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Theory of electron–phonon interaction effects on the spin susceptibility of conduction electrons

G S Tripathi and C M Misra
Department of Physics, Berhampur University, Berhampur 760007, Orissa, India

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Abstract. A theory of the spin susceptibility of conduction electrons is derived using a temperature Green function formalism in the presence of an electron–phonon interaction. It has been shown that the modifications to the spin susceptibility brought about by considering the magnetic field dependence of the electron self-energy are cancelled by the mass enhancement due to the electron–phonon interaction. However, by considering both the electron–electron and electron–phonon interactions we show that the exchange enhancement parameter (α) due to the electron–electron interaction changes to $\alpha(1+\gamma)^{-1}$ where γ is the electron–phonon mass enhancement parameter. In view of the present controversy concerning the role of the electron–phonon interaction in the magnetism of solids, our work is expected to pave the way for a better quantitative understanding of the effect.

1. Introduction

It is well known that the electron–phonon interaction plays an important role in the study of different solid state properties, the most remarkable of these being the explanation of the low-temperature superconductivity. However, the role of the electron–phonon interaction in the magnetism of solids is not understood completely and consequently has remained controversial (Herring 1966, Joshi and Rajagopal 1968, Enz and Mathias 1979, Fay and Appel 1979, Grimvall 1981, Pickett 1982, Zvrev and Silin 1987, Kim 1976, 1979, 1981, 1982, 1984, Kim and Tanaka 1986, 1988). The idea that the Pauli spin susceptibility is not affected by the electron–phonon interaction was first proposed by Herring (1966), and this was later supported by Grimvall (1981) and Pickett (1982). There have also been some attempts to assess the role of the electron–phonon interaction in itinerant electron magnetism. The findings are, however, not unanimous. For example Enz and Mathias (1979) have proposed that the electron–phonon interaction affects the Stoner factor and is responsible for the ferromagnetism of $ZrZn_2$. On the other hand, Fay and Appel (1979) have proposed that the electron–phonon correction to the Stoner factor is of the order of $(m/M)^{1/2}$, where m and M are the electron and atomic masses, respectively, and hence negligible.

Kim and co-workers have investigated extensively the role of the electron–phonon interaction in itinerant electron magnetism. They found that in the paramagnetic state of transition metals the electron–phonon interaction is the dominant mechanism of the temperature dependence of the magnetic susceptibility (Kim 1981, 1982, 1984). They also showed that in the ferromagnetic state the electron–phonon interaction affects the spontaneous magnetisation by as much as μ_B per atom (Kim and Tanaka 1986). These results were obtained from their earlier work on the magnetisation dependence of the phonon frequency arising from changes in the electronic screening of ion–ion interactions (Kim 1976, 1979).

It is clear from the foregoing discussion that the role of the electron–phonon interaction in the magnetism of solids still remains inconclusive. Different authors have emphasised different aspects of this problem, as outlined in the preceding paragraph. In this paper, therefore, we present a theory of electron–phonon interaction effects on the spin susceptibility of conduction electrons. Our work is distinguished from previous work in the sense that we consider a temperature Green function technique and solve an integral equation for the self-energy of electrons in the presence of electron–phonon interactions and a magnetic field. Spin–orbit interactions are also considered. This is an extension of a procedure adopted to derive first-principles theories of magnetic susceptibility (Misra *et al* 1982, Tripathi 1986, 1987), Knight shift (Tripathi *et al* 1981, 1982, 1987, Tripathi 1985a) and nuclear spin–spin interactions (Tripathi 1985b) in the presence of electron–electron interactions.

Furthermore, since the inertia of the ions is important, the interaction between electrons which is mediated by phonons is not instantaneous but retarded. This makes Green functions a particularly useful vehicle for describing them.

In § 2 we briefly review the general expression for the effective Pauli spin susceptibility in the presence of many-body interactions. Section 3 discusses the solution of the electron self-energy equations in the presence of electron–phonon interactions and a magnetic field. In § 4 we briefly discuss the mass enhancement due to the electron–phonon interaction in the light of our theory. Finally, § 5 concludes the work with a brief summary.

2. Effective spin susceptibility of conduction electrons

The effective Pauli spin susceptibility in the presence of many-body interactions (Misra *et al* 1982) is given by the expression

$$\chi_s = \sum_k (1+\delta_{\mu\nu}) \bigg(\frac{e^2\hbar^2}{8m^4c^2} \varepsilon_{\alpha\beta\mu}\varepsilon_{\gamma\delta\nu} \frac{\pi^{\alpha}_{n\rho,m\rho'}\pi^{\beta}_{m\rho',n\rho''}\pi^{\gamma}_{n\rho'',q\rho'''}\pi^{\delta}_{q\rho''',n\rho}}{E_{mn}E_{qn}} - \tfrac{1}{8}g^2\mu_B^2\sigma^{\mu}_{n\rho,n\rho'}F^{\nu}_{n\rho',n\rho} - \frac{\mathrm{i}eg\hbar\mu_B}{4m^2c}\varepsilon_{\alpha\beta\mu}\frac{J^{\mu}_{n\rho,n\rho'}\pi^{\alpha}_{n\rho',m\rho''}\pi^{\beta}_{m\rho'',n\rho}}{E_{mn}} \bigg) f'(E_{nk}) \tag{2.1}$$

