Many-body theory of magnetic susceptibility of electrons in solids

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We present a theory of the total magnetic susceptibility (χ) of interacting electrons in solids. We have included the effects of both the lattice potential and electron-electron interaction and constructed in $\vec{k}$ space, using the Bloch representation, the effective one-particle Hamiltonian and the equation of motion of the Green's function in the presence of a magnetic field. We have used a finite-temperature Green's-function formalism where the thermodynamic potential Ω is expressed in terms of the exact one-particle propagator G and have derived a general expression for χ by assuming the self-energy to be independent of frequency. We have calculated the many-body effects on orbital (χ_o), spin (χ_s), and spin-orbit (χ_{so}) contributions to χ. If we make simple approximations for the self-energy, our expression for χ_o reduces to the earlier results. If we make drastic assumptions while solving the matrix integral equations for the field-dependent part of the self-energy, our expression for χ_s is equivalent to the earlier results for exchange-enhanced spin susceptibility but with the g factor replaced by the effective g factor, a result which has been intuitively used but not yet rigorously derived. An important aspect of our work is the careful analysis of exchange and correlation effects on χ_{so}, the contribution to susceptibility from the effect of spin-orbit coupling on the orbital motion of Bloch electrons. Although χ_{so} is of the same order of magnitude as χ_s for some metals and semiconductors, its contribution has been hitherto completely ignored in all the many-body theories of magnetic susceptibility. We have also shown that if we neglect electron-electron interactions our expression for χ agrees with the well-known results for noninteracting Bloch electrons.

I. INTRODUCTION

The many-body theory of magnetic susceptibility of solids, in which the effects of both the lattice potential and electron-electron interactions are included, is one of the basic problems of solid-state physics that have not yet been satisfactorily resolved. Owing to the enormous complexity of the problem, the Hamiltonian is usually separated into orbital and spin components (thus neglecting spin-orbit interaction), and attention is focused on one of the two parts.

The many-body effects on the diamagnetism of free electrons have been studied by many authors.[1–8] The more recent calculations[3–8] all agree in the high-density, low-temperature limit. However, these calculations are carried out in the limit of very low or very high electron densities and are not appropriate for Bloch electrons. Fukuyama[9,10] calculated the orbital magnetism of interacting Bloch electrons, neglecting the current vertex corrections, and has shown that the interband effect between two bands separated by the Coulomb interaction has properties similar to Van Vleck paramagnetism.[11] He also included the effect of correlation in the framework of a random-phase approximation in the one-dimensional weak cosine-type periodic potential model. Philippas and McClure[12] established the validity of the Sampson-Seitz prescription[13] applied to the Landau-Peierls formula and obtained the quasiparticle prescription that the diamagnetism of interacting Bloch electrons is to be calculated using Misra-Roth theory,[14] i.e., by treating the self-energy operator as a nonlocal pseudopotential, ignoring the change of the transformed self-energy with the magnetic field. They have also shown that the explicit many-body corrections to the orbital paramagnetism is, in general, small. Mohanty and Misra[15] showed by using Bloch representation that the transformed self-energy in the effective one-particle Hamiltonian has the same translational properties as a nonlocal magnetic pseudopotential.[16,17] However, their expression for free energy contains only the quasiparticle term, and the vertex corrections have been neglected. Fukuyama and McClure[18] derived an expression for the orbital magnetism of an interacting free-electron gas, taking into account the exact functional form of the self-energy. Their result yields a generalized form of the Landau-Peierls formula. Thus the effects of exchange and correlations are not fully understood for orbital susceptibility (χ_o), but their contribution has been shown to be small.[19]

However, it is well known[20] that electron-electron interactions lead to an enhancement of the Pauli spin susceptibility. Sampson and Seitz[13] first calculated paramagnetic susceptibility (χ_s), including the effects of exchange and correlation. Pines[21] carried out a calculation similar to Sampson and Seitz,[13] but his results differ remarkably from theirs because of the use of the Bohm-Pines theory for correlation energy. Brueckner and Sawada[22] derived an expression for the magnetic susceptibility of an electron gas at high density using the exact theory of Gell-Mann and Brueckner.[23]

Silverstein[24] calculated the paramagnetic susceptibility by a similar method with the addition of a momentum transfer interpolation procedure designed to obtain relevant information in the region of metallic densities. Hamann and Overhauser[25] calculated the wave-vector-dependent spin susceptibility taking dynamically screened electron interactions into account, and their calculations agree with that of Dupree and Geldart[26] and Pizzimenti *et al.*[27] Lobo *et al.*[28] used a generalization of the random-phase approximation, which takes into account short-range correlations between the electrons, to obtain χ_s for an electron gas at metallic densities. Yafet[29] has calculated χ_s for a two-band model with δ-function interactions between the conduction electrons using a random-phase approximation. Isihara and Kojima[30] calculated both χ_o and χ_s of an electron fluid at low temperature by considering the free electrons, first- and second-order exchange, and the ring diagrams.

In a real metal, the background potential and the electron density are far from uniform. Kohn and Sham[31] have used the density-functional formalism[32] to derive an expression for χ_s valid for slowly varying density. The Hohenberg-Kohn-Sham theory of inhomogeneous electron gas has been generalized[33-35] to include the spin-dependent interaction. Recently, Vosko and Perdew[36] (VP) have calculated χ_s of metallic electrons based on a variational principle within the density-functional formalism.[31,32] This variational expression allows one to simultaneously treat band and exchange-correlation effects among the conduction electrons and also includes the influence of the core electrons on the lattice. Vosko *et al.*[37] calculated χ_s for the alkali metals, and there is good agreement with the experimental results. Using the theory of VP, Janak[38] calculated χ_s of a number of metals (including the transition metals) to study the enhancement of response which leads to ferromagnetic instability. His results are in good agreement with the results of Gunnarsson[39] but differ from those of Vosko *et al.*[37,40] because of the use of a different approximation for the exchange-correlation functional and because of the use of a different lattice parameter. However, the density-functional formalism works well for systems where the density varies slowly in space. Thus its validity is limited to nearly-free-electron metals with only one occupied band.

It may be noted that in all these derivations the entire effect of spin-orbit coupling was ignored. In fact, it has been hitherto assumed that the effect of spin-orbit coupling can be accounted for in χ_o through the modification of the Bloch functions and in χ_s by replacing the free-electron g factor by the effective g factor. However, recently it was shown by one of us[41] that there is an additional contribution from the effect of spin-orbit coupling (χ_{so}) on the orbital motion of Bloch electrons. It has also been shown that even in the absence of exchange and correlation effects the contribution of χ_{so} is of the same order of magnitude as χ_s for some metals[42] and semiconductors.[43] From these earlier results[41] *a priori* one cannot say anything about the effects of exchange and correlations on χ_{so}.

It is evident that the many-body effects on the spin-orbit contributions (both in χ_s and χ_{so}) to χ can be calculated by using the total crystal Hamiltonian including the spin-orbit interactions. Buot[44] recently attempted to derive an expression for the total magnetic susceptibility (χ) for interacting Bloch electrons. However, because of the complications due to the use of the lattice-Weyl transform,[45] he was not able to obtain a meaningful expression for χ except for the two simple cases of Fermi liquid and Hubbard limits.

It is clear from the foregoing remarks that there remains a need for a theory of total magnetic susceptibility (χ) of solids (including spin-orbit interaction) that will take into account both interband effects and many-body effects. In this paper we derive a theory for χ of interacting electrons in solids using a finite temperature Green's-function formalism where the thermodynamic potential Ω for an interacting electron system in the presence of a periodic potential, spin-orbit interaction, and external magnetic field is expressed in terms of the exact one-particle propagator G. We constructed in $\vec{k}$ space, using the Bloch representation, the equation of motion of the Green's function in the presence of the magnetic field and evaluated Ω. In our theory the effects of exchange and correlations on each of the three components of χ have been explicitly calculated. If we make a simple approximation for the self-energy, the first term of our expression for χ_o reduces to the earlier results.[12] If we make drastic assumptions while solving the matrix integral equations for the field-dependent part of the self-energy, our expression for χ_s is equivalent to the earlier results for the exchange-enhanced χ_s but with the g factor replaced by the effective g factor, a result which has been intuitively used but not yet rigorously derived. An important aspect of our work is the analysis of exchange and correlation effects on χ_{so} that are more subtle and cannot be included in an intuitive way. We note that our expression for χ agrees with the earlier results[41,46,47] for noninteracting Bloch electrons if we completely neglect electron-electron interactions.

The plan of the paper is as follows. In Sec. II, we construct in $\vec{k}$ space, using the Bloch representation, the effective one-particle Hamiltonian and the equation of motion for the Green's function in the presence of a magnetic field. In Sec. III, we derive a general expression for χ using a finite temperature Green's-function formalism and expanding Ω in terms of the exact one-particle propagator G. In Sec. IV, we carefully analyze the exchange and correlation effects on each component of χ and compare our results with the earlier results. In Sec. V, we summarize and discuss our results.

II. EQUATION OF MOTION IN THE BLOCH REPRESENTATION

We use a finite-temperature Green's-function formalism to express the thermodynamic potential $\Omega(T,V,\mu,\vec{B})$ for an interacting system in the presence of a periodic potential $V(\vec{r})$, spin-orbit interaction, and external magnetic field $\vec{B}$ in terms of the exact one-particle propagator G. G satisfies the equation

$$(\xi_l-H)G(\vec{r},\vec{r}\,',\xi_l)+\int d\vec{r}\,''\Sigma(\vec{r},\vec{r}\,'',\xi_l)G(\vec{r}\,'',\vec{r}\,',\xi_l)=\delta(\vec{r}-\vec{r}\,')\ , \tag{2.1}$$

where Σ is the exact proper self-energy operator, ξ_l is the complex energy,

$$\xi_l=(2l+1)i\Pi/\beta+\mu\ , \tag{2.2}$$

and H is the one-particle Hamiltonian given by

$$H=\frac{1}{2m}\left[\vec{p}+\frac{e\vec{A}}{c}\right]^2+\frac{\hbar^2}{4m^2c^2}\vec{\sigma}\cdot\vec{\nabla}V\times\left[\vec{p}+\frac{e\vec{A}}{c}\right]+V(\vec{r})+\frac{\hbar^2}{8m^2c^2}\nabla^2V+\tfrac{1}{2}g\mu_0\vec{B}\cdot\vec{\sigma}\ . \tag{2.3}$$

In Eq. (2.3), $\vec{A}(\vec{r})$ is the vector potential, $\vec{\sigma}$ is the Pauli spin matrix, μ_0 is the Bohr magneton, and g is the free-electron g factor. In the absence of the magnetic field, both G and Σ have the symmetry

$$G(\vec{r}+\vec{R},\vec{r}\,'+\vec{R},\xi_l)=G(\vec{r},\vec{r}\,',\xi_l) \tag{2.4a}$$

and

$$\Sigma(\vec{r}+\vec{R},\vec{r}\,'+\vec{R},\xi_l)=\Sigma(\vec{r},\vec{r}\,',\xi_l)\ . \tag{2.4b}$$

The vector potential in the Hamiltonian destroys this symmetry, but both G and Σ can be written as the product of a "Peierls phase factor" and a part which has the above symmetry. In the symmetric gauge $(\vec{A}=\frac{1}{2}\vec{B}\times\vec{r})$, we have[12,42]

$$G(\vec{r},\vec{r}\,',\xi_l,\vec{h})=e^{i\vec{h}\cdot\vec{r}\times\vec{r}\,'}\tilde{G}(\vec{r},\vec{r}\,',\xi_l,\vec{h}) \tag{2.5a}$$

and

$$\Sigma(\vec{r},\vec{r}\,',\xi_l,\vec{h})=e^{i\vec{h}\cdot\vec{r}\times\vec{r}\,'}\widetilde{\Sigma}(\vec{r},\vec{r}\,',\xi_l,\vec{h})\ , \tag{2.5b}$$

where

$$\vec{h}=\frac{e\vec{B}}{2\hbar c}\ . \tag{2.6}$$

Substituting Eq. (2.5) in (2.1) commuting the differential operator through the Peierls phase factor, and then multiplying the left-hand side by $e^{-i\vec{h}\cdot\vec{r}\times\vec{r}\,'}$, we obtain

$$\left[\xi_l-\frac{1}{2m}[\vec{p}+\hbar\vec{h}\times(\vec{r}-\vec{r}\,')]^2-\frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\vec{\nabla}V\times[\vec{p}+\hbar\vec{h}\times(\vec{r}-\vec{r}\,')]\right.$$
$$\left.-V(\vec{r})-\frac{\hbar^2}{8m^2c^2}\nabla^2V-\tfrac{1}{2}g\mu_0\vec{B}\cdot\vec{\sigma}\right]\widetilde{G}(\vec{r},\vec{r}\,',\xi_l,\vec{h})$$
$$-\int d\vec{r}\,''e^{i\vec{h}\cdot(\vec{r}\,'\times\vec{r}+\vec{r}\times\vec{r}\,''+\vec{r}\,''\times\vec{r}\,')}\widetilde{\Sigma}(\vec{r},\vec{r}\,'',\xi_l,\vec{h})\widetilde{G}(\vec{r}\,'',\vec{r}\,',\xi_l,\vec{h})=\delta(\vec{r}-\vec{r}\,')\ . \tag{2.7}$$

