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CONDUCTION ELECTRON SPIN POLARIZATION IN MAGNETIC SEMICONDUCTORS

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The first-order treatment of the s-f interaction in ferromagnetic semiconductors splits the conduction band into two spin-polarized subbands. This implies a well defined spin gap and predicts almost step-like behaviour of conduction electron spin polarization near T_C. By calculating the second-order, self-consistent self-energies, which include finite lifetime, we show that the spin gap does not exist and consequently, the spin polarization makes smoother transition below T_C.

I. Introduction

In the s-f model conduction electrons are by exchange interaction coupled to the spins of the magnetic lattice [1]. Exact solution for the model is known only in the strong-coupling limit, where the band width is small compared to the exchange interaction. In this limit the model reduces to the well known ionic case, which serves as a good starting point for the study of narrow band materials [2]. In the weak-coupling limit, where the band width is large compared to the exchange interaction, the conduction band is split into two spin-polarized subbands [1]. The lower band, called spin up band, is exact at zero temperature limit, but the spin down band is only an approximation. Improved by the second-order corrections [3, 4] this picture explains adequately the behaviour of the low lying states, e.g. the optical red shift of the band edge. However, for instance conduction electron spin polarization P, which depends on higher energy states, is not sufficiently well described. The spin-polarized bands predict almost step-like behaviour of P near T_C, whereas experiments show smoother transition.

The single-site coherent-potential approximation (CPA) has been applied to the s-f model [5]. It is valid for all band widths, but it does not include the correlation effects between the spins of the magnetic lattice. Thus its validity is limited to high temperatures or to the narrow band case. For more general cases the method of moments has also been used [6, 7]. In this method a strong-coupling structure for the spectral density of conduction electrons is assumed. The position of poles and their weights are determined by fitting a relevant number of moments. In this method the original conduction band is splitted into several subbands, which in general are not pure spin states.

Baltensperger [8] first pointed out that in the spin-polarized band picture the spin down band is metastable. An electron in the spin down band can always emit a magnon and make a transition into the lower lying spin up band. The lifetime due to this process is in the spin wave region typically of the order of $5 \cdot 10^{-13}$ s [8].

This gives a level broadening $4 \cdot 10^{-2}$ eV, which exceeds considerably the average thermal energy. Consequently, it is necessary to include the effects of finite lifetime to describe electrons in conduction band. This can be done by continuing the perturbation treatment to higher orders using proper decoupling or the ordinary diagrammatic methods [9, 10].

II. Conduction Electron Green's Function

The Hamiltonian for the s-f model reads

$$H = \sum_{\nu} E_{\nu} a_{\nu}^{+} a_{\nu} - \sum_{\nu,\nu',i} \vec{J}(\nu,\nu',i) \cdot \vec{S}_i a_{\nu}^{+} a_{\nu'} + H_M \, . \tag{1}$$

The first term represents conduction band electrons, the second one the s-f interaction and the third term is the Hamiltonian for the magnetic lattice. The index ν stands for the wave vector $\vec{k}$ and the spin index σ. In the s-f interaction part

$$\vec{J}(\nu,\nu',i) = J(\vec{k}' - \vec{k}) e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_i} \, 2 \langle \sigma | \vec{s} | \sigma' \rangle \tag{2}$$

$J(\vec{k}'-\vec{k})$ is the wave-vector-dependent exchange parameter.

In the calculation it is convenient to subtract first the thermal average of lattice spins by writing

$$\vec{S}_i = \langle \vec{S}_i \rangle + \vec{\xi}_i \, , \tag{3}$$

and treat the $\vec{\xi}$-dependent part as a perturbation. The conduction electron Green's function is defined by

$$G_{\nu} = \langle\langle a_{\nu} ; a_{\nu}^{+} \rangle\rangle = \frac{1}{\hbar\omega - E_{\nu} - \Sigma_{\nu}(\omega)} \, , \tag{4}$$

where

$$E_{\nu} = E_{\vec{k}\sigma} = \frac{\hbar^2 k^2}{2m^*} + \Delta E_{\sigma} \, ,$$

$$\Delta E_{\sigma} = -J(o) N \langle S^z \rangle (\delta_{\sigma,\uparrow} - \delta_{\sigma,\downarrow}) \, , \tag{5}$$

and Σ_{ν} denotes the self-energy. In other words E_{ν} gives the spin-polarized band picture, which is the first-order result.