where

$$\boldsymbol{\pi} = (\boldsymbol{p}+\hbar\boldsymbol{k}) + \frac{\hbar}{4mc^2}\boldsymbol{\sigma}\times\nabla V + \frac{m}{\hbar}\nabla_k\Sigma^0(\boldsymbol{k},E) \tag{2.2}$$

$$F^{\nu} = \sigma^{\nu} + (2/g\mu_B)\tilde{\Sigma}^{1,\nu} \tag{2.3}$$

$$J^{\mu} = \sigma^{\mu} + (1/g\mu_B)\tilde{\Sigma}^{1,\mu}. \tag{2.4}$$

The $\tilde{\Sigma}$ are defined through the expression (Misra *et al* 1982)

$$\tilde{\Sigma}(\boldsymbol{k},\boldsymbol{B},E_{nk}) = \Sigma^0(\boldsymbol{k},E_{nk}) + B^{\mu}\tilde{\Sigma}^{1,\mu}(\boldsymbol{k},E_{nk}) + B^{\mu}B^{\nu}\tilde{\Sigma}^{2,\mu\nu}(\boldsymbol{k},E_{nk}) + \ldots \tag{2.5}$$

The other symbols are as follows: $\varepsilon_{\alpha\beta\mu}$ is an antisymmetric tensor of third rank and we follow the Einstein summation convention, $f'(E_{nk})$ is the energy derivative of the Fermi function $f(E_{nk})$; n, m, q are band indices and the ρ are the spin indices (repeated band and spin indices here and elsewhere in the paper imply summation), μ_B is the Bohr magneton; the $\boldsymbol{\sigma}$ are the Pauli spin matrices and $E_{mn} = E_m(\boldsymbol{k}) - E_n(\boldsymbol{k})$; $\boldsymbol{F}$ and $\boldsymbol{J}$ are the renormalised spin vertices in the presence of many-body effects. The matrix elements occurring in equation (2.1) are taken between the periodic parts of the Bloch functions for different bands.

In the absence of many-body effects, $\chi_s^{\mu\nu}$ reduces to the expression given by Misra and Kleinman (1972), and if the spin–orbit interaction is neglected it would reduce to the Pauli paramagnetic susceptibility of the conduction electrons in a solid.

Using equations (2.3) and (2.4), equation (2.1) can be split into two parts:

$$\chi_s^{\mu\nu} = \sum_k (1+\delta_{\mu\nu})\left(\frac{e^2\hbar^2}{8m^4c^2}\varepsilon_{\alpha\beta\mu}\varepsilon_{\gamma\delta\nu}\frac{\pi^\alpha_{n\rho,m\rho'}\pi^\beta_{m\rho',n\rho''}\pi^\gamma_{n\rho'',q\rho'''}\pi^\delta_{q\rho''',n\rho}}{E_{mn}E_{qn}}\right.$$
$$\left. - \tfrac{1}{8}g^2\mu_B^2\sigma^\mu_{n\rho,n\rho'}\sigma^\nu_{n\rho',n\rho} - \frac{ieg\hbar\mu_B}{4m^2c}\varepsilon_{\alpha\beta\mu}\frac{\sigma^\mu_{n\rho,n\rho'}\pi^\alpha_{n\rho',m\rho''}\pi^\beta_{m\rho'',n\rho}}{E_{mn}}\right)$$
$$\times f'(E_{nk}) + \sum_k (1+\delta_{\mu\nu})\left(-\tfrac{1}{4}g\mu_B\sigma^\mu_{n\rho,n\rho'}\tilde{\Sigma}^{1,\mu}_{n\rho',n\rho}\right.$$
$$\left. - \frac{ie\hbar}{4m^2c}\varepsilon_{\alpha\beta\mu}\frac{\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}\pi^\alpha_{n\rho',m\rho''}\pi^\beta_{m\rho'',n\rho}}{E_{mn}}\right) f'(E_{nk}). \tag{2.6}$$

Equation (2.6) can further be rewritten as

$$\chi_s^{\mu\nu} = \chi_{s,1}^{\mu\nu} + \chi_{s,2}^{\mu\nu} \tag{2.7}$$

where

$$\chi_{s,1}^{\mu\nu} = -\tfrac{1}{8}(1+\delta_{\mu\nu})\mu_B^2\sum_k g^\mu_{nn}\sigma^\mu_{n\rho,n\rho'}g^\nu_{nn}\sigma^\nu_{n\rho',n\rho}f'(E_{nk}) \tag{2.8}$$

and

$$\chi_{s,2}^{\mu\nu} = -\tfrac{1}{4}(1+\delta_{\mu\nu})\mu_B\sum_k \tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}g^\nu_{nn}\,\sigma^\nu_{n\rho',n\rho}f'(E_{nk}). \tag{2.9}$$

Here the effective g factor is defined through the expression (Tripathi *et al* 1981, 1982, Misra *et al* 1981)

$$g^\mu_{nn}(\boldsymbol{k})\sigma^\mu_{n\rho,n\rho'}(\boldsymbol{k}) = g\sigma^\mu_{n\rho,n\rho'}(\boldsymbol{k}) + \frac{2i}{m}\varepsilon_{\alpha\beta\mu}\frac{\pi^\alpha_{n\rho,m\rho''}(\boldsymbol{k})\pi^\beta_{m\rho'',n\rho'}(\boldsymbol{k})}{E_{mn}(\boldsymbol{k})}. \tag{2.10}$$

In equation (2.7) we have separated the many-body contribution to the spin susceptibility and lumped it in $\chi_{s,2}^{\mu\nu}$. However, equation (2.9) is not in a form in which computations can be performed. This is because of the presence of the electron self-energy term. In order to express equation (2.7) in a physically meaningful form, we have to solve the integral equation for $\tilde{\Sigma}^{1,\mu}$. This has been done previously (Tripathi *et al* 1982, Misra *et al* 1982) in the case of exchange interactions between electrons. In the following section we solve an integral equation for $\tilde{\Sigma}^{1,\mu}$ in the presence of the electron–phonon interaction.