We can write the equation of motion in the Bloch representation, i.e., in terms of the basis functions

$$\phi_{n\vec{k}\rho}(\vec{r})=e^{i\vec{k}\cdot\vec{r}}U_{n\vec{k}\rho}(\vec{r})\ , \tag{2.8}$$

where $U_{n\vec{k}\rho}(\vec{r})$ is a periodic two-component function, n is the band index, $\vec{k}$ is the reduced wave vector, and ρ is the spin index. Using the Bloch representation, Eq. (2.7) can be written as

$$\sum_{n'',\rho'',\vec{k}\,',\vec{k}\,''}\int d\vec{r}\,d\vec{r}\,'d\vec{r}\,''e^{-i\vec{k}\cdot\vec{r}}U^*_{n\vec{k}\rho}(\vec{r})\left[\xi_l-\frac{1}{2m}[\vec{p}+\hbar\vec{h}\times(\vec{r}-\vec{r}\,')]^2\right.$$
$$\left.-\frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\vec{\nabla}V\times[\vec{p}+\hbar\vec{h}\times(\vec{r}-\vec{r}\,')]-V(\vec{r})-\frac{\hbar^2}{8m^2c^2}\nabla^2V-\tfrac{1}{2}g\mu_0\vec{B}\cdot\vec{\sigma}\right]$$
$$\times e^{i\vec{k}\,''\cdot(\vec{r}-\vec{r}\,'')}U_{n''\vec{k}\,''\rho''}(\vec{r})U^*_{n''\vec{k}\,''\rho''}(\vec{r}\,'')\widetilde{G}(\vec{r}\,'',\vec{r}\,',\xi_l,\vec{h})U_{n'\vec{k}\,'\rho'}(\vec{r}\,')e^{i\vec{k}\,'\cdot\vec{r}\,'}$$
$$+\sum_{n'',\rho'',\vec{k}\,',\vec{k}\,''}\int d\vec{r}\,d\vec{r}\,'d\vec{r}\,''\,d\vec{r}\,'''\,e^{-i\vec{k}\cdot\vec{r}}U^*_{nk\rho}(\vec{r})e^{i\vec{h}\cdot(\vec{r}\,'\times\vec{r}+\vec{r}\times\vec{r}\,''+\vec{r}\,''\times\vec{r}\,')}$$
$$\times\widetilde{\Sigma}(\vec{r},\vec{r}\,'')e^{i\vec{k}\,''\cdot(\vec{r}\,''-\vec{r}\,''')}U_{n''\vec{k}\,''\rho''}(\vec{r}\,'')U^*_{n''\vec{k}\,''\rho''}(\vec{r}\,''')$$
$$\times\widetilde{G}(\vec{r}\,''',\vec{r}\,',\xi_l,\vec{h})U_{n'\vec{k}\,'\rho'}(\vec{r}\,')e^{i\vec{k}\,'\cdot\vec{r}\,'}=\delta_{nn'}\delta_{\rho\rho'}\ . \tag{2.9}$$

By introducing change of variables $\vec{R}_1=\vec{r}\,''-\vec{r}\,'$, and $\vec{R}_2=\frac{1}{2}(\vec{r}\,'+\vec{r}\,'')$ in the first term, $\vec{R}_1=\vec{r}-\vec{r}\,''$, $\vec{R}_2=\frac{1}{2}(\vec{r}+\vec{r}\,'')$, $\vec{R}_3=\vec{r}\,'''-\vec{r}\,'$, and $\vec{R}_4=\frac{1}{2}(\vec{r}\,'+\vec{r}\,''')$ in the second term, and by using partial integration of the type

$$\sum_{\vec{k}\,''}(\vec{r}-\vec{r}\,')e^{i\vec{k}\,''\cdot(\vec{r}-\vec{r}\,')}e^{i\vec{k}\,''\cdot(\vec{r}\,'-\vec{r}\,'')}U_{n''\vec{k}\,''\rho''}(\vec{r})U^*_{n''\vec{k}\,''\rho''}(\vec{r}\,'')$$
$$=\sum_{\vec{k}\,''}e^{i\vec{k}\,''\cdot(\vec{r}-\vec{r}\,')}i\nabla_{\vec{k}\,''}e^{i\vec{k}\,''\cdot(\vec{r}\,'-\vec{r}\,'')}U_{n''\vec{k}\,''\rho''}(\vec{r})U^*_{n''\vec{k}\,''\rho''}(\vec{r}\,'')\ . \tag{2.10}$$

Equation (2.9) can be written in the form

$$\left.\sum_{n'',\rho''}[\xi_l-H(\vec{\kappa}\,',\xi_l)]_{n\vec{k}\rho,n''\vec{k}\rho''}\widetilde{G}_{n''\vec{k}\rho'',n'\vec{k}\rho'}(\vec{k}\,',\xi_l)\right|_{\vec{k}\,'=\vec{k}}=\delta_{nn'}\delta_{\rho\rho'}\ , \tag{2.11}$$

where

$$\vec{\kappa}=\vec{k}+i\hbar\nabla_k\ , \tag{2.12}$$

$$H(\vec{\kappa},\xi_l)=\frac{1}{2m}(\vec{p}+\hbar\vec{\kappa})^2+V(\vec{r})+\frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\vec{\nabla}V\times(\vec{p}+\hbar\vec{\kappa})+\frac{\hbar^2}{8m^2c^2}\nabla^2V+\tfrac{1}{2}g\mu_0\vec{B}\cdot\vec{\sigma}+\Sigma(\vec{\kappa},\xi_l)\ , \quad (2.13)$$

$$\widetilde{\Sigma}_{n\vec{k}\rho,n''\vec{k}\rho''}(\vec{\kappa}',\xi_l)=\int d\vec{r}\,d\vec{r}'\,U^*_{n''\vec{k}\rho''}(\vec{r})e^{-i\vec{\kappa}'\cdot(\vec{r}-\vec{r}')}\widetilde{\Sigma}(\vec{r},\vec{r}'\xi_l)U_{n''\vec{k}\rho''}(\vec{r}') \quad (2.14)$$

and

$$\widetilde{G}_{n''\vec{k}\rho'',n'\vec{k}\rho'}(\vec{k}',\xi_l)=\int d\vec{r}\,d\vec{r}'\,U^*_{n''\vec{k}\rho''}(\vec{r})\widetilde{G}(\vec{r},\vec{r}',\xi_l)e^{-i\vec{k}'\cdot(\vec{r}-\vec{r}')}U_{n'\vec{k}\rho'}(\vec{r}')\ . \quad (2.15)$$

Since the $U_{n\vec{k}\rho}$'s form a complete set for periodic functions, Eq. (2.14) can be written in an alternate form:

$$[\xi_l-H(\vec{\kappa},\xi_l)]\widetilde{G}(\vec{k},\xi_l)=I\ . \quad (2.16)$$

We note that similar Green's-function equations for the orbital motion of Bloch electrons were derived by Phillippas and McClure[12] in the Luttinger-Kohn representation[48] and Mohanty and Misra[15] in the Bloch representation. However, our equation of motion is more general and includes both spin and spin-orbit interaction.

III. DERIVATION OF GENERAL FORMULA FOR χ

The magnetic susceptibility (χ) is calculated from the expression

$$\chi^{\mu\nu}=-\frac{1}{V}\lim_{B\to 0}\frac{\partial^2\Omega}{\partial B^\mu\partial B^\nu}\ . \quad (3.1)$$

The thermodynamic potential Ω is evaluated using the Luttinger-Ward expression[44,49]

$$\Omega=\frac{1}{\beta}[\mathrm{Tr}\ln(-G_{\xi_l})-\mathrm{Tr}\Sigma(G_{\xi_l})G_{\xi_l}+\phi(G_{\xi_l})]\ . \quad (3.2)$$

Here $G_{\xi_l}\equiv G(\xi_l)$, Tr is defined as $\sum_l$ tr, where tr refers to summation over a complete one-particle set, and the functional $\phi(G_{\xi_l})$ is defined as[44,49]

$$\phi(G_{\xi_l})=\lim_{\lambda\to 1}\mathrm{Tr}\sum_n\frac{\lambda^n}{2n}\Sigma^{(n)}(G_{\xi_l})G_{\xi_l}\ . \quad (3.3)$$

Here $\Sigma^{(n)}(G_{\xi_l})$ is the nth-order self-energy part, where only the interaction parameter λ occurring explicitly in Eq. (3.3) is used to determine the order. In fact, $\phi(G_{\xi_l})$ is defined through the decomposition of $\Sigma^{(n)}(G_{\xi_l})$ into skeleton diagrams. There are $2n$ G_{ξ_l} lines for the nth-order diagrams in $\phi(G_{\xi_l})$. Differentiating $\phi(G_{\xi_l})$ with respect to G_{ξ_l} has the effect of "opening" any of the $2n$ lines of the nth-order diagram and each will give the same contribution when Tr is taken.[49] From Eqs. (3.1)–(3.3), it can be easily shown that[44]

$$\chi^{\mu\nu}=\frac{1}{V\beta}\left[-\frac{\partial^2}{\partial B^\mu\partial B^\nu}\mathrm{Tr}\ln(-G_{\xi_l})+\mathrm{Tr}\frac{\partial^2\widetilde{\Sigma}_{\xi_l}}{\partial B^\mu\partial B^\nu}\widetilde{G}_{\xi_l}+\mathrm{Tr}\frac{\partial\widetilde{\Sigma}_{\xi_l}}{\partial B^\mu}\frac{\partial\widetilde{G}_{\xi_l}}{\partial B^\nu}\right]_{B\to 0}\ . \quad (3.4)$$

The first term in the right-hand side of Eq. (3.4) has exactly the same form[44] as that of the noninteracting Fermi systems, except for the replacement of the "noninteracting G_{ξ_l}" by the exact G_{ξ_l} for the interacting Bloch electrons. Thus we denote this term as $\chi_{\rm qp}$ (qp represents quasiparticle) and the sum of the second and the third terms as $\chi_{\rm corr}$, which is the contribution due to exchange and correlation effects, and we have

$$\chi^{\mu\nu}=\chi^{\mu\nu}_{\rm qp}+\chi^{\mu\nu}_{\rm corr}\ . \quad (3.5)$$

In order to evaluate χ from Eq. (3.4), we expand $\widetilde{\Sigma}(\vec{\kappa},\vec{B},\xi_l)$, which is a (2×2) matrix, is an operator in $\vec{k}$ space, and has both explicit (through $\vec{\kappa}$) and implicit $\vec{B}$ dependence,

$$\widetilde{\Sigma}(\vec{\kappa},\vec{B},\xi_l)=\widetilde{\Sigma}(\vec{k},\vec{B},\xi_l)-ih_{\alpha\beta}\frac{\partial\widetilde{\Sigma}(\vec{k},\vec{B},\xi_l)}{\partial k^\alpha}\nabla_k^\beta-\tfrac{1}{2}h_{\alpha\beta}h_{\gamma\delta}\frac{\partial^2\widetilde{\Sigma}}{\partial k^\alpha\partial k^\gamma}\nabla_k^\beta\nabla_k^\delta+\cdots \quad (3.6)$$

and

$$\tilde{\Sigma}(\vec{k},\vec{B},\xi_l)=\Sigma^0(\vec{k},\xi_l)+B^\mu\Sigma^{1,\mu}(\vec{k},\xi_l)+B^\mu B^\nu\Sigma^{2,\mu\nu}(\vec{k},\xi_l)+\cdots , \tag{3.7}$$

where

$$h_{\alpha\beta}=\epsilon_{\alpha\beta\gamma}h^\gamma , \tag{3.8}$$

$\epsilon_{\alpha\beta\gamma}$ is the antisymmetric tensor of the third rank and we follow Einstein summation convention. From Eqs. (2.12), (2.13), (3.6), and (3.7), we write

$$H(\vec{\kappa},\xi_l)=H_0(\vec{k},\xi_l)+H'(\vec{k},\xi_l) , \tag{3.9}$$

where

$$H_0(\vec{k},\xi_l)=\frac{1}{2m}(\vec{p}+\hbar\vec{k})^2+V(\vec{r})+\Sigma^0(\vec{k},\xi_l)+\frac{\hbar^2}{8mc^2}\nabla^2V+\frac{\hbar}{4m^2c^2}\vec{\sigma}\cdot\vec{\nabla}V\times(\vec{p}+\hbar\vec{k}) \tag{3.10}$$

and

$$\begin{aligned}H'(\vec{k},\xi_l)=&-ih_{\alpha\beta}\Pi^\alpha\nabla_k^\beta+\tfrac{1}{2}g\mu_0B^\mu\sigma^\mu+B^\mu\Sigma^{1,\mu}(\vec{k},\xi_l)-ih_{\alpha\beta}B^\mu\frac{\partial\Sigma^{1,\mu}}{\partial k^\alpha}\nabla_k^\beta\\&-\tfrac{1}{2}h_{\alpha\beta}h_{\gamma\delta}\left[\frac{\hbar^2}{m}\delta_{\alpha\gamma}+\frac{\partial^2\Sigma^0}{\partial k^\alpha\partial k^\gamma}\right]\nabla_k^\beta\nabla_k^\delta+B^\mu B^\nu\Sigma^{2,\mu\nu}(\vec{k},\xi_l) ,\end{aligned} \tag{3.11}$$

where we have retained terms up to second order in the magnetic field. Here $\vec{\Pi}/\hbar$ is velocity operator

$$\vec{\Pi}(\vec{k},\xi_l)=\frac{\hbar}{m}(\vec{p}+\hbar\vec{k})+\frac{\hbar^2}{4m^2c^2}\vec{\sigma}\times\vec{\nabla}V+\nabla_k\Sigma^0(\vec{k},\xi_l) . \tag{3.12}$$

We make a perturbation expansion

$$\tilde{G}(\vec{k},\xi_l)=G_0(\vec{k},\xi_l)+G_0(\vec{k},\xi_l)H'G_0(\vec{k},\xi_l)+G_0(\vec{k},\xi_l)H'G_0(\vec{k},\xi_l)H'G_0(\vec{k},\xi_l)+\cdots , \tag{3.13}$$

where

$$G_0(\vec{k},\xi_l)=\frac{1}{\xi_l-H_0(\vec{k},\xi_l)} , \tag{3.14}$$

and we retain terms up to second order in magnetic field. It can be easily shown that[42]

$$\nabla_{\vec{k}}^\alpha G_0(\vec{k},\xi_l)=G_0(\vec{k},\xi_l)\Pi^\alpha G_0(\vec{k},\xi_l) \tag{3.15}$$

and

$$\begin{aligned}\nabla_{\vec{k}}^\alpha\nabla_{\vec{k}}^\gamma G_0(\vec{k},\xi_l)=&\ G_0(\vec{k},\xi_l)\left[\frac{\hbar^2}{m}\delta_{\alpha\gamma}+X^{\alpha\gamma}\right]G_0(\vec{k},\xi_l)+G_0(\vec{k},\xi_l)\Pi^\alpha G_0(\vec{k},\xi_l)\Pi^\gamma G_0(\vec{k},\xi_l)\\&+G_0(\vec{k},\xi_l)\Pi^\gamma G_0(\vec{k},\xi_l)\Pi^\alpha G_0(\vec{k},\xi_l) .\end{aligned} \tag{3.16}$$

