

An electron in the field of phonons and magnons

S S SHAH* and K P SINHA†

* Physics Department, Marathwada University, Aurangabad 431002

† Indian Institute of Science, Bangalore 560012

MS received 31 January 1974; in final form 4 March 1974.

Abstract. The behaviour of a conduction electron in the presence of two Bose fields, namely, phonons and magnons in ferromagnetic semiconductors is studied. The effects of both electron-magnon and electron-phonon interactions on the energy renormalization are calculated.

Keywords. Electron; phonons; magnons; magnetic semiconductors; magnetic polaron.

1. Introduction

Ferromagnetic semiconductors have generated considerable experimental and theoretical work owing to their interesting transport and optical properties (Methfessel and Mattis 1967). In pure state these materials are very good insulators. However, by appropriate doping, one can introduce carriers in the conduction band. The magnetic semiconductor thus produced (*e.g.*, doped EuO) is a system of interesting interactions involving the free carrier and other excitations such as phonons, magnons, etc. These magnetic systems (*e.g.*, rare earth chalcogenides), in addition to showing magnetic ordering, are also good examples of ionic solids. One therefore expects strong interactions of an electron (or a hole) with both magnons and phonons (Shah 1970, Klama and Klinger 1971). Following the analogy with the ionic polaron case, several theoretical studies of interaction between an electron and magnons have been made (Wolfram and Callaway 1962, Woolsey and White 1970, Izyumov and Medvedev 1970, Richmond 1970). These have also led to the concept of small or large magnetic polaron.

In what follows, we consider the behaviour of a conduction electron interacting with two Bose fields, namely, phonons and magnons in ferromagnetic semiconductors.

2. The Hamiltonian

The Hamiltonian of the system described above can be written as

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_m + \mathcal{H}_p + \mathcal{H}_{em} + \mathcal{H}_{ep} \quad (2.1)$$

where

$$\mathcal{H}_e = \sum_{k\sigma} \epsilon_{k\sigma} C_{k\sigma}^\dagger C_{k\sigma}, \quad \mathcal{H}_m = \sum_{\lambda} E_{\lambda}^m (a_{\lambda}^\dagger a_{\lambda} + \frac{1}{2})$$

$$\mathcal{H}_p = \sum_q E_q^p (b_q^\dagger b_q + \frac{1}{2}) \quad (2.2)$$

$$\mathcal{H}_{em} = - \sum_{k\lambda} I_m (C_{k\downarrow}^\dagger C_{k-\lambda\uparrow} a_\lambda + C_{k-\lambda\uparrow}^\dagger C_{k\downarrow} a_\lambda^\dagger) \quad (2.3)$$

$$\mathcal{H}_{ep} = \sum_{k,q\sigma} P_q C_{k+q\sigma}^\dagger C_{k\sigma} (b_q + b_{-q}^\dagger) \quad (2.4)$$

Here $(C_{k\sigma}^\dagger, C_{k\sigma})$, $(a_\lambda^\dagger, a_\lambda)$ and (b_q^\dagger, b_q) are the electron, magnon and phonon (creation, annihilation) operators respectively in corresponding states with k , λ and q representing the wave vectors; σ is the spin index. The single particle electron $\epsilon_{k\sigma}$ and magnon E_λ^m energies already incorporate the correction arising from the two magnon electron-magnon terms and the ferromagnetic ordering of the localised spins.