3. Self-energy equations

The problem of treating the retarded nature of the phonon interaction is a non-trivial one. However, the reason that one can give an essentially exact treatment of the problem

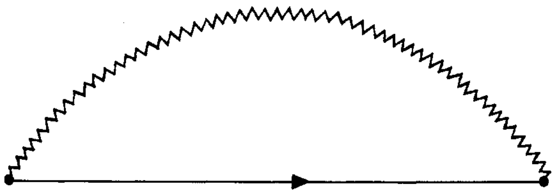

Figure 1. Lowest-order contribution to the self-energy $\Sigma(\boldsymbol{k}, \zeta_l)$. The full line represents the electron Green function $G(\boldsymbol{k}', \zeta_{l'})$. The wavy curve represents the phonon propagator $D(\boldsymbol{k}-\boldsymbol{k}', \zeta_l-\zeta_{l'})$ and the full circles stand for the coupling constant M.

follows from an important discovery by Migdal (1958) in his treatment of the coupled electron–phonon system in normal metals. In non-metals the electron and lattice motions are separated by using the Born–Oppenheimer approximation. Because of the smallness of m/M, where m and M are the electronic and ionic masses, respectively, the electrons move much faster than the ions. The electrons therefore move in a potential depending on the instantaneous positions of the ions while the ions are affected by an average potential due to the electrons. Mathematically, the approximation results in an expansion $(m/M)^{1/2}$ and is valid because of the smallness of $\omega/\Delta E$ where ω is a phonon energy and ΔE the energy difference between the electron states the phonon can connect. In metals, however, the ratio of energies is no longer small because electrons can make transitions near the Fermi surface with ΔE tending to zero. However, Migdal (1958) has shown that one can calculate the one-electron self-energy to an accuracy of order $(m/M)^{1/2} \sim 10^{-2}$ by what amounts to second-order self-consistent perturbation theory. This remarkable result does not depend on the strength of the electron–phonon coupling but rather depends on the existence of a small parameter $(m/M)^{1/2}$ in the problem.

From Migdal's theorem it suffices to consider the lowest-order diagram shown in figure 1 when calculating the self-energy $\Sigma(\boldsymbol{k}, \zeta_l)$. Here the phonon propagator appears only once. Then we can write (Schrieffer 1964)

$$\Sigma(\boldsymbol{k}, \zeta_l) = -\frac{1}{\beta}\sum_{\boldsymbol{k}',\zeta_{l'}} |M_{\boldsymbol{kk}'}|^2 D(\boldsymbol{k}-\boldsymbol{k}', \zeta_l-\zeta_{l'}) G(\boldsymbol{k}', \zeta_{l'}) \tag{3.1}$$

where $M_{\boldsymbol{kk}'}$ is the electron–phonon coupling function, D is the phonon propagator, G is the exact one-electron propagator and

$$\zeta_l = \frac{(2l+1)\mathrm{i}\pi}{\beta} + \mu \qquad l = 0, \pm 1, \pm 2, \ldots \tag{3.2}$$

in which μ is the chemical potential and $\beta = (k_\mathrm{B}T)^{-1}$. In the presence of a magnetic field both the electronic propagator and the self-energy are field dependent. Ignoring the field dependence of the phonon propagator, we have

$$\tilde{\Sigma}(\boldsymbol{k}, \zeta_l, \boldsymbol{B}) = -\frac{1}{\beta}\sum_{\boldsymbol{k}',\zeta_{l'}} |M_{\boldsymbol{kk}'}|^2 D(\boldsymbol{k}-\boldsymbol{k}', \zeta_l-\zeta_{l'}) \tilde{G}(\boldsymbol{k}', \boldsymbol{B}, \zeta_{l'}) \tag{3.3}$$

where $\tilde{G}(\boldsymbol{k}', \boldsymbol{B}, \zeta_{l'})$ is defined (Misra *et al* 1982) as

$$\tilde{G}(\boldsymbol{k}', \boldsymbol{B}, \zeta_{l'}) = G_0(\boldsymbol{k}', \zeta_{l'}) - \mathrm{i}(\hbar^2/m^2) h_{\alpha\beta} G_0(\boldsymbol{k}', \zeta_{l'}) \pi^\alpha G_0(\boldsymbol{k}', \zeta_{l'}) \pi^\beta G_0(\boldsymbol{k}', \zeta_{l'}) + \tfrac{1}{2} g\mu_\mathrm{B} B^\mu G_0(\boldsymbol{k}', \zeta_{l'}) F^\mu G_0(\boldsymbol{k}', \zeta_{l'}) + \text{higher-order terms in } B. \tag{3.4}$$