We obtain from Eqs. (3.11), (3.13), (3.15), and (3.16)

$$\begin{aligned}\tilde{G}(\vec{k},\xi_l)=G_0(\vec{k},\xi_l)-G_0\Bigg[&ih_{\alpha\beta}\Pi^\alpha G_0\Pi^\beta-\tfrac{1}{2}g\mu_0B^\nu F^\nu\\&+h_{\alpha\beta}h_{\gamma\delta}\Bigg[\frac{\hbar^4}{2m^2}G_0\delta_{\alpha\gamma}\delta_{\beta\delta}+(G_0\Pi^\beta G_0\Pi^\delta-\Pi^\beta G_0G_0\Pi^\delta+\Pi^\beta G_0\Pi^\delta G_0\\&+\tfrac{1}{2}X^{\beta\delta}G_0+\tfrac{1}{2}G_0X^{\beta\delta})\frac{\hbar^2\delta_{\alpha\gamma}}{m}+\tfrac{1}{2}X^{\alpha\gamma}G_0(X^{\beta\delta}+\Pi^\beta G_0\Pi^\delta+\Pi^\delta G_0\Pi^\beta)\end{aligned}$$

$$+\Pi^{\alpha}G_0(\Pi^{\beta}G_0\Pi^{\gamma}G_0\Pi^{\delta}+\Pi^{\gamma}G_0\Pi^{\beta}G_0\Pi^{\delta}+\Pi^{\gamma}G_0\Pi^{\delta}G_0\Pi^{\beta}+\Pi^{\gamma}G_0X^{\beta\delta}$$

$$\left.-\chi^{\beta\delta}G_0\Pi^{\gamma})\right]+\tfrac{1}{2}ih_{\alpha\beta}B^{\nu}[g\mu_0(\Pi^{\alpha}G_0\Pi^{\beta}G_0F^{\nu}$$

$$+\Pi^{\alpha}G_0F^{\nu}G_0\Pi^{\beta}+F^{\nu}G_0\Pi^{\alpha}G_0\Pi^{\beta})+2(Y^{\alpha\nu}G_0\Pi^{\beta}-\Pi^{\beta}G_0Y^{\alpha\nu})]$$

$$\left.+B^{\mu}B^{\nu}\left[\frac{g^2\mu_0^2}{4}F^{\mu}G_0F^{\nu}-\Sigma^{2,\mu\nu}\right]\right]G_0+\cdots\,, \tag{3.17}$$

where

$$Y^{\mu\nu}=\frac{\partial\Sigma^{1,\nu}}{\partial k^{\mu}} \tag{3.18}$$

and

$$F^{\nu}=\sigma^{\nu}+\frac{2}{g\mu_0}\Sigma^{1,\nu}\,. \tag{3.19}$$

A. Evaluation of $\chi_{\rm qp}$

We shall calculate $\chi_{\rm qp}^{\mu\nu}$ using Eqs. (3.4) and (3.19). We assume the self-energy to be independent of frequency, an approximation valid in the statistically screened exchange approximation.[50] To carry out the frequency sums appearing in $\chi_{\rm qp}^{\mu\nu}$, we use the identity[49]

$$\frac{1}{\beta}\sum_{\xi_l}\ln\left[\frac{1}{H-\xi_l}\right]=-\frac{1}{2\Pi i}\int_C\frac{d\xi}{e^{\beta(\xi-\mu)}+1}\ln\left[\frac{1}{H-\xi_l}\right], \tag{3.20}$$

where the contour C encircles the imaginary axis in a counterclockwise direction. We define

$$\phi_0(\xi)=-\frac{1}{\beta}\ln(1+e^{-\beta(\xi-\mu)})\,. \tag{3.21}$$

From Eqs. (3.2), (3.20), and (3.21), we obtain

$$\Omega_{\rm qp}=\frac{1}{2\Pi i}{\rm tr}\int_C\frac{d\phi_0(\xi)}{d\xi}\ln(H-\xi)d\xi\,, \tag{3.22}$$

where tr is taken over one-particle states only. By partial integration, we obtain from Eq. (3.22)

$$\Omega_{\rm qp}=\frac{1}{2\Pi i}{\rm tr}\left[\phi_0(\xi)\ln(H-\xi)-\int_C\phi_0(\xi)\frac{1}{\xi-H}d\xi\right]. \tag{3.23}$$

Since the first term is zero, we have

$$\Omega_{\rm qp}=-\frac{1}{2\Pi i}{\rm tr}\int_C\phi_0(\xi)G(\xi)d\xi\,. \tag{3.24}$$

The advantage of using Eq. (3.24) is that after substituting the perturbation expression for $\widetilde{G}(\xi)$ [Eq. (3.17)], the thermodynamic potential is easily evaluated. The results are precisely the same as obtained by using the inverse Laplace-transform technique,[42] but the present technique is simpler.

The one-particle trace is evaluated over the periodic part of $\psi_{n\vec{k}\rho}$, which are eigenfunctions of $H_0(\vec{k})$. In this basis G_0 is diagonal and is given by

$$G_0^{-1}=(\xi-E_{nk})\,. \tag{3.25}$$

After evaluating the trace, we perform the contour integration as prescribed in Eq. (3.24). We use the identity[41]

$$h_{\alpha\beta}h_{\gamma\delta}(M_l^\alpha M_2^\beta M_3^\gamma M_4^\delta + M_1^\alpha M_2^\gamma M_3^\delta M_4^\beta) = h_{\alpha\beta}h_{\gamma\delta}M_1^\alpha M_2^\gamma M_3^\beta M_4^\delta \,, \tag{3.26}$$

where M_1, M_2, M_3, and M_4 are any matrix elements and

$$\vec{\Pi}_{n\rho,n\bar{\rho}} = 0 \,, \tag{3.27}$$

where $\bar{\rho}$ is a spin state conjugate to ρ. We also adopt the convention that the running index means that the sum over all the bands and all the spin indices shall be taken except that all band terms equal to n have been explicitly separated out. After considerable algebra we obtain

$$\begin{aligned}
\mathrm{Tr}\ln(-G_{\xi_l}) = \sum_{\vec{k}} & ih_{\alpha\beta}(\Pi^\alpha_{n\rho,m\rho'}\Pi^\beta_{m\rho',n\rho} - B^\mu \Pi^\beta_{n\rho,m\rho'}Y^{\alpha\mu}_{m\rho',n\rho} \\
& + B^\mu Y^{\alpha\mu}_{n\rho,m\rho'}\Pi^\beta_{m\rho',n\rho})\left[\frac{f(E_n)}{E_{mn}} + \frac{2\phi_0(E_n)}{E_{mn}^2}\right] + \tfrac{1}{2}g\mu_0 B^\mu F^\mu_{n\rho,n\rho}f(E_n) \\
& + h_{\alpha\beta}h_{\gamma\delta}\left[-\frac{1}{6}\left[\frac{\hbar^2}{m}\delta_{\beta\delta} + X^{\beta\delta}_{n\rho,n\rho}\right]\Pi^\alpha_{n\rho,n\rho}\Pi^\gamma_{n\rho,n\rho}f''(E_n)\right. \\
& \quad - \left[\frac{\hbar^4}{4m^2}\delta_{\alpha\gamma}\delta_{\beta\delta} + \frac{\hbar^2}{2m}X^{\alpha\gamma}_{n\rho,n\rho}\delta_{\beta\delta} - \tfrac{1}{4}X^{\alpha\gamma}_{n\rho,n\rho}X^{\beta\delta}_{n\rho,n\rho}\right]f'(E_n) \\
& \quad + \Pi^\alpha_{n\rho,n\rho}\Pi^\gamma_{n\rho,n\rho}\Pi^\beta_{n\rho,m\rho'}\Pi^\delta_{m\rho',n\rho}\left[\frac{f''(E_n)}{3E_{mn}} + \frac{2f'(E_n)}{E_{mn}^2} + \frac{6f(E_n)}{E_{mn}^3} + \frac{8\phi_0(E_n)}{E_{mn}^4}\right] \\
& \quad + \frac{\hbar^2}{m}\Pi^\alpha_{n\rho,m\rho'}\Pi^\gamma_{m\rho',n\rho}\delta_{\beta\delta}\left[\frac{f'(E_n)}{E_{mn}} + \frac{4f(E_n)}{E_{mn}^2} + \frac{8\phi_0(E_n)}{E_{mn}^3}\right] \\
& \quad - \Pi^\alpha_{n\rho,m\rho'}\Pi^\gamma_{m\rho',n\rho''}\Pi^\beta_{n\rho'',q\rho'''}\Pi^\delta_{q\rho''',n\rho}\left[\frac{f'(E_n)}{E_{mn}E_{qn}} + \frac{6f(E_n)}{E_{mn}^2E_{qn}} + \frac{8\phi_0(E_n)}{E_{mn}^3E_{qn}} + \frac{4\phi_0(E_n)}{E_{mn}^2E_{qn}^2}\right] \\
& \quad + \Pi^\alpha_{n\rho,m\rho'}\Pi^\gamma_{m\rho',q\rho''}\Pi^\beta_{q\rho'',l\rho'''}\Pi^\delta_{l\rho''',n\rho}\left[\frac{2f(E_n)}{E_{\ln}E_{qn}E_{mn}} + \frac{4\phi_0(E_n)}{E_{mn}^2E_{\ln}E_{qn}} + \frac{4\phi_0(E_n)}{E_{\ln}^2E_{mn}E_{qn}}\right] \\
& \quad \left. + \Pi^\alpha_{n\rho,n\rho}\Pi^\gamma_{n\rho,m\rho'}\Pi^\beta_{m\rho',q\rho''}\Pi^\delta_{q\rho'',n\rho}\left[-\frac{2f(E_n)}{E_{mn}E_{qn}^2} + \frac{2f(E_n)}{E_{mn}^2E_{qn}} - \frac{4\phi_0(E_n)}{E_{mn}E_{qn}^3} + \frac{4\phi_0(E_n)}{E_{mn}^3E_{qn}}\right]\right] \\
& + \tfrac{1}{4}g^2\mu_0^2B^\mu B^\nu\left[\tfrac{1}{2}F^\mu_{n\rho,n\rho'}F^\nu_{n\rho',n\rho}f'(E_n) - \frac{F^\mu_{n\rho,m\rho'}F^\nu_{m\rho',n\rho}}{E_{mn}}f(E_n)\right] \\
& + (\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^\mu F^\mu_{n\rho,n\rho'}\Pi^\alpha_{n\rho',m\rho''}\Pi^\beta_{m\rho'',n\rho} + h_{\alpha\beta}h_{\gamma\delta}X^{\alpha\gamma}_{n\rho,n\rho}\Pi^\beta_{n\rho,m\rho'}\Pi^\delta_{m\rho',n\rho}) \\
& \times\left[\frac{f'(E_n)}{E_{mn}} + \frac{3f(E_n)}{E_{mn}^2} + \frac{4\phi_0(E_n)}{E_{mn}^3}\right] - (\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^\mu\Pi^\alpha_{n\rho,m\rho'}\Pi^\beta_{m\rho',q\rho''}F^\mu_{q\rho'',n\rho} \\
& \qquad + h_{\alpha\beta}h_{\gamma\delta}\Pi^\beta_{n\rho,m\rho'}\Pi^\delta_{m\rho',q\rho''}X^{\alpha\gamma}_{q\rho'',n\rho})\left[\frac{f(E_n)}{E_{qn}E_{mn}} + \frac{2\phi_0(E_n)}{E_{mn}^2E_{qn}}\right]
\end{aligned}$$

$$-(\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^{\mu}\pi^{\alpha}_{n\rho,m\rho'}F^{\mu}_{m\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho}-h_{\alpha\beta}h_{\gamma\delta}\pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\pi^{\delta}_{q\rho'',n\rho})$$

$$\times\left[\frac{f(E_n)}{E_{qn}E_{mn}}+\frac{2\phi_0(E_n)}{E^2_{mn}E_{qn}}+\frac{2\phi_0(E_n)}{E^2_{qn}E_{mn}}\right]-(\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^{\mu}F^{\mu}_{n\rho,m\rho'}\pi^{\alpha}_{m\rho',q\rho''}\pi^{\beta}_{q\rho'',n\rho}$$

$$+h_{\alpha\beta}h_{\gamma\delta}X^{\alpha\gamma}_{n\rho,m\rho'}\pi^{\beta}_{m\rho',q\rho''}\pi^{\delta}_{q\rho'',n\rho})\left[\frac{f(E_n)}{E_{mn}E_{qn}}+\frac{2\phi_0(E_n)}{E_{mn}E^2_{qn}}\right]$$

$$+(\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^{\mu}\Pi^{\alpha}_{n\rho,m\rho'}F^{\mu}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}-h_{\alpha\beta}h_{\gamma\delta}\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho})$$

$$\times\left[\frac{f(E_n)}{E^2_{mn}}+\frac{2\phi_0(E_n)}{E^3_{mn}}\right]-(\tfrac{1}{2}ih_{\alpha\beta}g\mu_0B^{\mu}F^{\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}$$

$$+h_{\alpha\beta}h_{\gamma\delta}X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho})\left[\frac{f(E_n)}{E_{mn}E_{qn}}+\frac{2\phi_0(E_n)}{E_{mn}E^2_{qn}}\right]$$