Approximations for the self-energy can be obtained by a decoupling method or by perturbation theory [9, 10]. In the present case the first relevant approximation, which includes the effects of finite lifetime, is the second-order, self-consistent self-energy given by [9, 10]

$$\Sigma_{\nu} = \sum_{\nu',i,j} \vec{J}(\nu,\nu',i) \cdot \langle \vec{\xi}_i \vec{\xi}_j \rangle \cdot \vec{J}(\nu',\nu,j) G_{\nu'} \, . \tag{6}$$

The two-spin correlation function needed in eq. (6) is calculated by the mean-field theory [11]. As a result

$$\langle \vec{\xi}_i \vec{\xi}_j \rangle = \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)} \overleftrightarrow{\Gamma}(\vec{q}) \, , \tag{7}$$

where

$$\Gamma^{\alpha\beta}(\vec{q}) = \frac{4S(S+1)T}{T_C} \frac{\delta_{\alpha\beta}}{\kappa_\alpha^2 + a^2q^2} \quad ; \quad \alpha,\beta = x, y, z \ , \tag{8}$$

and

$$\kappa_z^2 = 12\left(\frac{T\, B_S'(o)}{T_C\, B_S(\bar{x})} - 1\right) , \quad \kappa_x^2 = \kappa_y^2 = 12\left(\frac{T\bar{x}B_S'(o)}{T_C B_S(\bar{x})} - 1\right) . \tag{9}$$

Here B_S' denotes the derivative of the Brillouin function and a is the lattice constant. The wave-vector-dependent exchange parameter is approximated by

$$J(q) = \frac{J}{1 + l^2q^2} \ , \tag{10}$$

where l is of the order of the radius of the magnetic shell. When Σ is assumed to be independent of wave vector eq. (6) gives in the long wavelength limit

$$\Sigma_\sigma = -\frac{J^2N^2}{16\pi E_o}\frac{4S(S+1)T}{T_C} \sum_{\sigma'} c(\sigma,\sigma')\left(\frac{1}{\kappa(\sigma,\sigma') - i\Omega_{\sigma'}} - \frac{1}{\kappa(\sigma,\sigma') + a/l} - \frac{a}{2l(\kappa(\sigma,\sigma') + a/l)^2}\right) , \tag{11}$$

where

$$\Omega_{\sigma'} = (\hbar\omega - \Delta E_{\sigma'} - \Sigma_{\sigma'})^{1/2} E_o^{-1/2}, \quad E_o = \frac{\hbar^2}{2m^*a^2} \ , \tag{12}$$

and

$$c(\sigma,\sigma') = \begin{cases} 1 & ; \ \sigma = \sigma' \\ 2 & ; \ \sigma \neq \sigma' \end{cases} , \qquad \kappa(\sigma,\sigma') = \begin{cases} \kappa_z & ; \ \sigma = \sigma' \\ \kappa_x & ; \ \sigma = \sigma' \end{cases} . \tag{13}$$

Equation (11) is a coupled equation for $\Sigma_\uparrow$ and $\Sigma_\downarrow$, which has to be solved numerically.

III. Results and Discussion

Figure (1) shows the calculated self-energies for EuS slightly below T_C. The values of parameters are S = 7/2, a = 5,96 Å, $m^* = m_o$, T_C = 16 K, and l = 0,3 Å. The maximum band-splitting energy is taken to be $\Delta E = 2J(o)NS = 0.66$ eV, which corresponds to the atomic value of the exchange parameter. The most important result in Fig. (1) is that the imaginary part of $\Sigma_\downarrow$ is non-zero down to the band edge. Consequently, the spin gap predicted by the first order theory does not exist. The density of states is shown in Fig. (2). Owing to the finite lifetime the spin down band has a tail, which extends to the band edge. The conduction electron spin polarization is shown in Fig. (3) for a non-degenerate