Here

$$h_{\alpha\beta} = \varepsilon_{\alpha\beta\mu} h^{\mu} \qquad h^{\mu} = eB^{\mu}/2\hbar c \tag{3.5}$$

and G_0 is the electron propagator in the absence of the magnetic field, and is diagonal in the periodic part of the Bloch function. Using equations (2.5) and (3.4) in equation (3.3), and comparing the coefficients of B^{μ}, we have

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}(\boldsymbol{k}, \zeta_l) = &-\frac{1}{\beta}\sum_{\boldsymbol{k}',\zeta_{l'}} |M_{\boldsymbol{k}\boldsymbol{k}'}|^2 D(\boldsymbol{k}-\boldsymbol{k}', \zeta_l - \zeta_{l'}) \\ &\times \Big(-\frac{\mathrm{i}e\hbar}{2m^2c} \varepsilon_{\alpha\beta\mu} G_0(\boldsymbol{k}', \zeta_{l'})\pi^{\alpha} G_0(\boldsymbol{k}', \zeta_{l'})\pi^{\beta} G_0(\boldsymbol{k}', \zeta_{l'}) \\ &+ \tfrac{1}{2} g\mu_{\mathrm{B}} G_0(\boldsymbol{k}', \zeta_{l'})\sigma^{\mu} G_0(\boldsymbol{k}', \zeta_{l'}) \\ &+ G_0(\boldsymbol{k}', \zeta_{l'})\tilde{\Sigma}^{1,\mu}(\boldsymbol{k}', \zeta_{l'}) G_0(\boldsymbol{k}', \zeta_{l'})\Big).\end{aligned} \tag{3.6}$$

Equation (3.6) can be written with the introduction of the band and spin indices as

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}, E_{n\boldsymbol{k}}) = &-\frac{1}{\beta}\sum_{\boldsymbol{k}',\zeta_{l'}} |M_{n\boldsymbol{k},n\boldsymbol{k}'}|^2 D(\boldsymbol{k}-\boldsymbol{k}', E_{n\boldsymbol{k}} - \zeta_{l'}) \\ &\times \Big(-\frac{\mathrm{i}e\hbar}{2m^2c} \varepsilon_{\alpha\beta\mu} G_0\pi^{\alpha} G_0\pi^{\beta} G_0 + \tfrac{1}{2} g\mu_{\mathrm{B}} G_0\sigma^{\mu} G_0 + G_0\tilde{\Sigma}^{1,\mu} G_0\Big)_{n\boldsymbol{k}'\rho,\, n\boldsymbol{k}'\rho'}.\end{aligned} \tag{3.7}$$

Using the completeness properties of the $u_{n\boldsymbol{k}\rho}$ and replacing the phonon propagator D by the bare phonon propagator D_0, where

$$D_0 = 2\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'}/[(E_{n\boldsymbol{k}} - \zeta_{l'})^2 - (\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'})^2], \tag{3.8}$$

we can write

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}, E_{n\boldsymbol{k}}) = &-\frac{1}{\beta}\sum_{\boldsymbol{k}',\zeta_{l'}} |M_{n\boldsymbol{k},n\boldsymbol{k}'}|^2 \frac{2\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'}}{(E_{n\boldsymbol{k}} - \zeta_{l'})^2 - (\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'})^2} \\ &\times \Big(-\frac{\mathrm{i}e\hbar}{2m^2c} \varepsilon_{\alpha\beta\mu} \frac{\pi^{\alpha}_{n\rho,m\rho''}(\boldsymbol{k}')\,\pi^{\beta}_{m\rho'',n\rho'}(\boldsymbol{k}')}{(\zeta_{l'} - E_{n\boldsymbol{k}'})^2\,(\zeta_{l'} - E_{m\boldsymbol{k}'})} \\ &+ \tfrac{1}{2} g\mu_{\mathrm{B}}(\sigma^{\mu}_{n\rho,n\rho'}(\boldsymbol{k}') + \tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}'))\frac{1}{(\zeta_{l'} - E_{n\boldsymbol{k}'})^2}\Big)\end{aligned} \tag{3.9}$$

where, as before, repeated band and spin indices imply summation. The frequency summations on the left can be carried out by using Luttinger–Ward (1960) identity

$$\frac{1}{\beta}\sum_{\zeta_{l'}} \frac{1}{(\zeta_{l'} - E_n)^m} = -\frac{1}{2\pi\mathrm{i}}\oint_{\Gamma} \frac{1}{(\zeta' - E_n)^m} f(\zeta')\,\mathrm{d}\zeta' \tag{3.10}$$

where the contour Γ encircles the imaginary axis in an anticlockwise direction. Substituting equation (3.10) in equation (3.9) and neglecting the terms proportional to f, which are not expected to be important for the intraband matrix element, we obtain

$$\begin{aligned}\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}, E_n) \simeq &-\sum_{\boldsymbol{k}'} \frac{|M_{n\boldsymbol{k},n\boldsymbol{k}'}|^2\, 2\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'}}{(E_{n\boldsymbol{k}} - E_{n\boldsymbol{k}'})^2 - (\hbar\omega_{\boldsymbol{k}-\boldsymbol{k}'})^2} \\ &\times (\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}') + \tfrac{1}{2}\mu_{\mathrm{B}} g^{\mu}_{nn}(\boldsymbol{k}')\sigma^{\mu}_{n\rho,n\rho'}(\boldsymbol{k}'))f'(E_{n\boldsymbol{k}'}).\end{aligned} \tag{3.11}$$