$$-ih_{\alpha\beta}B^{\mu}(\Pi^{\beta}_{n\rho,m\rho'}Y^{\alpha\gamma}_{m\rho',n\rho}-Y^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho})\left[\frac{f(E_n)}{E_{mn}}+\frac{2\phi_0(E_n)}{E^2_{mn}}\right]+B^{\mu}B^{\nu}\Sigma^{2,\mu\nu}_{n\rho,n\rho}f(E_n)\,, \tag{3.28}$$

where, as indicated earlier, sums will be taken over all indices n, m, q, l, ρ, and ρ', but $n\neq m,q,l$. In the above, we have also used the notation

$$E_{mn}=E_m(\vec{k})-E_n(\vec{k})\,. \tag{3.29}$$

In Appendix A, we derive the following identity:

$$\sum_{\vec{k}}\left[2h_{\alpha\beta}h_{\gamma\delta}\left[\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}\right.\right.$$
$$\left.-2\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^3_{mn}}\right]$$
$$\left.+ih_{\alpha\beta}g\mu_0B^{\mu}\left[\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}F^{\mu}_{m\rho',n\rho}}{E^2_{mn}}-\frac{\Pi^{\alpha}_{n\rho,n\rho}F^{\mu}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^2_{mn}}\right]\right]f(E_n)$$
$$=\sum_{\vec{k}}\left\{4h_{\alpha\beta}h_{\gamma\delta}\left[2\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^4_{mn}}+\frac{2\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^3_{mn}}\delta_{\beta\delta}\right.\right.$$
$$-\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}\left[\frac{2}{E^3_{mn}E_{qn}}+\frac{1}{E^2_{mn}E^2_{qn}}\right]$$
$$+\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',l\rho'''}\Pi^{\delta}_{l\rho''',n\rho}\left[\frac{1}{E^2_{mn}E_{\ln}E_{qn}}+\frac{1}{E^2_{\ln}E_{mn}E_{qn}}\right]$$

$$-\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\left[\frac{1}{E_{mn}E_{qn}^3}-\frac{1}{E_{mn}^3E_{qn}}\right]\Bigg]$$

$$+\left[\frac{2ih_{\alpha\beta}g\mu_0B^{\mu}F^{\mu}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}+4h_{\alpha\beta}h_{\gamma\delta}X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E_{mn}^3}\right]$$

$$-\left[\frac{ih_{\alpha\beta}g\mu_0B^{\mu}\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}F^{\mu}_{q\rho'',n\rho}+2h_{\alpha\beta}h_{\gamma\delta}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}X^{\alpha\gamma}_{q\rho'',n\rho}}{E_{mn}^2E_{qn}}\right]$$

$$-(ih_{\alpha\beta}g\mu_0B^{\mu}\Pi^{\alpha}_{n\rho,m\rho'}F^{\mu}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}-2h_{\alpha\beta}h_{\gamma\delta}\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho})$$

$$\times\left[\frac{1}{E_{mn}^2E_{qn}}+\frac{1}{E_{qn}^2E_{mn}}\right]$$

$$-\left[\frac{ih_{\alpha\beta}g\mu_0B^{\mu}F^{\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}+2h_{\alpha\beta}h_{\gamma\delta}X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E_{qn}^2}\right]$$

$$+\left[\frac{ih_{\alpha\beta}g\mu_0B^{\mu}\Pi^{\alpha}_{n\rho,n\rho}F^{\mu}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}-2h_{\alpha\beta}h_{\gamma\delta}\Pi^{\beta}_{n\rho,n\rho}X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E_{mn}^3}\right]$$

$$-\left[\frac{ih_{\alpha\beta}g\mu_0B^{\mu}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}F^{\mu}_{m\rho',n\rho}+2h_{\alpha\beta}h_{\gamma\delta}\Pi^{\beta}_{n\rho,n\rho}\Pi^{\delta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',n\rho}}{E_{mn}^3}\right]$$

$$-2ih_{\alpha\beta}\left[\frac{\Pi^{\beta}_{n\rho,m\rho'}Y^{\alpha\gamma}_{m\rho',n\rho}-Y^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E_{mn}^2}\right]\Bigg\}\phi_0(E_n)\ . \qquad (3.30)$$

In Appendix B we show that

$$\sum_{\vec{k}}h_{\alpha\beta}h_{\gamma\delta}\Bigg\{\Bigg[-\frac{1}{6}\left[\frac{\hbar^2}{m}\delta_{\beta\delta}+X^{\beta\delta}_{n\rho,n\rho}\right]\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{3E_{mn}}\Bigg]f''(E_n)$$

$$-\Bigg[\left[\frac{\hbar^4}{4m^2}\delta_{\alpha\gamma}\delta_{\beta\delta}+\frac{\hbar^2}{2m}X^{\alpha\gamma}_{n\rho,n\rho}\delta_{\beta\delta}-\tfrac{1}{4}X^{\alpha\gamma}_{n\rho,n\rho}X^{\beta\delta}_{n\rho,n\rho}\right]-\left[\frac{\hbar^2}{m}\delta_{\beta\delta}+X^{\beta\delta}_{n\rho,n\rho}\right]\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{2E_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\delta}_{n\rho'',q\rho'''}\Pi^{\beta}_{q\rho''',n\rho}}{2E_{mn}E_{qn}}\Bigg]f'(E_n)\Bigg\}$$

$$=-\tfrac{1}{12}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_nf'(E_n)\ . \qquad (3.31)$$

It can also be shown by a partial integration similar to that shown in Appendix A for Eq. (3.30):

$$2h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^2_{mn}}f'(E_n)$$

$$=h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\left[2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}+2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\delta}_{n\rho,q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}\right.$$

$$-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}-\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\left\{\frac{1}{E_{qn}E^2_{mn}}-\frac{1}{E_{mn}E^2_{qn}}\right.$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}-2\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^3_{mn}}$$

$$-\frac{2\hbar^2}{m}\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^2_{mn}}\delta_{\alpha\gamma}-2\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^2_{mn}}$$

$$\left.+\frac{\Pi^{\beta}_{n\rho,n\rho}X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^2_{mn}}+\frac{\Pi^{\delta}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',n\rho}}{E^2_{mn}}\right]f(E_n)\ . \tag{3.32}$$

It can be easily shown from time-reversal symmetry[41] that

$$\Pi_{n\rho,m\rho'}(\vec{k})=\pm\Pi_{m\bar{\rho},n\bar{\rho}'}(-\vec{k}) \tag{3.33}$$

and

$$F_{n\rho,n\rho}(\vec{k})=-F_{n\bar{\rho},n\bar{\rho}}(-\vec{k})\ . \tag{3.34}$$

Using $h_{\alpha\beta}=-h_{\beta\alpha}$ and the above, we have for nonferromagnetic crystals

$$\sum_{\substack{n,m,\rho,\rho',\vec{k}\\ n\neq m}} ih_{\alpha\beta}\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}\left[\frac{f(E_n)}{E_{mn}}+\frac{2\phi_0(E_n)}{E^2_{mn}}\right]+\tfrac{1}{2}g\mu_0B^{\mu}F^{\mu}_{n\rho,n\rho}f(E_n)=0\ . \tag{3.35}$$

From Eqs. (3.1), (3.28), (3.30), (3.31), (3.32), and (3.35), we obtain

$$\chi^{\mu\nu}_{\rm qp}=\sum_{\vec{k}}(1+\delta_{\mu\nu})\left\{\left[\frac{e^2}{48\hbar^2c^2}\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_n\right.\right.$$

$$+\frac{e^2}{8\hbar^2c^2}\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}$$

$$\left.-\tfrac{1}{8}g^2\mu_0^2F^{\mu}_{n\rho,n\rho'}F^{\nu}_{n\rho',n\rho}-\frac{ieg\mu_0}{4\hbar c}\epsilon_{\alpha\beta\nu}\frac{F^{\mu}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}}{E_{mn}}\right]f'(E_n)$$

$$+\left[\frac{e^2}{4\hbar^2c^2}\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}\left\{-\frac{2\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^2_{mn}}\delta_{\beta\delta}+2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E_{qn}}\right.\right.$$

$$+2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E_{qn}}-2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',l\rho'''}\Pi^{\delta}_{l\rho''',n\rho}}{E_{ln}E_{qn}E_{mn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}$$

$$-2\frac{\Pi^{\beta}_{np,mp'}X^{\alpha\gamma}_{mp',qp''}\Pi^{\delta}_{qp'',np}}{E_{mn}E_{qn}}+2\frac{\Pi^{\beta}_{np,mp'}\Pi^{\delta}_{mp',qp''}X^{\alpha\gamma}_{qp'',np}}{E_{mn}E_{qn}}$$

$$+2\frac{X^{\alpha\gamma}_{np,mp'}\Pi^{\beta}_{mp',qp''}\Pi^{\delta}_{qp'',np}}{E_{mn}E_{qn}}-2\frac{X^{\alpha\gamma}_{np,np}\Pi^{\beta}_{np,mp'}\Pi^{\delta}_{mp',np}}{E^2_{mn}}\Bigg]+\tfrac{1}{4}g^2\mu_0^2\frac{F^{\mu}_{np,mp'}F^{\nu}_{mp',np}}{E_{mn}}$$

$$+\frac{ieg\mu_0}{4\hbar c}\epsilon_{\alpha\beta\nu}\Bigg[-3\frac{F^{\mu}_{np,np'}\Pi^{\alpha}_{np',mp''}\Pi^{\beta}_{mp'',np}}{E^2_{mn}}+\frac{\Pi^{\alpha}_{np,mp'}\Pi^{\beta}_{mp',qp''}F^{\mu}_{qp'',np}}{E_{qn}E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{np,mp'}F^{\mu}_{mp',qp''}\Pi^{\beta}_{qp'',np}}{E_{qn}E_{mn}}+\frac{F^{\mu}_{np,mp'}\Pi^{\alpha}_{mp',qp''}\Pi^{\beta}_{qp'',np}}{E_{qn}E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{np,np}F^{\mu}_{np,mp'}\Pi^{\beta}_{mp',np}}{E^2_{mn}}-\frac{\Pi^{\alpha}_{np,np}\Pi^{\beta}_{np,mp'}F^{\mu}_{mp',np}}{E^2_{mn}}\Bigg]$$

$$+\frac{ie}{2\hbar c}\epsilon_{\alpha\beta\nu}\left[\frac{\Pi^{\beta}_{np,mp'}Y^{\alpha\mu}_{mp',np}-Y^{\alpha\mu}_{np,mp'}\Pi^{\beta}_{mp',np}}{E_{mn}}\right]-\Sigma^{2,\mu\nu}_{np,np}\Bigg]f(E_n)\Bigg\}\,. \tag{3.36}$$

We note that in the absence of an electron-electron interaction $F=\sigma$, $X=0$, $Y=0$, and E_n and Π reduce to the corresponding values for noninteracting Bloch electrons. In such limits, it can be easily shown that our expression for χ_{qp} reduces to the earlier results of χ obtained for noninteracting Bloch electrons.[41,46,47]

B. Derivation of χ_{corr}

We shall now derive an expression for χ_{corr}. From Eqs. (3.7) and (3.17), we obtain

$$\chi^{\mu\nu}_{\text{corr}}=\frac{1}{\beta}\text{Tr}\left[\frac{\partial^2\tilde{\Sigma}_{\xi_l}}{\partial B_\mu\partial B_\nu}\tilde{G}_{\xi_l}+\frac{\partial\tilde{\Sigma}_{\xi_l}}{\partial B_\mu}\frac{\partial\tilde{G}_{\xi_l}}{\partial B_\nu}\right]_{B\to 0}$$

$$=\frac{1}{\beta}\text{Tr}\Bigg[(1+\delta_{\mu\nu})\Bigg\{\Sigma^{2,\mu\nu}_{\xi_l}G_0(\vec{k},\xi_l)-\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\Sigma^{1,\mu}_{\xi_l}G_0(\vec{k},\xi_l)\Pi^{\alpha}G_0(\vec{k},\xi_l)\Pi^{\beta}G_0(\vec{k},\xi_l)$$

$$+\tfrac{1}{4}g\mu_0\Sigma^{1,\mu}_{\xi_l}G_0(\vec{k},\xi_l)F^{\nu}G_0(\vec{k},\xi_l)\Bigg\}\Bigg]\,. \tag{3.37}$$

As before, we assume the self-energy to be independent of frequency. We carry out the frequency sums as per prescription of Luttinger and Ward[49]:

$$\frac{1}{\beta}\sum_l\frac{1}{(\xi_l-E_n)^m}=\frac{1}{2\Pi i}\int_{\Gamma_0}\frac{1}{(\xi-E_n)^m}\frac{1}{e^{\beta(\xi-\mu)}+1}d\xi\,. \tag{3.38}$$

We obtain

$$\chi^{\mu\nu}_{\text{corr}}=\sum_{\vec{k}}(1+\delta_{\mu\nu})\Bigg\{\Bigg[\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\Bigg[\frac{\Sigma^{1,\mu}_{np,np'}\Pi^{\alpha}_{np',mp''}\Pi^{\beta}_{mp'',np}}{E_{mn}}+\frac{\Sigma^{1,\mu}_{np,mp'}\Pi^{\alpha}_{mp',np}\Pi^{\beta}_{np,np}}{E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',n\rho}}{E_{mn}}\Bigg]+\tfrac{1}{4}g\mu_0\Sigma^{1,\mu}_{n\rho,n\rho'}F^{\nu}_{n\rho',n\rho}\Bigg]f'(E_n)$$

$$+\Bigg[\Sigma^{2,\mu\nu}_{n\rho,n\rho}+\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\Bigg[\frac{\Sigma^{1,\mu}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}}{E^2_{mn}}+\frac{\Sigma^{1,\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,n\rho}}{E^2_{mn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',n\rho}}{E^2_{mn}}-\frac{\Sigma^{1,\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E_{qn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Sigma^{1,\mu}_{q\rho'',n\rho}}{E_{qn}E_{mn}}-\frac{\Pi^{\beta}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',q\rho''}\Pi^{\alpha}_{q\rho'',n\rho}}{E_{mn}E_{qn}}\Bigg]$$

$$-\tfrac{1}{4}g\mu_0\Bigg[\frac{\Sigma^{1,\mu}_{n\rho,m\rho'}F^{\nu}_{m\rho',n\rho}}{E_{mn}}+\frac{F^{\nu}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',n\rho}}{E_{mn}}\Bigg]\Bigg]f(E_n)\Bigg\}\;. \tag{3.39}$$