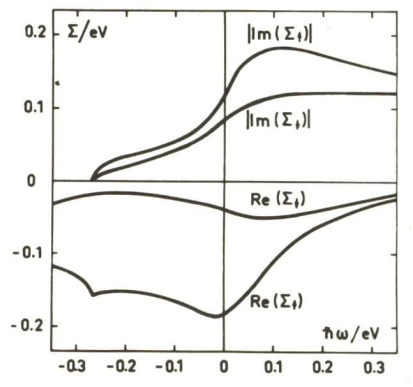

Fig. 1 Conduction electron self-energies in EuS at T = 0.95 T_C

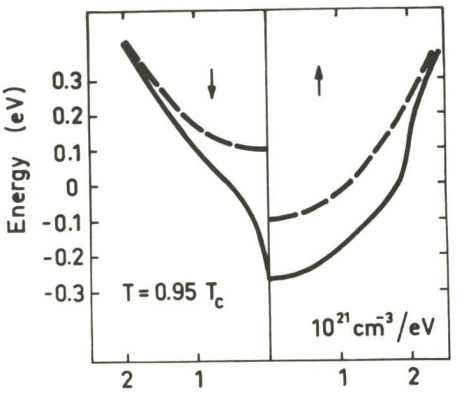

Fig. 2 Density of states (——), first order theory (---)

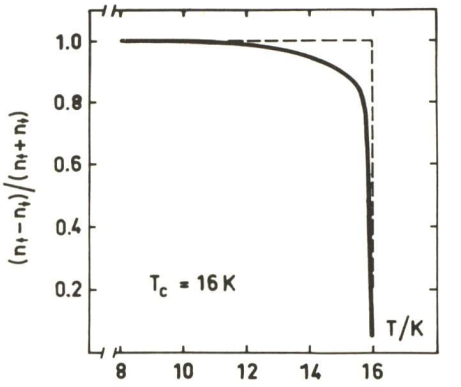

Fig. 3 Spin polarization (——), first order theory (---)

case. The first order theory predicts almost step-like behaviour of P near T_C, whereas the present calculation gives smoother transition. Well below T_C P approaches 1. This is a consequence of the fact that the imaginary parts of self-energies become smaller than kT and then the spectral densities become δ-function-like peaked at the poles of the Green's functions. The spin polarization in Fig. (3) compares rather well with the results of Nolting and Reihl [12] obtained by the method of moments and also with the experimental results reported by Kisker et al. [13]. However, the experimental value of P is 90 % at $T \simeq 11$ K whereas Fig. (3) gives practically 100 % polarization. This may arise from the fact that the spin correlation functions derived from the mean-field theory decrease too rapidly below T_C. Use of spin wave representation would possibly improve the result. On the other hand, the present theory cannot be strictly compared to the experimental results. We have calculated the thermal equilibrium value for P, but the experimental results [13] are obtained by the field emission from W-EuS junction. This process is controlled by the tunneling trough the internal potential barrier at the junction.

In conclusion, we have shown that the spin gap predicted by the first-order theory does not exist, but the spin down band has a tail, which extends down to the band edge. As the result of band tailing the spin polarization decreases from the first-order result.

1) S. Methfessel and D.C. Mattis: Encyclopedia of Physics, XVIII/1, (1968) 389.
2) E.L. Nagaev: Phys. Status Solidi (b) 65 (1974) 11.
3) F. Rys, J.S. Helman, and W. Baltensperger: Phys. konden. Mater. 6 (1967) 105.
4) C. Haas: Phys. Rev. 168 (1968) 531.
5) A. Rangette, A. Yanase and J. Kübler: Solid State Commun. 12 (1973) 171.
6) W. Nolting: Phys. Status Solidi (b) 79 (1977) 573.
7) W. Nolting: J. Phys. C 11 (1978) 1427.
8) W. Baltersperger: J. appl. Phys. 41 (1970) 1052.
9) J. Sinkkonen: Phys. Rev. B 19 (1979) 6407.
10) J. Sinkkonen: to be published.
11) P.G. de Gennes and J. Villain: J. Phys. Chem. Solids 13 (1960) 10.
12) W. Nolting and B. Reihl: J. Magn. magn. Mater. 10 (1979) 1.
13) E. Kisker, G. Baum, A.H. Mahan, W. Raith and B. Reihl: Phys. Rev. B 18 (1978) 2256.