Following an average interaction ansatz in which the self-energy is independent of $\boldsymbol{k}$, we obtain

$$\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}, E_n) \simeq (\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'}(\boldsymbol{k}, E_n) + \tfrac{1}{2}\mu_B g^{\mu}_{nn}(\boldsymbol{k}))\beta_n(\boldsymbol{k}) \tag{3.12}$$

where

$$\beta_n(\boldsymbol{k}) = -\sum_{k'} \frac{2\hbar\omega_{k-k'}|M_{nk,nk'}|^2}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2} f'(E_{nk'}). \tag{3.13}$$

The apparent singularity in equation (3.13) is due to the fact that, in evaluating frequency summations, we have considered only the real part of the energy. The imaginary part is proportional to the lifetime, which is not of interest here. From equation (3.12) we have

$$\tilde{\Sigma}^{1,\mu}_{n\rho,n\rho'} = \tfrac{1}{2}\mu_B \frac{\beta_n(\boldsymbol{k})}{1 - \beta_n(\boldsymbol{k})} g^{\mu}_{nn}(\boldsymbol{k})\sigma^{\mu}_{n\rho,n\rho'} g^{\nu}_{nn}(\boldsymbol{k})\sigma^{\nu}_{n\rho',n\rho} f'(E_{nk}). \tag{3.14}$$

Substituting equation (3.14) in equation (2.9) we have

$$\chi^{\mu\nu}_{s,2} = -\tfrac{1}{8}(1 + \delta_{\mu\nu})\mu_B^2 \sum_k \frac{\beta_n(\boldsymbol{k})}{1 - \beta_n(\boldsymbol{k})} g^{\mu}_{nn}(\boldsymbol{k})\sigma^{\mu}_{n\rho,n\rho'} g^{\nu}_{nn}(\boldsymbol{k})\sigma^{\nu}_{n\rho',n\rho} f'(E_{nk}). \tag{3.15}$$

Now, from equations (2.7), (2.8) and (3.15) we obtain

$$\chi^{\mu\nu}_{s} = -\tfrac{1}{8}(1 + \delta_{\mu\nu})\mu_B^2 \sum_k \frac{1}{1 - \beta_n(\boldsymbol{k})} g^{\mu}_{nn}(\boldsymbol{k})\sigma^{\mu}_{n\rho,n\rho'} g^{\nu}_{nn}(\boldsymbol{k})\sigma^{\nu}_{n\rho',n\rho} f'(E_{nk}). \tag{3.16}$$

Since only the diagonal components are of interest, we have

$$\chi^{\mu\mu}_{s} = -\tfrac{1}{4}\mu_B^2 \sum_k \frac{1}{1 - \beta_n(\boldsymbol{k})} g^{\mu}_{nn}(\boldsymbol{k})\sigma^{\mu}_{n\rho,n\rho'} g^{\mu}_{nn}(\boldsymbol{k})\sigma^{\mu}_{n\rho',n\rho} f'(E_{nk}). \tag{3.17}$$

Thus, by considering the magnetic field dependence of the self-energy, we have seen that $\chi^{\mu\mu}_s$ is modified by a factor $(1 - \beta_n(\boldsymbol{k}))^{-1}$. In order to see how the modification affects the susceptibility, let us write equation (3.13) in the form

$$\beta_n(\boldsymbol{k}) = -\sum_{k'} v_{nn}(\boldsymbol{k}, \boldsymbol{k}') f'(E_{nk'}) \tag{3.18}$$

where $v_{nn}(\boldsymbol{k}, \boldsymbol{k}')$ is the effective interaction between electrons mediated by phonons and is

$$v_{nn}(\boldsymbol{k}, \boldsymbol{k}') = \frac{2\hbar\omega_{k-k'}|M_{nk,nk'}|^2}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2}. \tag{3.19}$$

Unlike the case of exchange interactions between electrons, which are positive, $v_{nn}(\boldsymbol{k}, \boldsymbol{k}')$ can be either positive or negative depending on whether $E_{nk} - E_{nk'}$ is greater or less than $\hbar\omega_{k-k'}$.

4. Mass renormalisation

The electron–phonon mass enhancement has different effects on different properties (Grimvall 1981). Thus far, we have only partially considered its effects on the spin susceptibility. Let the renormalised energy, in the presence of the electron–phonon interaction, be E^{R} and

$$E_{nk}^{\mathrm{R}} = E_{nk} + \Sigma^0(\boldsymbol{k}, E_{nk}) \tag{4.1}$$

where

$$\Sigma^0(\boldsymbol{k}, E_{nk}) = -\frac{1}{\beta}\sum_{k',\zeta_{l'}} \frac{|M_{nk,nk'}|^2\, 2\hbar\omega_{k-k'}}{(\zeta_{l'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2}\, G_0(\boldsymbol{k}', \zeta_{l'}). \tag{4.2}$$

Performing the frequency summation as per the Luttinger–Ward prescription (equation (3.10)), we obtain

$$E_{nk}^{\mathrm{R}} = E_{nk} - \sum_{k'} \frac{|M_{nk,nk'}|^2\, 2\hbar\omega_{k-k'} f(E_{nk'})}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2}. \tag{4.3}$$