C. General expression for magnetic susceptibility

It can be shown by partial integration method outlined in Appendix A that

$$\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\sum_{\vec{k}}\Bigg[\frac{\Sigma^{1,\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,n\rho}}{E_{mn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',n\rho}}{E_{mn}}\Bigg]f'(E_n)$$

$$=\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\sum_{\vec{k}}\Bigg[\Bigg[2\frac{\Pi^{\beta}_{n\rho,m\rho'}\Sigma^{1,\mu}_{m\rho',q\rho''}\Pi^{\alpha}_{q\rho'',n\rho}}{E_{mn}E_{qn}}-2\frac{\Sigma^{1,\mu}_{n\rho,n\rho'}\Pi^{\beta}_{n\rho',m\rho''}\Pi^{\alpha}_{m\rho'',n\rho}}{E^2_{mn}}\Bigg]$$

$$+\Bigg[\frac{\Pi^{\alpha}_{n\rho,m\rho'}Y^{\beta\mu}_{m\rho',n\rho}}{E_{mn}}-\frac{Y^{\beta\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',n\rho}}{E_{mn}}\Bigg]\Bigg]f(E_n)\;. \tag{3.40}$$

From Eqs. (3.5), (3.36), (3.39), and (3.40), we obtain the general expression for total magnetic susceptibility, which we write in an alternate form:

$$\chi^{\mu\nu}=\chi^{\mu\nu}_{o}+\chi^{\mu\nu}_{s}+\chi^{\mu\nu}_{\rm so}\;, \tag{3.41}$$

where $\chi^{\mu\nu}_{o}$ is the orbital contribution to the susceptibility,

$$\chi^{\mu\nu}_{o}=\sum_{\vec{k}}(1+\delta_{\mu\nu})\Bigg\{\frac{e^2\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}}{48\hbar^2c^2}\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_nf'(E_n)$$

$$+\Bigg[\frac{e^2\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}}{4\hbar^2c^2}\Bigg[-\frac{2\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^2_{mn}}\delta_{\beta\delta}+2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E_{qn}}$$

$$-2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',l\rho'''}\Pi^{\delta}_{l\rho''',n\rho}}{E_{\rm ln}E_{qn}E_{mn}}-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}-\frac{\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E_{qn}}$$

$$+\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}X^{\alpha\gamma}_{q\rho'',n\rho}}{E_{mn}E_{qn}}+\frac{X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E_{qn}}-\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^2_{mn}}\Bigg]$$

$$+\frac{ie}{4\hbar c}\epsilon_{\alpha\beta\nu}\left[\frac{\Pi^{\beta}_{n\rho,m\rho'}Y^{\alpha\mu}_{m\rho',n\rho}}{E_{mn}}-\frac{Y^{\alpha\mu}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E_{mn}}\right]\Bigg]f(E_n)\Bigg\}, \tag{3.42}$$

$\chi^{\mu\nu}_s$ is the effective Pauli spin susceptibility including exchange and correlation effects,

$$\chi^{\mu\nu}_s=\sum_{\vec{k}}(1+\delta_{\mu\nu})\Bigg[\frac{e^2\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}}{8\hbar^2c^2}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}-\tfrac{1}{8}g^2\mu_0^2\sigma^{\mu}_{n\rho,n\rho'}F^{\nu}_{n\rho',n\rho}$$

$$-\frac{ieg\mu_0}{4\hbar c}\epsilon_{\alpha\beta\nu}\frac{J^{\mu}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}}{E_{mn}}\Bigg]f'(E_n), \tag{3.43}$$

and $\chi^{\mu\nu}_{\rm so}$ is the additional spin-orbit contribution to the magnetic susceptibility,

$$\chi^{\mu\nu}_{\rm so}=\sum_{\vec{k}}(1+\delta_{\mu\nu})\Bigg[\frac{e^2\epsilon_{\alpha\beta\mu}\epsilon_{\gamma\delta\nu}}{2\hbar^2c^2}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E_{qn}}$$

$$+\frac{ieg\mu_0}{4\hbar c}\epsilon_{\alpha\beta\nu}\Bigg[-3\frac{J^{\mu}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}}{E^2_{mn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}J^{\mu}_{q\rho'',n\rho}}{E_{qn}E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,m\rho'}J^{\mu}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{qn}E_{mn}}+\frac{J^{\mu}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{qn}E_{mn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho'}J^{\mu}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^2_{mn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}J^{\mu}_{m\rho',n\rho}}{E^2_{mn}}\Bigg]+\tfrac{1}{8}g^2\mu_0^2\left[\frac{\sigma^{\mu}_{n\rho,m\rho'}F^{\nu}_{m\rho',n\rho}}{E_{mn}}+\frac{F^{\mu}_{n\rho,m\rho'}\sigma^{\nu}_{m\rho',n\rho}}{E_{mn}}\right]\Bigg]f(E_n). \tag{3.44}$$

Here

$$\vec{J}=\vec{\sigma}+\frac{1}{g\mu_0}\Sigma^1, \tag{3.45}$$

$E_{mn}=E_m-E_n$, and the other symbols have their usual meanings. We would like to make a few remarks. Had we kept only the quasiparticle contribution to χ, both spin vertices σ^{μ} and σ^{ν} appearing in χ_s would have been renormalized to F^{μ} and F^{ν} by the exchange-correlation effect. The addition of $\chi_{\rm corr}$ results in cancelling the renormalization effects of one spin vertex keeping only one renormalized spin vertex. Similarly in $\chi_{\rm so}$, every spin matrix $\vec{\sigma}$ appearing in $\sigma\Pi\Pi$ terms gets renormalized by $\vec{J}$, which is equivalent to the vertex correction of one of the two spin vertices. Had we considered only the quasiparticle term, each $\vec{\sigma}$ would have been renormalized by $\vec{F}$. Similarly in the $\sigma\sigma$ terms, one of the $\vec{\sigma}$ gets modified to $\vec{F}$. There are also additional contributions due to self-energy terms.

We can also rewrite $\chi^{\mu\nu}_s$ in Eq. (3.43) as

$$\chi^{\mu\nu}_s=-\tfrac{1}{8}(1+\delta_{\mu\nu})\mu_0^2\sum_{n,\vec{k},\rho,\rho'}g^{\nu}_{nn}(\vec{k})\sigma^{\nu}_{n\rho,n\rho'}\left[g^{\mu}_{nn}(\vec{k})\sigma^{\mu}_{n\rho',n\rho}+\frac{2}{\mu_0}\Sigma^{1,\mu}_{n\rho',n\rho}\right]f'(E_n), \tag{3.46}$$

where the effective g matrix is defined as

$$g_{nn}^{\nu}(\vec{k})\sigma_{n\rho,n\rho'}^{\nu}=\frac{ie}{\mu_0\hbar c}\epsilon_{\alpha\beta\nu}\sum_{m,\rho''}\frac{\Pi_{n\rho,m\rho''}^{\alpha}\Pi_{m\rho'',n\rho'}^{\beta}}{E_{mn}}+g\sigma_{n\rho,n\rho'}^{\nu} . \tag{3.47}$$

In the absence of many-body effects, Eq. (3.46) is identical to the expression for effective Pauli spin susceptibility. The exchange and correlation effects are included through the vertex correction, i.e., σ^{μ} is corrected to $(2/g_{\text{eff}}\mu_0)\Sigma^{1,\mu}+\sigma^{\mu}$.

IV. MANY-BODY EFFECTS ON MAGNETIC SUSCEPTIBILITY

A. Exchange self-energy in the band model

The exchange contribution to the self-energy is local in $\vec{r}$ space

$$\Sigma(\vec{r},\vec{r}\,',\xi_l)=-\frac{1}{\beta}\sum_{\xi_{l'}}v_{\text{eff}}(\vec{r},\vec{r}\,')G(\vec{r},\vec{r}\,',\xi_l-\xi_{l'}) , \tag{4.1}$$

where a simple static screening approximation is made in obtaining $v_{\text{eff}}(\vec{r},\vec{r}\,')$ from $v(\vec{r},\vec{r}\,')$. In this approximation the self-energy is independent of ξ_l and one has

$$\Sigma(\vec{r},\vec{r}\,')=-\frac{1}{\beta}\sum_{\xi_l}v_{\text{eff}}(\vec{r},\vec{r}\,')G(\vec{r},\vec{r}\,',\xi_l) . \tag{4.2}$$

We also assume that $v_{\text{eff}}(\vec{r},\vec{r}\,')$ is field independent, i.e., neglecting the field dependence of screening, we obtain

$$\tilde{\Sigma}(\vec{r},\vec{r}\,')=-\frac{1}{\beta}\sum_{\xi_l}v_{\text{eff}}(\vec{r},\vec{r}\,')\tilde{G}(\vec{r},\vec{r}\,',\xi_l) . \tag{4.3}$$

$\tilde{\Sigma}$ and $\tilde{G}$ can be expanded in terms of Bloch states as follows:

$$\tilde{\Sigma}(\vec{r},\vec{r}\,')=\sum_{n,m,\vec{k},\rho,\rho'}\tilde{\Sigma}_{n\rho,m\rho'}(\vec{k})\psi_{n\vec{k}\rho}(\vec{r})\psi^{*}_{m\vec{k}\rho'}(\vec{r}\,') \tag{4.4a}$$

and

$$\tilde{G}(\vec{r},\vec{r}\,')=\sum_{n,m,\vec{k},\rho,\rho'}\tilde{G}_{n\rho,m\rho'}(\vec{k})\psi_{n\vec{k}\rho}(\vec{r})\psi^{*}_{m\vec{k}\rho'}(\vec{r}\,') . \tag{4.4b}$$

Substituting Eqs. (4.4a) and (4.4b) in Eq. (4.3), we obtain

$$\sum_{n,m,\rho,\rho'}\tilde{\Sigma}_{n\rho,m\rho'}(\vec{k})\psi_{n\vec{k}\rho}(\vec{r})\psi^{*}_{m\vec{k}\rho'}(\vec{r}\,')$$
$$=-\frac{1}{\beta}\sum_{\xi_l}\sum_{p,q,\vec{k}',\bar{\rho},\bar{\rho}'}v_{\text{eff}}(\vec{r},\vec{r}\,')\tilde{G}_{p\bar{\rho},q\bar{\rho}'}(\vec{k}')\psi_{p\vec{k}'\bar{\rho}}(\vec{r})\psi^{*}_{q\vec{k}'\bar{\rho}'}(\vec{r}\,') . \tag{4.5}$$

If the effective electron-electron interaction is spin independent, then $\rho=\bar{\rho},\rho'=\bar{\rho}'$ and we have

$$\tilde{\Sigma}_{n\rho,m\rho'}(\vec{k})=-\frac{1}{\beta}\sum_{\vec{k}',\xi_l,p,q}\langle nm\,|\,v_{\text{eff}}(\vec{k},\vec{k}')\,|\,pq\rangle_{\rho\rho'}\tilde{G}_{p\rho,q\rho'}(\vec{k}',\xi_l) , \tag{4.6}$$

where

$$\langle nm\,|\,v_{\text{eff}}(\vec{k},\vec{k}')\,|\,pq\rangle_{\rho\rho'}=\int\psi^{*}_{n\vec{k}\rho}(\vec{r})\psi_{m\vec{k}\rho'}(\vec{r}\,')v_{\text{eff}}(\vec{r},\vec{r}\,')\psi_{p\vec{k}'\rho}(\vec{r})\psi^{*}_{q\vec{k}'\rho'}(\vec{r}\,')d\vec{r}\,d\vec{r}\,' . \tag{4.7}$$

Equation (4.6) is the expression for exchange self-energy in the band model. We can obtain $\Sigma^0,\Sigma^1,\Sigma^2$, etc., by expanding $\tilde{G}$. However, the resulting expressions become very complicated, and we have to make further approximations to obtain reasonably tractable expressions. We shall now evaluate $\Sigma^{1}_{n\rho,n\rho'}$ and $\Sigma^{1}_{n\rho,m\rho'}$, which occur in χ_s and χ_{so}. We make the approximation

$$\langle nn \mid v_{\text{eff}}(\vec{k},\vec{k}') \mid pq \rangle_{\rho\rho'} \simeq \langle nn \mid v_{\text{eff}}(\vec{k},\vec{k}') \mid pp \rangle \delta_{pq} = v_{np}(\vec{k},\vec{k}')\delta_{pq} \; . \tag{4.8}$$

From Eqs. (4.6) and (4.8), we obtain

$$\tilde{\Sigma}_{n\rho,n\rho'}(\vec{k}) = -\frac{1}{\beta} \sum_{\vec{k}',\xi_l,p} v_{np}(\vec{k},\vec{k}')\tilde{G}_{p\rho,p\rho'}(\vec{k}',\xi_l) \; . \tag{4.9}$$

Substituting the value of $\tilde{G}$ from Eq. (3.17) in Eq. (4.9), summing over ξ_l, expanding $\tilde{\Sigma}(\vec{k})$ as in Eq. (3.7), and comparing first-order terms in magnetic fields, we obtain

$$\begin{aligned}\Sigma^{1,\mu}_{n\rho,n\rho'}(\vec{k}) = &-\sum_{m,\vec{k}'} v_{nm}(\vec{k},\vec{k}')\Sigma^{1,\mu}_{m\rho,m\rho'}(\vec{k}')f'_m(\vec{k}') - \tfrac{1}{2}\mu_0 \sum_{m,\vec{k}'} v_{nm}(\vec{k},\vec{k}')g^{\mu}_{mm}(\vec{k}')\sigma^{\rho}_{m\rho,m\rho'}f'_m(\vec{k}') \\ &-\frac{ie}{2\hbar c}\epsilon_{\alpha\beta\mu} \sum_{\substack{m\,\vec{k},q\rho'' \\ q\neq m}} v_{nm}(\vec{k},\vec{k}')\frac{\Pi^{\alpha}_{m\rho,q\rho''}\Pi^{\beta}_{q\rho'',m\rho'}}{E^2_{qm}}[f_m(\vec{k}')-f_q(\vec{k}')] \; .\end{aligned} \tag{4.10}$$

