rangle -\frac{4i\mu_B^2N}{\hbar^2(G_x^2+G_y^2)}\sum_{n,n',\mathbf{k}}\frac{f_{n\mathbf{k}}-f_{n'\mathbf{k}}}{E_{n\mathbf{k}}-E_{n'\mathbf{k}}}\langle n\mathbf{k}\,|\,e^{-i\mathbf{G}\cdot\mathbf{r}}(G_xp_y-G_yp_x)\,|\,n'\mathbf{k}\rangle\langle n'\mathbf{k}\,|\,L_z\,|\,n\mathbf{k}\rangle\ , \tag{4.5}$$

where N is the number of unit cells and we have multiplied by a factor of 2 for spin degeneracy. The first term in Eq. (4.5) is the diamagnetic form factor[14] and the second term is the Van Vleck form factor.[4] It may be noted that if $\mathbf{G}$ is along the y direction (as approximated in Ref. 4), our Eq. (4.5) is identical with Eqs. (2.43) and (2.44) of Ref. 4.

V. SUMMARY AND CONCLUSION

The principal result of this paper is to derive an expression for the neutron form factors using a relativistic formulation. Our expression for the neutron form factor has been written as the sum of orbital $[\chi_o(\mathbf{G},\mathbf{0})]$, spin $[\chi_s(\mathbf{G},\mathbf{0})]$, and spin-orbit $[\chi_{so}(\mathbf{G},\mathbf{0})]$ contributions, although spin-orbit effects are also present in both $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$. $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_s(\mathbf{G},\mathbf{0})$ reduce to the earlier results in the nonrelativistic case if we also use the same approximations. However, our results are more general and are valid for any arbitrary $\mathbf{G}$ direction, while in the earlier theories $\mathbf{G}$ was restricted to be parallel to $\mathbf{q}$ (perpendicular to $\mathbf{B}$). Our expressions for $\chi_o(\mathbf{G},\mathbf{0})$ and $\chi_{so}(\mathbf{G},\mathbf{0})$ are also free from any divergences, unlike the earlier theories.

In addition, we obtain a new contribution to the neutron form factor $[\chi_{so}(\mathbf{G},\mathbf{0})]$ which is entirely due to relativistic effects. This term, which has been heretofore neglected, should be important in the analysis of the neutron scattering data for heavy transition metals in which spin-orbit effects are large.[15]

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APPENDIX

We shall now prove that if $j \neq i$,

$$\langle j \mid (q_x \alpha_y - q_x \alpha_x) \mid i \rangle = 0 \ . \tag{A1}$$

The four-component function can be written as

$$\Psi_{n\mathbf{k}s}(\mathbf{r}) = N \begin{bmatrix} U \\ \frac{c\sigma\cdot\mathbf{p}}{mc^2+\varepsilon} U \end{bmatrix} \psi_{n\mathbf{k}}(\mathbf{r}) \ , \tag{A2}$$

where $\psi_{n\mathbf{k}}(\mathbf{r})$ is a Bloch function, U is a two-component spin function,

$$U = \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} ,$$

and N is a normalization constant. The orthonormality condition of the four-component functions is

$$\int \Psi^\dagger_{n\mathbf{k}s}(\mathbf{r}) \Psi_{m\mathbf{k}s'}(\mathbf{r}) d^3r = \delta_{nm} \delta_{ss'} \ . \tag{A3}$$

If $| j \rangle = \Psi_{n\mathbf{k}s}$ and $| i \rangle = \Psi_{m\mathbf{k}s'}$, it is evident, from the fact that the Bloch functions are orthogonal, that Eq. (A1) is satisfied for $n \neq m$. In order to prove Eq. (A1) for $n = m$, we first note that s and s' correspond to two-component spin functions U and U', where

$$(U_1^\dagger U_1' + U_2^\dagger U_2') = 0 \ , \tag{A4}$$

such that Eq. (A3) is satisfied. By using Eq. (A2), one can show, after straightforward algebra,

$$\int \Psi^\dagger_{n\mathbf{k}s}(\mathbf{r})(q_x \alpha_y - q_y \alpha_x) \Psi_{n\mathbf{k}s'}(\mathbf{r}) d^3r = \frac{2N^2C}{mc^2+\varepsilon} (U_1^\dagger U_1' + U_2^\dagger U_2') \int \psi^*_{n\mathbf{k}}(\mathbf{r})(p_y q_x - p_x q_y) \times \psi_{n\mathbf{k}}(\mathbf{r}) d^3r \ . \tag{A5}$$

From Eqs. (A4) and (A5), we obtain

$$\int \Psi^\dagger_{n\mathbf{k}s}(\mathbf{r})(q_x \alpha_y - q_y \alpha_x) \Psi_{n\mathbf{k}s'}(\mathbf{r}) d^3r = 0 \ . \tag{A6}$$

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