Since the electron states near the Fermi surface are of interest, we can write

$$\begin{aligned} \nabla_k E_{nk}^{\mathrm{R}} &\simeq \nabla_k E_{nk} - \sum_{k'} \frac{|M_{nk,nk'}|^2\, 2\hbar\omega_{k-k'} \nabla_{k'} f(E_{nk'})}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2} \\ &= \nabla_k E_{nk} - \sum_{k'} \frac{|M_{nk,nk'}|^2\, 2\hbar\omega_{k-k'} \nabla_{k'} E_{nk'}}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2} f'(E_{nk'}). \end{aligned} \tag{4.4}$$

Replacing $\nabla_{k'} E_{nk'}^{\mathrm{R}}$ by $\nabla_k E_{nk}$, we obtain

$$\nabla_k E_{nk}^{\mathrm{R}} = \nabla_k E_{nk}(1 - \gamma(\boldsymbol{k})) \tag{4.5}$$

where

$$\gamma(\boldsymbol{k}) = \sum_{k'} \frac{|M_{nk,nk'}|^2\, 2\hbar\omega_{k-k'}}{(E_{nk'} - E_{nk})^2 - (\hbar\omega_{k-k'})^2} f'(E_{nk'}) = -\beta(\boldsymbol{k}). \tag{4.6}$$

Since the density of states is proportional to $|\nabla_k E|^{-1}$, we have to first order in $\gamma(\boldsymbol{k})$

$$N^{\mathrm{R}}(E_{nk}) = N(E_{nk})(1 + \gamma(\boldsymbol{k})) \tag{4.7}$$

where N^{R} is the renormalised density of states and N is the density of states in the absence of the electron–phonon interaction. The increase in the density of states implies a change in the effective mass by the same factor:

$$m_{\text{el-ph}} = m(1 + \gamma(\boldsymbol{k})) \tag{4.8}$$

where $m_{\text{el-ph}}$ is the renormalised mass due to the electron–phonon interaction. Now we shall further simplify $\gamma(\boldsymbol{k})$. Since the electron–phonon interaction is short ranged we can consider $|M_{nk,nk'}|^2$ as a constant, $|M|^2$. Again, since in the low-temperature limit $\hbar\omega_{k-k'}$ is greater than $E_{nk} - E_{nk'}$, we replace the phonon frequency by an average frequency, say the Debye frequency ω_{D}. In this limit, the value of $\gamma(\boldsymbol{k})$ averaged over the Fermi surface is given by

$$\bar{\gamma} = |M|^2\, N(\varepsilon_{\mathrm{F}})/\hbar\omega_{\mathrm{D}} \tag{4.9}$$

which is a positive quantity. Thus $\bar{\gamma}$ is the mass enhancement factor.

In order to see the effect of the mass renormalisation on χ_s let us write equation (3.17) as

$$\chi_s^{\mu\mu} = -\tfrac{1}{4}\mu_B^2 \sum_k \frac{1}{1-\beta_n(k)} g_{nn}^{\mu}(k)\sigma_{n\rho,n\rho'}^{\mu} g_{nn}^{\mu}(k)\sigma_{n\rho',n\rho}^{\mu} \nabla_k f(E_{nk}^{R})(\nabla_k E_{nk}^{R})^{-1}. \tag{4.10}$$

Using equations (4.5) and (4.6) in equation (4.10), and assuming $\nabla_k f(E_{nk}^{R}) \simeq \nabla_k f(E_{nk})$, we obtain

$$\chi_s^{\mu\mu} = -\tfrac{1}{4}\mu_B^2 \sum_k g_{nn}^{\mu}(k)\sigma_{n\rho,n\rho'}^{\mu}(k) g_{nn}^{\mu}(k)\, \sigma_{n\rho',n\rho}^{\mu} f'(E_{nk}). \tag{4.11}$$

This is a remarkable result in the sense that the modifications caused in χ_s due to the magnetic field dependence of the electron self-energy are cancelled by the mass enhancement. In other words, there is apparently no explicit effect of the electron–phonon interaction on the spin susceptibility, except through the modifications of the one-electron eigenvalues and eigenfunctions. However, as we shall now see, the picture would be different if we consider the combined effects of both the electron–electron and electron–phonon interactions. $\chi_s^{\mu\mu}$, in the presence of the electron–electron interaction only, is given (Misra *et al* 1982) by

$$\chi_s^{\mu\mu} = -\tfrac{1}{4}\mu_B^2 \sum_k \frac{1}{1-\alpha_n(k)} g_{nn}^{\mu}(k)\sigma_{n\rho,n\rho'}^{\mu} g_{nn}^{\mu}(k)\sigma_{n\rho',n\rho}^{\mu} f'(E_{nk}) \tag{4.12}$$

where $\alpha_n(k)$ is the exchange-enhanced function

$$\alpha_n(k) = -\sum_{k'} \bar{v}_{nn}(k, k') f'(E_{nk'}) \tag{4.13}$$

where $\bar{v}$ is the strength of an average exchange interaction. It is now easy to see that by considering both the electron–electron and the electron–phonon interactions in the self-energy equations, we would finally obtain

$$\chi_s^{\mu\mu} = -\tfrac{1}{4}\mu_B^2 \sum_k \frac{1}{1+\gamma(k)-\alpha_n(k)} g_{nn}^{\mu}(k)\sigma_{n\rho,n\rho'}^{\mu} g_{nn}^{\mu}(k)\sigma_{n\rho',n\rho}^{\mu} f'(E_{nk}). \tag{4.14}$$

Replacing E_{nk} by E_{nk}^{R}, and following the procedure used to obtain equation (4.11), we obtain

$$\chi_s^{\mu\mu} = \frac{\chi_s^{\mu\mu}(0)}{1-[\bar{\alpha}/(1+\bar{\gamma})]} \tag{4.15}$$

where $\chi_s^{\mu\mu}(0)$ is the susceptibility in the absence of the electron–electron and electron–phonon interactions, and the overbars above α and γ denote average values.