Explicitly

$$\epsilon_{k\sigma} = \frac{\hbar^2 k^2}{2m^*} - \mu_B \mathcal{H}_{ext\sigma} - \frac{I}{2} \left(S - \frac{1}{N} \sum_\lambda \langle N_\lambda^m \rangle \right) \quad (2.5)$$

$$E_\lambda^m = \hbar\omega_\lambda + \frac{I}{2N} (\langle n_\uparrow \rangle - \langle n_\downarrow \rangle) \quad (2.6)$$

where m^* is the effective electron mass, H_{ext} is the external magnetic field, σ takes the values ± 1 and I is exchange constant of the contact type between conduction electron and localised spins of magnitude S . Here N_λ^m is the average magnon occupation number and $\langle n_\uparrow \rangle - \langle n_\downarrow \rangle$ is the net spin polarisation of the conduction electrons. Furthermore, $E_q^p = \hbar\omega_q$ is the phonon energy. The remaining electron-magnon interaction term \mathcal{H}_{em} involves emission or absorption of a magnon along with spin flip scattering of a conduction electron with $I_m \equiv \frac{1}{2}(2S/N)^{\frac{1}{2}} I$. In equation (2.4) \mathcal{H}_{ep} represents the electron-phonon interaction term wherein the general form of the coupling constant P_q can be written as (Shankar and Sinha 1973)

$$P_q = \frac{1}{\sqrt{N}} \left(\frac{\hbar}{2M\omega_q} \right)^{\frac{1}{2}} F \quad (2.7)$$

where F is the deformation potential field, M is the atomic mass and N the number of unit cells. We have ignored any direct interaction between phonons and magnons (Sinha and Upadhyaya 1962, Shah 1970).

3. Electron Green's function

We calculate the Green's function for an electron in the field of phonons and magnons. We follow the method of double time thermal Green's function technique for computing the relevant single particle and higher order Green's functions (Zubarev 1960). These calculations are rather lengthy and involved. Accordingly, we will be content with writing significant results and conclusions. The Green's functions will contain information about relevant properties of the electron, *i.e.*, renormalisation of energy, effective mass, life time, etc.

The electron Green's function is denoted as follows (Zubarev 1960):

$$G_{kk'}^{\sigma\sigma'} = \langle\langle C_{k\sigma}(t); C_{k'\sigma'}^\dagger(t') \rangle\rangle \quad (3.1)$$

Setting up the equations of motion of these Green's functions and taking their Fourier transform we get the following chain of equations:

$$\begin{aligned}
 (E - \epsilon_{k\sigma}) \langle\langle C_{k\sigma}; C_{k'\sigma}^\dagger \rangle\rangle &= \frac{\hbar}{2\pi} \delta_{\sigma\sigma'} \delta_{kk'} - \sum_{\lambda} I_m(k, \lambda) \delta_{\sigma\uparrow} \langle\langle C_{k+\lambda\downarrow} a_{\lambda\uparrow}; C_{k'\sigma'}^\dagger \rangle\rangle \\
 &\quad - \sum_{\lambda} I_m(k, \lambda) \delta_{\sigma\downarrow} \langle\langle C_{k-\lambda\uparrow} a_{\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle \\
 &\quad + \sum_q P_q \{ \langle\langle C_{k+a, \sigma} b_q^\dagger; C_{k'\sigma'}^\dagger \rangle\rangle + \langle\langle C_{k-a, \sigma} b_q; C_{k'\sigma'}^\dagger \rangle\rangle \} \quad (3.2)
 \end{aligned}$$

The right hand side contains four higher order Green's functions. The equations of motion of these will in turn contain still higher order Green's functions.

At this state it will be expedient to reduce these by appropriate decoupling. For example some of the Green's functions involved at this stage are decoupled in the following manner:

$$\begin{aligned}
 \delta_{\lambda, \lambda+a} \langle\langle a_{\lambda_1+a_1}^\dagger b_q b_{a_1}^\dagger C_{k+\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle &= \langle b_q b_{a_1}^\dagger \rangle \langle\langle a_{\lambda_1}^\dagger C_{k+\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle \\
 &= (1 + N_q^p) \langle\langle a_{\lambda_1}^\dagger C_{k+\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle
 \end{aligned}$$