In order to calculate $\Sigma^{1}_{n\rho,m\rho'}(\vec{k})$, from Eq. (4.6), we assume

$$\langle nm \mid v_{\text{eff}}(\vec{k},\vec{k}') \mid pq \rangle_{\rho\rho'} = \bar{v}_{nm}(\vec{k},\vec{k}')\delta_{np}\delta_{mq} \; . \tag{4.11}$$

From Eqs. (4.6) and (4.11) we have

$$\tilde{\Sigma}_{n\rho,m\rho'}(\vec{k}) = -\frac{1}{\beta}\sum_{\vec{k}',\xi_l} \bar{v}_{nm}(\vec{k},\vec{k}')\tilde{G}_{n\rho,m\rho'}(\vec{k}',\xi_l) \; . \tag{4.12}$$

Substituting the value of $\tilde{G}$ from Eq. (3.17) in Eq. (4.12), summing over ξ_l, and comparing first-order terms in magnetic field, we obtain

$$\Sigma^{1,\mu}_{n\rho,m\rho'}(\vec{k}) = -\sum_{\vec{k}'} \bar{v}_{nm}(\vec{k},\vec{k}')\Sigma^{1,\mu}_{n\rho,m\rho'}\left[\frac{f(E_n)-f(E_m)}{E_{nm}}\right] - \tfrac{1}{2}\mu_0 \sum_{\vec{k}'} \bar{v}_{nm}(\vec{k},\vec{k}')g_{nm}\sigma^{\mu}_{n\rho,m\rho'}\left[\frac{f(E_n)-f(E_m)}{E_{nm}}\right] , \tag{4.13}$$

where we have defined a nondiagonal g matrix g_{nm} as

$$g_{nm}\sigma^{\mu}_{n\rho,m\rho'} = g\sigma^{\mu}_{n\rho,m\rho'} + \frac{ie}{\mu_0\hbar c}\epsilon_{\alpha\beta\mu}\sum_{\substack{q,\rho'' \\ q\neq m}} \frac{\Pi^{\alpha}_{n\rho,q\rho''}\Pi^{\beta}_{q\rho'',m\rho'}}{E_{qm}} \; . \tag{4.14}$$

B. Exchange enhancement of χ_s

Let us see how $\chi^{\mu\mu}_s$ gets exchange enhanced. We can write Eq. (3.46) in the alternate form,

$$\chi^{\mu\mu}_s = \chi^{\mu\mu}_{0,s} + \chi^{\mu\mu}_{1,s} \; , \tag{4.15}$$

where

$$\chi^{\mu\mu}_{0,s} = -\tfrac{1}{4}\mu_0^2 \sum_{n,\vec{k},\rho,\rho'} g^{\mu}_{nn}\sigma^{\mu}_{n\rho,n\rho'}g^{\mu}_{nn}\sigma^{\mu}_{n\rho',n\rho}f'(E_n) \; , \tag{4.16}$$

is the effective Pauli spin susceptibility for noninteracting Bloch electrons,[41] and

$$\chi^{\mu\mu}_{1,s} = -\tfrac{1}{2}\mu_0 \sum_{n,\vec{k},\rho,\rho'} g^{\mu}_{nn}\Sigma^{1,\mu}_{n\rho,n\rho'}\sigma^{\mu}_{n\rho',n\rho}f'(E_n) \; , \tag{4.17}$$

is the contribution due to exchange and correlation. First we consider individual band enhancement and neglect interband interactions in the expression for $\Sigma^{1,\mu}_{n\rho,n\rho'}$ in Eq. (4.10). We also neglect terms proportional to f, make an average exchange enhancement ansatz, and assume $v_{nm} \simeq v_{nn}\delta_{nm}$, which is equivalent to the assumption that $\Sigma^{1,\mu}$ is independent of $\vec{k}$, to obtain

$$\Sigma^{1,\mu}_{n\rho,n\rho'}=\frac{1}{2}\frac{\alpha_n}{1-\alpha_n}\mu_0 g^{\mu}_{nn}\sigma^{\mu}_{n\rho,n\rho'} , \tag{4.18}$$

where

$$\alpha_n=-\sum_{\vec{k}',m} v_{nm}(\vec{k},\vec{k}')f'(E_m(k')) . \tag{4.19}$$

From Eqs. (4.15)–(4.18), we obtain

$$\chi^{\mu\mu}_s=\sum_n \frac{\chi^{\mu\mu}_{0s,n}}{(1-\alpha_n)} , \tag{4.20}$$

where $\chi^{\mu\mu}_{0s,n}$ is the contribution to effective Pauli susceptibility for each band. We note that the intuitive result of Eq. (4.20), which gives rise to the well-known Stoner enhancement,[51] is only valid if one makes drastic assumptions while solving the matrix integral equations for $\Sigma^{1,\mu}_{n\rho,n\rho'}$. However, the neglect of interband terms, i.e., coupling between the $\Sigma^{1,\mu}_{n\rho,n\rho'}$ for different occupied bands might be too drastic for systems such as Be, Cd, etc.

We now consider exchange enhancement in a two-band model. We define

$$\Sigma_m=\Sigma^{1,\mu}_{m\rho,m\rho'} , \tag{4.21a}$$

$$a_m=\tfrac{1}{2}\mu_0 g^{\mu}_{mm}\sigma^{\mu}_{m\rho,m\rho'} , \tag{4.21b}$$

and

$$N_m=-\sum_{\vec{k}'} f'(E_m) . \tag{4.21c}$$

From Eqs. (4.10) and (4.21), we obtain (neglecting f terms)

$$\Sigma_n=v_{nn}N_n\Sigma_n+v_{nm}N_m\Sigma_m+v_{nn}a_nN_n+v_{nm}a_mN_m \tag{4.22}$$

and

$$\Sigma_m=v_{mn}N_n\Sigma_n+v_{mm}N_m\Sigma_m+v_{mn}a_nN_n+v_{mm}a_mN_m . \tag{4.23}$$

Equations (4.22) and (4.23) can be solved self-consistently, and we obtain

$$\Sigma_n=\frac{v_{nn}a_nN_n+v_{nm}a_mN_m-v_{nn}v_{mm}a_nN_nN_m+|v_{nm}|^2a_nN_nN_m}{1-v_{nn}N_n-v_{mm}N_m+(v_{nn}v_{mm}-|v_{nm}|^2)N_nN_m} \tag{4.24}$$

and

$$\Sigma_m=\frac{v_{mn}a_nN_n+v_{mm}a_mN_m-v_{nn}v_{mm}a_mN_nN_m+|v_{nm}|^2a_mN_nN_m}{1-v_{nn}N_n-v_{mm}N_m+(v_{nn}v_{mm}-|v_{nm}|^2)N_nN_m} . \tag{4.25}$$

We can write Eq. (3.46) in the alternate form,

$$\chi^{\mu\mu}_s=a_n^2N_n+a_m^2N_m+a_nN_n\Sigma_n+a_mN_m\Sigma_m . \tag{4.26}$$

From Eqs. (4.24)–(4.26), we obtain

$$\chi^{\mu\mu}_s\simeq\frac{\chi^{\mu\mu}_{0s,n}(1-v_{mm}N_m)+\chi^{\mu\mu}_{0s,m}(1-v_{nn}N_n)+\frac{1}{2}(\chi^{\mu\mu}_{0s,n}N_m+\chi^{\mu\mu}_{0s,m}N_n)(v_{nm}+v_{mn})}{1-v_{nn}N_n-v_{mm}N_m+(v_{nn}v_{mm}-|v_{nm}|^2)N_nN_m} \tag{4.27}$$

where we have assumed

$$a_n^2+a_m^2 \simeq 2a_n a_m \ . \tag{4.28}$$

Thus we see that even in a simple two-band model, the exchange enhancement of χ_s is quite different from the simple form obtained in Eq. (4.20). A realistic calculation of exchange enhancement in metals such as Be, Cd, etc. should at least be done in a two-band model.

C. Exchange and correlation effects on χ_{so}

It is interesting to note that the effect of electron-electron interactions is different on the various terms in χ_{so} of Eq. (3.44). For example, the effect of electron-electron interactions on the first term in χ_{so} comes from the $\Pi\Pi\Pi\Pi$ term, which contains $\nabla_k \Sigma^0$. In order to calculate the exchange and correlation effects on the second term, we have from Eqs. (3.45) and (4.18)

$$J^{\mu}_{n\rho,n\rho'} = A^{\mu}_{nn} \sigma^{\mu}_{n\rho,n\rho'} \ , \tag{4.29}$$

where

$$A^{\mu}_{nn} = 1 + \frac{\alpha_n g^{\mu}_{nn}}{2g(1-\alpha_n)} \ . \tag{4.30}$$

In order to obtain the exchange enhancement in the third—seventh terms in χ_{so}, we note that we can write Eq. (4.13) in alternate form,

$$\Sigma^{1,\mu}_{n\rho,m\rho'}(\vec{k}) = \frac{\mu_0 \alpha_{nm} g^{\mu}_{nm} \sigma^{\mu}_{n\rho,m\rho'}}{2(1-\alpha_{nm})} \ , \tag{4.31}$$

where α_{nm} is an exchange-enhancement parameter defined by

$$\alpha_{nm} = -\sum_{\vec{k}'} \bar{v}_{nm}(\vec{k},\vec{k}') \frac{f(E_n)-f(E_m)}{E_{nm}} \ . \tag{4.32}$$

From Eqs. (3.45) and (4.32), we obtain

$$J^{\mu}_{n\rho,m\rho'} = A^{\mu}_{nm} \sigma^{\mu}_{n\rho,m\rho'} \ , \tag{4.33}$$

where

$$A^{\mu}_{nm} = 1 + \frac{\alpha_{nm} g^{\mu}_{nm}}{2g(1-\alpha_{nm})} \ . \tag{4.34}$$

In order to calculate the exchange enhancement of the last two terms in χ_{so} we have from Eqs. (3.19) and (4.32)

$$F^{\mu}_{n\rho,m\rho'} = B^{\mu}_{nm} \sigma^{\mu}_{n\rho,m\rho'} \ , \tag{4.35}$$

where

$$B^{\mu}_{nm} = 1 + \frac{\alpha_{nm} g^{\mu}_{nm}}{g(1-\alpha_{nm})} \ . \tag{4.36}$$

We can now rewrite Eq. (3.44) with the help of Eqs. (4.29), (4.33), and (4.35) as

$$\chi^{\mu\mu}_{so} = \sum_{\substack{\vec{k},n,m,q,\rho,\rho' \\ n \neq m,q}} \left[\frac{e^2 \epsilon_{\alpha\beta\mu} \epsilon_{\gamma\delta\nu}}{\hbar^2 c^2} \frac{\Pi^{\alpha}_{n\rho,m\rho'} \Pi^{\beta}_{m\rho',n\rho''} \Pi^{\gamma}_{n\rho'',q\rho'''} \Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn} E_{qn}} \right.$$
$$+ \frac{ieg\mu_0}{2\hbar c} \epsilon_{\alpha\beta\mu} \left[-3 \frac{A^{\mu}_{nn} \sigma^{\mu}_{n\rho,n\rho'} \Pi^{\alpha}_{n\rho',m\rho''} \Pi^{\beta}_{m\rho'',n\rho}}{E^2_{mn}} + \frac{A^{\mu}_{qn} \Pi^{\alpha}_{n\rho,m\rho'} \Pi^{\beta}_{m\rho',q\rho''} \sigma^{\mu}_{q\rho'',n\rho}}{E_{qn} E_{mn}} \right.$$
$$+ \frac{A^{\mu}_{mq} \Pi^{\alpha}_{n\rho,m\rho'} \sigma^{\mu}_{m\rho',q\rho''} \Pi^{\beta}_{q\rho'',n\rho}}{E_{qn} E_{mn}} + \frac{A^{\mu}_{nm} \sigma^{\mu}_{n\rho,m\rho'} \Pi^{\alpha}_{m\rho',q\rho''} \Pi^{\beta}_{q\rho'',n\rho}}{E_{qn} E_{mn}}$$
$$\left. + \frac{A^{\mu}_{nm} \Pi^{\alpha}_{n\rho,n\rho} \sigma^{\mu}_{n\rho,m\rho'} \Pi^{\beta}_{m\rho',n\rho}}{E^2_{mn}} - \frac{A^{\mu}_{mn} \Pi^{\alpha}_{n\rho,n\rho} \Pi^{\beta}_{n\rho,m\rho'} \sigma^{\mu}_{m\rho' n\rho}}{E^2_{mn}} \right]$$
$$\left. + \tfrac{1}{4} g^2 \mu_0^2 \left[\frac{B^{\mu}_{mn} \sigma^{\mu}_{n\rho,m\rho'} \sigma^{\beta}_{m\rho',n\rho}}{E_{mn}} + \frac{B^{\mu}_{nm} \sigma^{\mu}_{n\rho,m\rho'} \sigma^{\mu}_{m\rho',n\rho}}{E_{mn}} \right] \right] f(E_n) \ . \tag{4.37}$$

We note that except for the first term, each term in χ_{so} gets exchange enhanced through the exchange enhancement parameters A's and B's defined earlier, but the enhancement factors are different for different terms. From the earlier results,[41] *a priori* one could not say anything about the effects of exchange and correlation. Even in the absence of exchange and correlation effects, the contribution of χ_{so} is of the same order of magnitude as χ_s for some metals[42] and semiconductors[43]; hence the exchange enhancement parameters A's and B's would play an important role for determination of susceptibility of these solids.