Thus we have seen that the Stoner factor $(1-\bar{\alpha})^{-1}$ becomes $\{1-[\bar{\alpha}/(1+\bar{\gamma})]\}^{-1}$ in the presence of the electron–phonon interaction. The apparent modification of $\chi_s^{\mu\mu}$ in equation (4.15) as distinguished from equation (4.11) arises from the fact that, while both the electron–electron and electron–phonon interactions modify the susceptibility through the factors $(1-\bar{\alpha})^{-1}$ and $(1+\bar{\gamma})^{-1}$, the mass enhancements are different. While the mass enhancement due to the electron–phonon interaction is appreciable and is taken into account, the same effect due to the electron–electron interaction is negligible and is ignored. Since $\bar{\gamma}$ is a positive quantity, it reduces the exchange-enhancement parameter. Furthermore $\bar{\gamma}$ varies from a value of about 0.23 in the case of beryllium to a value of 1.12 in the case of lead (McMillan 1968). Thus the modification brought about by the electron–phonon interaction in the exchange-enhancement parameter appears to be significant. However, the extent to which the spin susceptibility is modified depends on both $\bar{\alpha}$ and $\bar{\gamma}$. Let us now estimate the effect in a free-electron-like system, sodium. The mass enhancement parameter $\bar{\gamma}$ in sodium is about 0.26 and $\bar{\alpha}$ is about 0.4 (Kittel 1976). With these data it is easy to see that the exchange-enhancement parameter is affected by about 13%. In general, $\bar{\gamma}$ varies by about 20–40% in simple metals. Thus $\bar{\alpha}$ would be correspondingly reduced by about 20–30% in these systems.

Thus far, we have confined our discussion to low temperatures. However, it is important to consider how $\gamma_n(\boldsymbol{k})$ varies with temperature. Let us assume that the electron–phonon matrix elements and the phonon frequency are constants. Dropping the band index, equation (4.6) can be written as

$$\gamma(\boldsymbol{k}) = 2\hbar\omega_D|M|^2 \sum_{k'} \frac{f'_T(E_{k'} - \mu)}{(E_{k'} - E_k)^2 - (\hbar\omega_D)^2}. \tag{4.16}$$

Replacing the summation over $\boldsymbol{k}'$ by an integration over energy, we have

$$\gamma(\boldsymbol{k}) = 2\hbar\omega_D|M|^2 \int_0^\infty \frac{N(E_{k'})}{(E_{k'} - E_k)^2 - (\hbar\omega_D)^2} f'_T(E_{k'} - \mu)\, dE_{k'}. \tag{4.17}$$

Integrating by parts, we have

$$\gamma(\boldsymbol{k}) = 2\hbar\omega_D|M|^2 \left[\frac{N(E_{k'})}{(E_{k'} - E_k)^2 - (\hbar\omega_D)^2} f_T(E_{k'} - \mu)\bigg|_0^\infty - \int \frac{d}{dE_{k'}}\left(\frac{N(E_{k'})}{(E_{k'} - E_k)^2 - (\hbar\omega_D)^2}\right) f_T(E_{k'} - \mu)\, dE_{k'}\right]. \tag{4.18}$$

We note that the first term vanishes and we have

$$\gamma(\boldsymbol{k}) = -2\hbar\omega_D|M|^2 \int \Phi(E_{k'}, E_k, \hbar\omega_D) f_T(E_{k'} - \mu)\, dE_{k'} \tag{4.19}$$

where

$$\Phi(E_{k'}, E_k, \hbar\omega_D) = \frac{d}{dE_{k'}}\left(\frac{N(E_{k'})}{(E_{k'} - E_k)^2 - (\hbar\omega_D)^2}\right). \tag{4.20}$$

Using the relation (Ziman 1973)

$$\int dE\,\Phi(E) f_T(E - \mu) = \int \Phi(E)\, dE + \tfrac{1}{6}\pi^2 (k_B T)^2 \frac{d\Phi(E)}{dE}\bigg|_{E=\mu} \tag{4.21}$$

and assuming $N(E_{k'})$ to be equal to $N(\mu)$, we obtain

$$\gamma(\boldsymbol{k}) \simeq -|M|^2\hbar\omega_D N(\mu) \left[\frac{1}{(E_k - \mu)^2 - (\hbar\omega_D)^2} - \tfrac{1}{3}\pi^2 (k_B T)^2 \times \frac{1}{[(E_k - \mu)^2 - (\hbar\omega_D)^2]^2}\left(1 - \frac{4(E_k - \mu)^2}{(E_k - \mu)^2 - (\hbar\omega_D)^2}\right)\right]. \tag{4.22}$$

At low temperatures the second term in the square bracket is neglected and $\hbar\omega_D \gg (E_k - \mu)$. In this limit $\gamma(\boldsymbol{k})$ becomes $\gamma(0)$:

$$\gamma(0) = |M|^2 N(\mu_0)/\hbar\omega_D \tag{4.23}$$

where μ_0 is the Fermi energy.