also

$$\begin{aligned}
 \langle\langle a_{\lambda_1+a_1} a_{\lambda+a_1}^\dagger a_{\lambda+a_1} C_{k+\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle \delta_{a_1-a_2} &= \langle N_{\lambda+a}^m \rangle \langle\langle a_{\lambda_1}^\dagger C_{k+\lambda\downarrow}; C_{k'\sigma'}^\dagger \rangle\rangle
 \end{aligned}$$

where (N_q^p) , (N_λ^m) , etc., are phonon and magnon occupation numbers. Further the average values of $\langle b_q \rangle$, $\langle b_q^\dagger \rangle$, $\langle a_{\lambda_1}^\dagger \rangle$, etc., and of products of two creation or two annihilation operators will be taken as zero. After decoupling these higher order Green's functions the various lower order Green's functions are solved.

For example

$$\begin{aligned}
 (E - \epsilon_{k+\lambda\downarrow} + E_\lambda^m - A(E, k + \lambda_\downarrow)) \langle\langle C_{k+\lambda\downarrow} a_{\lambda\uparrow}; C_{k'\sigma'}^\dagger \rangle\rangle &= -I_m [\langle N_\lambda^m \rangle + \langle n_{k+\lambda\downarrow} \rangle] \langle\langle C_{k\uparrow}; C_{k'\sigma'}^\dagger \rangle\rangle \\
 &\quad - \sum_q P_q I_m \left\{ \frac{\langle N_\lambda^m \rangle + \langle n_{k+\lambda-q\downarrow} \rangle}{E - \epsilon_{k+\lambda-q\downarrow} + E_\lambda^m - E_q^p} \langle\langle C_{k-q\downarrow} b_q; C_{k'\sigma'}^\dagger \rangle\rangle \right. \\
 &\quad \left. + \frac{\langle N_\lambda^m \rangle + \langle n_{k+q\uparrow\lambda\downarrow} \rangle}{E - \epsilon_{k+\lambda+q\downarrow} + E_\lambda^m + E_q^p} \langle\langle C_{k+q\uparrow} b_q^\dagger; C_{k'\sigma'}^\dagger \rangle\rangle \right\} \quad (3.3)
 \end{aligned}$$

where

$$\begin{aligned}
 A(E, k + \lambda_\downarrow) &= \sum_q P_q^2 \left\{ \frac{\langle 1 + N_q^p \rangle - \langle n_{k+\lambda+q\downarrow} \rangle}{E - \epsilon_{k+\lambda+q\downarrow} + E_\lambda^m - E_q^p} + \frac{\langle N_q^p \rangle + \langle n_{k+\lambda-q\downarrow} \rangle}{E - \epsilon_{k+\lambda+q\downarrow} + E_\lambda^m + E_q^p} \right\} \quad (3.4)
 \end{aligned}$$

Similarly, we can solve the equations of motion for the remaining three higher order Green's function on the right hand side of equation (3.2). Substituting

these in equation (3.2), we finally get two equations from equation (3.2), one for up spin electron and the other for down spin electron. Explicitly,

$$\langle\langle C_{k\uparrow}; C_{k\uparrow}^\dagger \rangle\rangle = \frac{\hbar}{2\pi[E - \epsilon_{k\uparrow} - \Sigma(E, k\uparrow)]} \quad (3.5)$$