D. Many-body effects on χ_o

The effect of electron-electron interaction on χ_o is quite different from that on χ_s and χ_{so}. The first term of χ_o in Eq. (3.42) is the Landau-Peierls susceptibility for quasiparticle (χ_{LP}^{qp}) since the energy in the Landau-Peierls term is the quasiparticle energy. This is the well-known Sampson-Seitz prescription[13] which has been proved by Philippas and McClure.[12] If we include the effects of electron-electron interaction through an effective mass and ignore the band effects, we obtain the well-known result[51] for χ_o in the Fermi-liquid theory

$$\chi_{LP}^{qp}=\frac{\chi_{LP}}{1+A_1/3}\ , \tag{4.38}$$

where A_1 is the Fermi-liquid parameter. Philippas and McClure[12] have shown that if a static Thomas-Fermi potential is used and the band effects are ignored, χ_{LP}^{qp} yields all the recent many-body results[6–8] of χ_o for free electrons. Thus we note that our χ_{LP}^{qp} agrees with all the earlier results of χ_o for both band and free electrons. The second—fifth terms are corrections to the Landau-Peierls term and agree with the results of Misra and Roth[14] except that the electron-electron interaction is included in the Π's through $\nabla_k\Sigma^0$. These terms, which are zero for free electrons, are of the same order as χ_{LP} for band electrons[14] even in the absence of electron-electron interactions. Therefore, while considering many-body effects on χ_o, it is wrong only to consider χ_{LP}^{qp} as has been done in all the earlier calculations.

The sixth—ninth terms are interaction terms between the Π's and the electron-electron effective mass. The tenth and eleventh terms are also explicit many-body correction terms through $\partial\Sigma^{1,\mu}/\partial k^{\alpha}$. However, in our approximation, these terms are small.

It may be noted that since the explicit many-body correction terms to χ_o are small, χ_o can be calculated treating the self-energy as a one-particle nonlocal pseudopotential and ignoring the change with magnetic field of the transformed self-energy. Since the theory of Misra and Roth[14] does just that, if the correct pseudopotential is used, their theory includes both the band-structure and many-body effects. The same conclusion has also been reached by Philippas and McClure.[12]

V. SUMMARY AND CONCLUSION

The principal result of this work is the obtaining of a tractable expression for the total magnetic susceptibility (χ) of interacting electrons in solids. We included the effects of both the lattice potential and electron-electron interaction and constructed in $\vec{k}$ space, using the Bloch representation, the effective one-particle Hamiltonian, and the equation of motion of the Green's function in the presence of a magnetic field. We used a finite-temperature Green's-function formalism where the thermodynamic potential Ω is expressed in terms of the exact one-particle propagator G and derived a general expression for χ by assuming the self-energy to be independent of frequency, an approximation valid in the statically screened exchange approximation. In our theory the effects of exchange and correlations on each of the three components of χ have been explicitly calculated. If we make simple approximations for the self-energy, our expression for orbital susceptibility (χ_o) essentially reduces to the earlier results.[17] If we neglect the coupling between self-energy terms for different occupied bands while solving the matrix integral equations for the field-dependent part of the self-energy, our expression for spin susceptibility (χ_s) is equivalent to the earlier results for the exchange-enhanced χ_s but with the g factor replaced by the effective g factor, a result which has been intuitively used but not yet rigorously derived. However, since these assumptions are too drastic for metals such as Be, Cd, etc., and for semiconductors, we made a careful analysis of exchange and correlation effects in a two-band model and solved the integral equations for self-energy terms taking into account the interband couplings. Our results indicate that the exchange-enhancement effects do not appear in the simple form obtained in the earlier results.

An important aspect of our work is the analysis of exchange and correlation effects on χ_{so}, the contribution to magnetic susceptibility from the effect of spin-orbit coupling on the orbital motion of Bloch electrons. In all the earlier many-body theories of magnetic susceptibility, these effects had been ignored, since attention had been focused either on the orbital part or on the spin part of the Hamiltonian. It has been assumed that the effect of spin-orbit coupling could be accounted for in χ_o through the modifications of the Bloch functions and in χ_s by replacing the free-electron g factor by the effective g factor, thereby neglecting many-body effects on χ_{so}. However, even for noninteracting electrons, χ_{so} is of the same order as χ_s for solids with large g factors.[48,49] Since from these earlier results *a priori* one cannot say anything about the effects of exchange and correlations on χ_{so}, our present work is the first of its kind where these effects have been analyzed using a statically screened exchange approximation.

Our results indicate that the effects of exchange and correlations are different for the various terms in χ_{so}. The leading $\Pi\Pi\Pi\Pi\Pi\Pi$ term in χ_{so} becomes exchange enhanced in a similar way as χ_s. However, this term is proportional to the nondiagonal terms of the effective g factor g_{nm}, which involve the interband matrix elements of $\tilde{\Sigma}^1$ operator. The other terms in χ_{so} are also exchange enhanced, but quite differently from χ_s. In the absence of spin-orbit interaction, the many-body contributions to χ_{so} vanish, as they should.

We have noted that our results agree with the earlier many-body results for χ_o if we make simple approximations and for χ_s if we make drastic assumptions. However, it is not possible to compare χ_{so} since there has been no many-body calculation for χ_{so}. It may also be noted that if we neglect electron-electron interaction, our expression for χ agrees with the results for noninteracting Bloch electrons.[1,2,4]

APPENDIX A

We shall now prove the partial integrations in Eq. (3.30) by generalizing a procedure used earlier by one of us[42] for noninteracting electrons. We have

$$\begin{aligned}\nabla_k^\alpha \Pi^\beta_{n\rho,m\rho'} &= \nabla_k^\alpha \int d\vec{r}\, U^*_{n\vec{k}\rho}(\nabla_k^\beta H_0)U_{m\vec{k}\rho'} \\ &= \int d\vec{r}(\nabla_k^\alpha U^*_{n\vec{k}\rho})(\nabla_k^\beta H_0)U_{m\vec{k}\rho'} + \int d\vec{r}\, U^*_{n\vec{k}\rho}(\nabla_k^\alpha\nabla_k^\beta H_0)U_{m\vec{k}\rho'} + \int d\vec{r}\, U^*_{n\vec{k}\rho}(\nabla_k^\beta H_0)\nabla_k^\alpha U_{m\vec{k}\rho'}\ .\end{aligned} \tag{A1}$$

Since $U_{n\vec{k}\rho}$ are a complete set for periodic functions, we insert the complete set $|U_{q\vec{k}\rho''}\rangle\langle U_{q\vec{k}\rho''}|$ in the first and third terms. Therefore we have

$$\begin{aligned}\nabla_k^\alpha \Pi^\beta_{n\rho,m\rho'} = &\sum_{\substack{q,\rho'' \\ q\neq n}} \int d\vec{r}(\nabla_k^\alpha U^*_{n\vec{k}\rho})U_{q\vec{k}\rho''}\int d\vec{r}\,' U^*_{q\vec{k}\rho''}(\nabla_k^\beta H_0)U_{m\vec{k}\rho'} \\ &+\sum_{\rho''}\int d\vec{r}(\nabla_k^\alpha U^*_{n\vec{k}\rho})U_{n\vec{k}\rho''}\int d\vec{r}\,' U^*_{n\vec{k}\rho''}(\nabla_k^\beta H_0)U_{m\vec{k}\rho'} \\ &+\sum_{\substack{q,\rho'' \\ q\neq m}}\int d\vec{r}\, U^*_{n\vec{k}\rho}(\nabla_k^\beta H_0)U_{q\vec{k}\rho''}\int d\vec{r}\,' U^*_{q\vec{k}\rho''}\nabla_k^\alpha U_{m\vec{k}\rho'} \\ &+\sum_{\rho''}\int d\vec{r}\, U^*_{n\vec{k}\rho}(\nabla_k^\beta H_0)U_{m\vec{k}\rho''}\int d\vec{r}\,' U^*_{m\vec{k}\rho''}\nabla_k^\alpha U_{m\vec{k}\rho'} + \frac{\hbar^2}{m}\delta_{\alpha\beta}\delta_{n\rho,m\rho'} + X^{\alpha\beta}_{n\rho,m\rho'}\ .\end{aligned} \tag{A2}$$

We also have

$$\nabla_k^\alpha \int d\vec{r}\, U^*_{n\vec{k}\rho}H_0 U_{q\vec{k}\rho'} = 0\ , \tag{A3}$$

from which we obtain

$$E_q\int d\vec{r}(\nabla_k^\alpha U^*_{n\vec{k}\rho})U_{q\vec{k}\rho'} + E_n\int d\vec{r}\, U^*_{n\vec{k}\rho}\nabla_k^\alpha U_{q\vec{k}\rho'} + \Pi^\alpha_{n\rho,q\rho'} = 0 \tag{A4}$$

and

$$\nabla_k^\alpha \int d\vec{r}\, U^*_{n\vec{k}\rho} U_{q\vec{k}\rho'} = 0 \;, \tag{A5}$$

from which we obtain

$$\int d\vec{r} (\nabla_k^\alpha U^*_{n\vec{k}\rho}) U_{q\vec{k}\rho'} = -\int d\vec{r}\, U^*_{n\vec{k}\rho} \nabla_k^\alpha U_{q\vec{k}\rho'} \;. \tag{A6}$$

From Eqs. (A4) and (A6) we have for $q \neq n$

$$\int d\vec{r}\, U^*_{n\vec{k}\rho} \nabla_k^\alpha U_{q\vec{k}\rho'} = \frac{\Pi^\alpha_{n\rho,q\rho'}}{E_{qn}} \;. \tag{A7}$$

We define

$$\vec{D}_{n\rho,n\rho'} \equiv \int d\vec{r}\, U^*_{n\vec{k}\rho} \nabla_k U_{n\vec{k}\rho'} \;. \tag{A8}$$

From Eqs. (A2), (A7), and (A8) we obtain

$$\nabla_k^\alpha \Pi^\beta_{n\rho,m\rho'} = \sum_{\substack{q,\rho'' \\ q\neq n}} \frac{\Pi^\alpha_{n\rho,q\rho''}\Pi^\beta_{q\rho'',m\rho'}}{E_{nq}} + \sum_{\substack{q,\rho'' \\ q\neq m}} \frac{\Pi^\beta_{n\rho,q\rho''}\Pi^\alpha_{q\rho'',m\rho'}}{E_{mq}} + \frac{\hbar^2}{m}\delta_{\alpha\beta}\delta_{n\rho,m\rho'} + X^{\alpha\beta}_{n\rho,m\rho'}$$
$$- \sum_{\rho''} (D^\alpha_{n\rho,n\rho''}\Pi^\beta_{n\rho'',m\rho'} - \Pi^\beta_{n\rho,m\rho''}D^\alpha_{m\rho'',m\rho'}) \;. \tag{A9}$$

Similarly we can prove

$$\nabla_k^\alpha F^\beta_{n\rho,n\rho'} = \sum_{\substack{q,\rho'' \\ q\neq n}} \frac{\Pi^\alpha_{n\rho,q\rho''}F^\beta_{q\rho'',m\rho'}}{E_{nq}} + \sum_{\substack{q,\rho'' \\ q\neq m}} \frac{F^\beta_{n\rho,q\rho''}\Pi^\alpha_{q\rho'',m\rho'}}{E_{mq}} + \frac{2}{g\mu_0} Y^{\alpha\beta}_{n\rho,m\rho'} - \sum_{\rho''} (D^\alpha_{n\rho,n\rho''}F^\beta_{n\rho'',m\rho'} - F^\beta_{n\rho,m\rho''}D^\alpha_{m\rho'',m\rho'}) \;. \tag{A10}$$

The partial integrations can be done in the following way. We first differentiate

$$h_{\alpha\beta}h_{\gamma\delta}\nabla_k^\alpha \left[\sum_{\substack{m,\rho',q,\rho'' \\ m,q\neq n}} \frac{\Pi^\beta_{n\rho,m\rho'}\Pi^\gamma_{m\rho',q\rho''}\Pi^\delta_{q\rho'',n\rho}}{E^2_{mn}E_{qn}} \phi_0(E_n) \right] \;. \tag{A11}$$