In the high-temperature limit, $(E_k - \mu) \gg k_B T$ and consequently $(E_k - \mu) \gg \hbar\omega_D$. In this limit

$$|\gamma(\boldsymbol{k})| \simeq \frac{|M|^2 N(\mu)}{\hbar\omega_D}\left(\frac{\hbar\omega_D}{E_k - \mu}\right)^2\left[1 + \pi^2\left(\frac{k_B T}{E_k - \mu}\right)^2\right]. \tag{4.24}$$

The second term in the square bracket is small and can be neglected, and since μ does not differ significantly from μ_0 we have

$$|\gamma(\boldsymbol{k})| = \gamma(0)\left(\frac{\hbar\omega_D}{E_k - \mu_0}\right)^2, \tag{4.25}$$

which is a very small quantity. At room temperature $T \sim \theta_D$ and $\mu_0 \sim 10^2 k_B T$. Thus the mass enhancement at room temperature is of the order of $10^{-4}\gamma(0)$. Thus there is no mass enhancement when the temperature is of the order of the Debye temperature and beyond. It may be noted that the temperature dependence of the mass enhancement has also been considered previously (Grimvall 1968, 1981, Eliashberg 1963).

5. Summary and conclusion

In this paper we have analysed carefully the effect of the electron–phonon interaction on the spin susceptibility of conduction electrons. The method is distinguished from earlier works in the sense that we have used a temperature Green formalism and solved an integral equation for the electron self-energy in the presence of a magnetic field and the electron–phonon interaction. The modifications caused due to the magnetic field dependence of the electron self-energy are cancelled by the mass enhancement due to the electron–phonon interaction. In this aspect, our findings are in agreement with the results obtained by Grimvall (1981) and Pickett (1982). However, by considering both the electron–electron and electron–phonon interactions, we have shown that the Stoner factor is affected by the electron–phonon interactions. Thus whether or not the effect is important depends on both the strengths of the exchange interaction among conduction electrons and the effective electron–electron interaction mediated by the phonon. We have also considered the temperature dependence of the mass enhancement due to the electron–phonon interaction.

In conclusion, we would like to state that the theory can be applied to metals, intermetallic compounds and semiconductors with suitable modifications. Furthermore, in view of the present controversy regarding the effect of electron–phonon interaction in the magnetism of solids, our theory paves the way towards a better quantitative understanding of the effect.

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References

Eliashberg G M 1963 *Sov. Phys.-JETP* **16** 780

Enz C P and Mathias B T 1979 *Z. Phys.* B **33** 129
Fay D and Appel J 1979 *Phys. Rev.* B **20** 3705
Grimvall G 1968 *J. Phys. Chem. Solids* **29** 1221
—— 1981 *The Electron–Phonon Interaction in Metals* (Amsterdam: North-Holland) p 140
Herring C 1966 *Magnetism* vol 4, ed. G T Rado and H Suhl (New York: Academic) p 290
Joshi S K and Rajagopal A K 1968 *Solid State Phys.* **22** 159 (New York: Academic)
Kim D J 1976 *J. Phys. Soc. Japan* **40** 1250
—— 1979 *Solid State Commun.* **30** 249
—— 1981 *Phys. Rev. Lett.* **47** 1213
—— 1982 *Phys. Rev.* B **25** 6919
—— 1984 *J. Appl. Phys.* **55** 2347
Kim D J and Tanaka C 1986 *J. Magn. Magn. Mater.* **58** 254
—— 1988 *Phys. Rev.* B **37** 3948
Kittel C 1976 *Introduction to Solid State Physics* (New York: Wiley) p 451
Luttinger J M and Ward J C 1960 *Phys. Rev.* **118** 1417
McMillan W L 1968 *Phys.Rev.* **167** 331
Migdal A B 1958 *Sov. Phys.-JETP* **7** 996
Misra P K and Kleinman L 1972 *Phys. Rev.* B **5** 4531
Misra S K, Misra P K and Mahanti S D 1982 *Phys. Rev.* B **26** 1903
Pickett W E 1982 *Phys. Rev.* B **26** 1186
Schrieffer J 1964 *Theory of Superconductivity* (New York: Benjamin) p 198
Tripathi G S 1985a *J. Phys. C: Solid State Phys.* **18** L1157
—— 1985b *Phys. Rev.* B **31** 5143
—— 1986 *Phys. Lett.* **115A** 169
—— 1987 *Phys. Rev.* B **35** 5247
Tripathi G S, Das L K, Misra P K and Mahanti S D 1981 *Solid State Commun.* **39** 58
—— 1982 *Phys. Rev.* B **35** 5247
Tripathi G S, Misra B and Misra P K 1987 *J. Magn. Magn. Mater.* **67** 271
Ziman J M 1973 *Principles of the Theory of Solids* (Cambridge: Cambridge University Press) p 144
Zvrev V M and Silin V P 1987 *JETP Lett.* **45** 178