where the full form of $\Sigma(E, k\uparrow)$ is given by

$$\begin{aligned} \Sigma(E, k\uparrow) &= \sum_{\lambda} \frac{I_m^2 [\langle N_{\lambda}^m \rangle + \langle n_{k+\lambda\downarrow} \rangle]}{E - \epsilon_{k+\lambda\downarrow} + E_{\lambda}^m - A(E, k + \lambda\downarrow)} \\ &+ \sum_{q} P_q^2 \left\{ \frac{[\langle N_q^p \rangle + \langle n_{k+q\uparrow} \rangle]}{E - \epsilon_{k+q\uparrow} + E_q^p - B(E, k + q\uparrow)} \right. \\ &+ \left. \frac{[(1 + N_q^p) - \langle n_{k-q\uparrow} \rangle]}{E - \epsilon_{k-q\uparrow} - E_q^p - B(E, k - q\uparrow)} \right\} \\ &+ \sum_{\lambda q} P_q^2 I_m^2 \frac{[\langle N_{\lambda}^m \rangle + \langle n_{k+\lambda\downarrow} \rangle]}{E - \epsilon_{k+\lambda\downarrow} + E_{\lambda}^m - A(E, k + \lambda\downarrow)} \times \\ &\times \left\{ \frac{[\langle N_q^p \rangle + \langle N_{k+\lambda+q\downarrow} \rangle]}{E - \epsilon_{k+\lambda+q\downarrow} + E_{\lambda}^m + E_q^p} (E - \epsilon_{k+q\uparrow} - E_q^p - B(E, k + q\uparrow)) \right. \\ &+ \left. \frac{[(1 + N_q^p) - \langle n_{k+\lambda-q\downarrow} \rangle]}{(E - \epsilon_{k+\lambda-q\downarrow} + E_{\lambda}^m - E_q^p) (E - \epsilon_{k-q\uparrow} - E_q^p - B(E, k - q\uparrow))} \right\} \end{aligned} \quad (3.6)$$

Similarly we get

$$\langle\langle C_{k\downarrow}; C_{k\downarrow}^\dagger \rangle\rangle = \frac{\hbar}{2\pi[E - \epsilon_{k\downarrow} - \Sigma(E, k\downarrow)]} \quad (3.7)$$

where $\Sigma(E, k\downarrow)$ is given by

$$\begin{aligned} \Sigma(E, k\downarrow) &= \sum_{\lambda} \frac{I_m^2 [\langle N_{\lambda}^m \rangle + \langle 1 - n_{k-\lambda\uparrow} \rangle]}{E - \epsilon_{k-\lambda\uparrow} - E_{\lambda}^m - A(E, k - \lambda\uparrow)} \\ &+ \sum_{q} P_q^2 \left\{ \frac{[\langle N_q^p \rangle + \langle n_{k+q\downarrow} \rangle]}{E - \epsilon_{k+q\downarrow} + E_q^p - B(E, k + q\downarrow)} + \right. \\ &\quad \left. + \frac{[(1 + N_q^p) - \langle n_{k-q\downarrow} \rangle]}{E - \epsilon_{k-q\downarrow} - E_q^p - B(E, k - q\downarrow)} \right\} \\ &+ \sum_{\lambda q} \frac{P_q^2 I_m^2 [\langle N_{\lambda}^m \rangle + \langle 1 - n_{k-\lambda\uparrow} \rangle]}{E - \epsilon_{k-\lambda\uparrow} - E_{\lambda}^m - A(E, k - \lambda\uparrow)} \times \\ &\times \left\{ \frac{[\langle N_q^p \rangle + \langle n_{k-\lambda+q\uparrow} \rangle]}{(E - \epsilon_{k-\lambda+q\uparrow} - E_{\lambda}^m + E_q^p) (E - \epsilon_{k+q\downarrow} + E_q^p - B(E, k + q\downarrow))} \right. \\ &+ \left. \frac{[(1 + N_q^p) - \langle n_{k-\lambda-q\uparrow} \rangle]}{(E - \epsilon_{k-\lambda-q\uparrow} - E_{\lambda}^m - E_q^p) (E - \epsilon_{k-q\downarrow} - E_q^p - B(E, k - q\downarrow))} \right\} \end{aligned} \quad (3.8)$$

where $A(E, k - \lambda \uparrow)$ is defined in the same way as in equation (3.4) by reversing the spin index and changing sign wherever λ occurs.

$$B(E, k \pm q \uparrow) = \frac{\sum_{\lambda} I_m^2 [\langle N_{\lambda}^m \rangle + \langle n_{k+\lambda \pm q \downarrow} \rangle]}{E - \epsilon_{k+\lambda \pm q \downarrow} + E_{\lambda}^m \pm E_q^p} \quad (3.9)$$