When we differentiate the $q \neq m$ terms, we obtain the following (where $l=m$ and $l=q$ terms are displayed explicitly):

$$h_{\alpha\beta}h_{\gamma\delta} \Bigg[\Bigg(\frac{\Pi^\alpha_{n\rho,l\rho'''}\Pi^\beta_{l\rho''',m\rho'}}{E_{nl}} + \frac{\Pi^\alpha_{n\rho,m\rho'}\Pi^\beta_{m\rho',m\rho'}}{E_{nm}} + \frac{\Pi^\alpha_{n\rho,q\rho'''}\Pi^\beta_{q\rho''',m\rho'}}{E_{nq}} + \frac{\Pi^\beta_{n\rho,l\rho'''}\Pi^\alpha_{l\rho''',m\rho'}}{E_{ml}} + \frac{\Pi^\beta_{n\rho,n\rho}\Pi^\alpha_{n\rho,m\rho'}}{E_{mn}}$$
$$+ \frac{\Pi^\beta_{n\rho,q\rho'''}\Pi^\alpha_{q\rho''',m\rho'}}{E_{mq}} + X^{\alpha\beta}_{n\rho,m\rho'} - D^\alpha_{n\rho,n\rho'''}\Pi^\beta_{n\rho''',m\rho'} + \Pi^\beta_{n\rho,m\rho'''}D^\alpha_{m\rho''',m\rho'} \Bigg) \frac{\Pi^\gamma_{m\rho',q\rho''}\Pi^\delta_{q\rho'',n\rho}}{E^2_{mn}E_{qn}} \phi_0(E_n)$$
$$+ \frac{\Pi^\beta_{n\rho,m\rho'}}{E^2_{mn}E_{qn}} \Bigg(\frac{\Pi^\alpha_{m\rho',l\rho'''}\Pi^\gamma_{l\rho''',q\rho''}}{E_{ml}} + \frac{\Pi^\alpha_{m\rho',q\rho''}\Pi^\gamma_{q\rho'',q\rho''}}{E_{mq}}$$
$$+ \frac{\Pi^\alpha_{m\rho',n\rho'''}\Pi^\gamma_{n\rho''',q\rho''}}{E_{mn}} + \frac{\Pi^\gamma_{m\rho',l\rho'''}\Pi^\alpha_{l\rho''',q\rho''}}{E_{ql}} + \frac{\Pi^\gamma_{m\rho',m\rho'}\Pi^\alpha_{m\rho',q\rho''}}{E_{qm}}$$
$$+ \frac{\Pi^\gamma_{m\rho',n\rho'''}\Pi^\alpha_{n\rho''',q\rho''}}{E_{qn}} + X^{\alpha\gamma}_{m\rho',q\rho''} - D^\alpha_{m\rho',m\rho'''}\Pi^\gamma_{m\rho''',q\rho''} + \Pi^\gamma_{m\rho',q\rho'''}D^\alpha_{q\rho''',q\rho''} \Bigg) \Pi^\delta_{q\rho'',n\rho}\phi_0(E_n)$$
$$+ \frac{\Pi^\beta_{n\rho,m\rho'}\Pi^\gamma_{m\rho',q\rho''}}{E^2_{mn}E_{qn}} \Bigg(\frac{\Pi^\alpha_{q\rho'',l\rho'''}\Pi^\delta_{l\rho''',n\rho}}{E_{ql}} + \frac{\Pi^\alpha_{q\rho'',n\rho}\Pi^\delta_{n\rho,n\rho}}{E_{qn}}$$

$$+\frac{\Pi^{\alpha}_{q\rho'',m\rho'''}\Pi^{\delta}_{m\rho''',n\rho}}{E_{qm}}+\frac{\Pi^{\delta}_{q\rho'',l\rho'''}\Pi^{\alpha}_{l\rho''',n\rho}}{E_{nl}}+\frac{\Pi^{\delta}_{q\rho'',q\rho''}\Pi^{\alpha}_{q\rho'',n\rho}}{E_{nq}}$$

$$+\frac{\Pi^{\delta}_{q\rho'',m\rho'''}\Pi^{\alpha}_{m\rho''',n\rho}}{E_{nm}}+X^{\alpha\delta}_{q\rho'',n\rho}-D^{\alpha}_{q\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}+\Pi^{\delta}_{q\rho'',n\rho'''}D^{\alpha}_{n\rho''',n\rho}\Bigg]\phi_0(E_n)$$

$$-2\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^3_{nm}E_{qn}}\phi_0(E_n)+2\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^3_{nm}E_{qn}}\phi_0(E_n)$$

$$+\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^2_{mn}E^2_{qn}}\phi_0(E_n)$$

$$-\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^2_{nm}E^2_{qn}}\phi_0(E_n)+\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^2_{mn}E_{qn}}f(E_n)\Bigg]\ . \qquad \text{(A12)}$$

Here the summation is over all the band indices except for $n\neq m\neq q\neq l$. We also differentiate the $q=m$ terms in Eq. (A11) and then add these terms to the terms in Eq. (A12). We simplify the sum by interchanging band indices (except n) wherever necessary and by using the identity (3.26). Then the diagonal terms in the band indices l, q, and m are grouped together with the nondiagonal terms. Finally, the summation over $\vec{k}$ is changed to an integration, the volume integral over $\vec{k}$ space is changed to a surface integral, and since the integrand is periodic in $\vec{k}$, the surface integral vanishes. Thus the term proportional to $f(E_n)$ will be equal and opposite to all the terms proportional to $\phi_0(E_n)$ and we obtain

$$-h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}f(E_n)$$

$$=h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Bigg[2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',l\rho'''}\Pi^{\delta}_{l\rho''',n\rho}}{E^2_{mn}E_{qn}E_{\ln}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^3_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E^2_{qn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^3_{mn}E_{qn}}-\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E^2_{qn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E^2_{qn}}+\frac{\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^3_{mn}}\delta_{\beta\delta}$$

$$+\frac{\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}-\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}X^{\alpha\gamma}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}\Bigg]\phi_0(E_n)\ , \qquad \text{(A13)}$$

where the sums are over $m,\rho',q,\rho'',l,\rho'''$ but $m,q,l\neq n$. Similarly we obtain

$$-h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}f(E_n)$$

$$=h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Bigg[-2\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',l\rho'''}\Pi^{\delta}_{l\rho''',n\rho}}{E^2_{ln}E_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^2_{mn}E^2_{qn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}\Pi^{\gamma}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^3_{qn}E_{mn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E^2_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{mn}E^2_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}$$

$$-\frac{\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^3_{mn}}\delta_{\beta\delta}+\frac{X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}-\frac{\Pi^{\delta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^2_{qn}}\Bigg]\phi_0(E_n)\ , \qquad \text{(A14)}$$

$$-h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^3_{nm}}f(E_n)$$

$$=h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Bigg[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\delta}_{n\rho,q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{qn}E^3_{mn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{qn}E^2_{mn}}-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^3_{mn}E_{qn}}-2\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^4_{mn}}$$

$$-\frac{\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^3_{mn}}\delta_{\beta\delta}+\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\delta}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^3_{nm}}-\frac{\Pi^{\delta}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}X^{\alpha\gamma}_{m\rho',n\rho}}{E^3_{nm}}\Bigg]\phi_0(E_n)\ , \qquad \text{(A15)}$$

$$-h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\delta}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^3_{nm}}f(E_n)$$

$$=h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Bigg[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\delta}_{n\rho,q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}$$

$$+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{mn}E^3_{qn}}+\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E^2_{mn}E^2_{qn}}-2\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\delta}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^4_{mn}}$$

$$-\frac{\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E^3_{mn}}\delta_{\beta\delta}+\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E^3_{nm}}-\frac{\Pi^{\delta}_{n\rho,n\rho}X^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^3_{nm}}\Bigg]\phi_0(E_n)\ , \qquad \text{(A16)}$$

$$-h_{\alpha\beta}\lambda^{\gamma}\sum_{\vec{k}}\frac{\Pi^{\alpha}_{n\rho,m\rho'}F^{\gamma}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,n\rho}}{E^2_{mn}}f(E_n)$$

$$=h_{\alpha\beta}\lambda^{\gamma}\sum_{\vec{k}}\Bigg[-\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',q\rho''}F^{\gamma}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}F^{\gamma}_{m\rho',n\rho}\Pi^{\beta}_{n\rho,n\rho}}{E^3_{mn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho''}F^{\gamma}_{n\rho'',n\rho}}{E^3_{mn}}$$

$$-\frac{\Pi^{\alpha}_{n\rho,m\rho'}F^{\gamma}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{mn}E_{qn}}+\frac{2}{g\mu_0}\frac{\Pi^{\beta}_{n\rho,m\rho'}Y^{\alpha\gamma}_{m\rho',n\rho}}{E^2_{mn}}\Bigg]\phi_0(E_n)\ , \qquad \text{(A17)}$$

and

$$-h_{\alpha\beta}\lambda^{\gamma}\sum_{\vec{k}}\frac{F^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^2_{mn}}f(E_n)$$

$$=h_{\alpha\beta}\lambda^{\gamma}\sum_{\vec{k}}\Bigg[-\frac{\Pi^{\alpha}_{n\rho,q\rho''}F^{\gamma}_{q\rho'',m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E_{qn}E^2_{mn}}+\frac{F^{\gamma}_{n\rho,n\rho'}\Pi^{\alpha}_{n\rho',m\rho''}\Pi^{\beta}_{m\rho'',n\rho}}{E^3_{mn}}-\frac{F^{\gamma}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E^2_{qn}E_{mn}}$$

$$+\frac{F^{\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}\Pi^{\alpha}_{n\rho,n\rho}}{E^3_{mn}}-\frac{2}{g\mu_0}\frac{Y^{\alpha\gamma}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E^2_{mn}}\Bigg]\phi_0(E_n)\ . \tag{A18}$$

Using Eqs. (A13)–(A18) and the identities

$$h_{\alpha\beta}h_{\gamma\delta}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E^3_{mn}E_{qn}}=h_{\alpha\beta}h_{\gamma\delta}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E^3_{qn}}\ , \tag{A19}$$

which is obtained by interchanging m and q and ρ and ρ'' in the summation, and

$$h_{\alpha\beta}h_{\gamma\delta}\sum_{\substack{m,q,\rho',\rho'',\rho'''\\ \rho''\neq\rho}}\left[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\delta}_{n\rho'',q\rho'''}\Pi^{\beta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}\right]=0\ , \tag{A20}$$

we obtain the desired result of Eq. (3.30).

APPENDIX B

We shall now prove Eq. (3.40). We have

$$h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\left[-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{3E_{mn}}+\frac{\hbar^2}{6m}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\delta_{\beta\delta}+\tfrac{1}{6}X^{\beta\delta}_{n\rho,n\rho}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\right]f''(E_n)$$

$$=\tfrac{1}{6}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\left[\frac{\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E_{nm}}+\frac{\Pi^{\delta}_{n\rho,m\rho'}\Pi^{\beta}_{m\rho',n\rho}}{E_{nm}}+\frac{\hbar^2}{m}\delta_{\beta\delta}+X^{\beta\delta}_{n\rho,n\rho}\right]f''(E_n)\ . \tag{B1}$$

Further,

$$\nabla^{\alpha}_{k}E_n=\Pi^{\alpha}_{n\rho,n\rho}\ . \tag{B2}$$

From Eqs. (B2) and (A9), we obtain

$$\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n=\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E_{nm}}+\frac{\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',n\rho}}{E_{nm}}+\frac{\hbar^2}{m}\delta_{\alpha\gamma}+X^{\alpha\gamma}_{n\rho,n\rho}\ . \tag{B3}$$

Equation (B1) can thus be rewritten as

$$h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\left[-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{3E_{mn}}+\frac{\hbar^2}{6m}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\delta_{\beta\delta}+\tfrac{1}{6}X^{\beta\delta}_{n\rho,n\rho}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\right]f''(E_n)$$

$$=\tfrac{1}{6}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}(\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_n)f''(E_n)\ . \tag{B4}$$

The right-hand side of Eq. (B4) can be shown by partial integration to be equal to

$$-\tfrac{1}{6}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}(\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n)(\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_n)f'(E_n)\ . \tag{B5}$$

From Eqs. (B4) and (B5) we write

$$h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}\left[-\frac{\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{3E_{mn}}+\frac{\hbar^2}{6m}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\delta_{\beta\delta}+\tfrac{1}{6}X^{\beta\delta}_{n\rho,n\rho}\Pi^{\alpha}_{n\rho,n\rho}\Pi^{\gamma}_{n\rho,n\rho}\right]f''(E_n)$$

$$=-\tfrac{1}{6}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}(\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n)(\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_n)f'(E_n)\ . \tag{B6}$$

Further, we can write

$$\frac{1}{2}h_{\alpha\beta}h_{\gamma\delta}\left[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\delta}_{n\rho'',q\rho'''}\Pi^{\beta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}\right.$$

$$\left.+\frac{2\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E_{nm}}\delta_{\beta\delta}+\frac{\hbar^4}{2m^2}\delta_{\alpha\gamma}\delta_{\beta\delta}+\frac{\hbar^2}{m}X^{\alpha\gamma}_{n\rho,n\rho}\delta_{\beta\delta}-2\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E_{mn}}+\frac{1}{2}X^{\alpha\gamma}_{n\rho,n\rho}X^{\beta\delta}_{n\rho,n\rho}\right]f'(E_n)$$

$$=\frac{1}{4}h_{\alpha\beta}h_{\gamma\delta}\left[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E_{nm}}+\frac{\Pi^{\gamma}_{n\rho,m\rho'}\Pi^{\alpha}_{m\rho',n\rho}}{E_{nm}}+\frac{\hbar^2}{m}\delta_{\alpha\gamma}+X^{\alpha\gamma}_{n\rho,n\rho}\right]$$

$$\times\left[\frac{\Pi^{\beta}_{n\rho,q\rho''}\Pi^{\delta}_{q\rho'',n\rho}}{E_{nq}}+\frac{\hbar^2}{m}\delta_{\beta\delta}+\frac{\Pi^{\delta}_{n\rho,q\rho''}\Pi^{\beta}_{q\rho'',n\rho}}{E_{nq}}+X^{\beta\delta}_{n\rho,n\rho}\right]f'(E_n)\ . \qquad \text{(B7)}$$

From Eqs. (B3) and (B7) we have

$$\frac{1}{2}h_{\alpha\beta}h_{\gamma\delta}\left[\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\beta}_{n\rho'',q\rho'''}\Pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}+\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho''}\Pi^{\delta}_{n\rho'',q\rho'''}\Pi^{\beta}_{q\rho''',n\rho}}{E_{mn}E_{qn}}+\frac{2\hbar^2}{m}\frac{\Pi^{\alpha}_{n\rho,m\rho'}\Pi^{\gamma}_{m\rho',n\rho}}{E_{nm}}\delta_{\beta\delta}\right.$$

$$\left.+\frac{\hbar^4}{2m^2}\delta_{\alpha\gamma}\delta_{\beta\delta}+\frac{\hbar^2}{m}X^{\alpha\gamma}_{n\rho,n\rho}\delta_{\beta\delta}+\frac{1}{2}X^{\alpha\gamma}_{n\rho,n\rho}X^{\beta\delta}_{n\rho,n\rho}-2\frac{X^{\alpha\gamma}_{n\rho,n\rho}\Pi^{\beta}_{n\rho,m\rho'}\Pi^{\delta}_{m\rho',n\rho}}{E_{mn}}\right]f'(E_n)$$

$$=\frac{1}{4}h_{\alpha\beta}h_{\gamma\delta}\sum_{\vec{k}}(\nabla^{\alpha}_{k}\nabla^{\gamma}_{k}E_n)(\nabla^{\beta}_{k}\nabla^{\delta}_{k}E_n)f'(E_n)\ . \qquad \text{(B8)}$$

From Eqs. (B6), (B8), and (A20), we obtain the desired result in Eq. (3.40).

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