Similarly

$$B(E, k \pm q \downarrow) = \frac{\sum_{\lambda} I_m^2 [\langle 1 + N_{\lambda}^m \rangle - \langle n_{k-\lambda \pm q \uparrow} \rangle]}{E - \epsilon_{k-\lambda \pm q \uparrow} - E_{\lambda}^m \pm E_q^p} \quad (3.10)$$

4. Renormalization effects

4.1 Renormalization of electron energy

From equations (3.5) and (3.7) we obtain the energy of the conduction electron in the \uparrow and \downarrow spin states, *i.e.*, from the poles of the two Green's functions.

$$E_{k\uparrow} = \epsilon_{k\uparrow} + \Sigma(E, k \uparrow) \quad (4.1)$$

$$E_{k\downarrow} = \epsilon_{k\downarrow} + \Sigma(E, k \downarrow) \quad (4.2)$$

where the explicit forms of $\Sigma(E, k \uparrow)$ and $\Sigma(E, k \downarrow)$ are given by equations (3.6) and (3.8). The real parts of these terms give the renormalization of electron self-energy. We can also get the effective mass enhancement from these terms. $\Sigma(E, k\sigma)$ contains three type of terms:

$$(i) \Sigma I_m^2(\dots), \quad (ii) \Sigma P_q^2(\dots) \quad \text{and} \quad (iii) \Sigma P_q^2 I_m^2(\dots).$$

Their explicit forms are given in equations (3.6) and (3.8); (i) and (ii) are the self-energy corrections owing to electron-magnon and electron-phonon interactions respectively. They depend implicitly on each other and on the occupation number of electrons and relevant bosons. One important conclusion emanating from the above two interactions is that the energy of the spin up electron is further lowered relative to $\epsilon_{k\uparrow}$ even at the absolute zero of temperature. This will be seen in the calculations given later in this paper. This is in contradistinction to the situation when only electron-magnon interactions are taken into account (Woolsey and White 1970, Richmond 1970).

The term (iii) mentioned above is a consequence of our consideration of simultaneous presence of two boson fields (Sinha 1973). Energy renormalization owing to these processes become comparable to that due to the terms (i) and (ii). This will give rise to different power laws (temperature dependences) in specific heats, relaxation time and some of the transport phenomena.

It turns out that contributions from (i) and (ii) neutralize each other (see concluding remarks for spin down case). A similar situation obtains for terms involving P_q^4 and I_m^4 . Thus terms like (iii) are expected to play an important role.

4.2 Calculations

Keeping in view the formation of polaron with up spin electron even at absolute zero, we calculate the renormalization energies $\Sigma(E, k\sigma)$ at $T = 0$ K. This

simplifies the task very much. We can take the boson occupation numbers to be zero. Only terms involving interaction with zero point phonons survive.

Thus at $T=0$ equation (3.6) reduces to

$$\sum (E, k \uparrow) = \sum_q P_q^2 \frac{1}{E \uparrow - \epsilon_{k-q} - E_q^p} \quad (4.3)$$

We take the case of EuO for our numerical estimates. This has the rock salt structure with lattice constant $a = 5.14 \text{ \AA}$, $S = 7/2$, $I = 0.3 \times 10^{-12} \text{ erg}$ (Rys *et al* 1967).

Further, $F \sim 10^{-3}$ dynes and $\omega_q \simeq \omega_0 \sim 10^{14}$ c/s for optical phonons (Shankar and Sinha 1973). Changing the summation to integration and using the above parameters, equation (4.3) reduces to

$$\sum (E, k \uparrow) \simeq - \frac{a^2 m^* F^2}{8\pi\hbar M \omega_0} \quad (4.4)$$

$\simeq -6.25 \times 10^{-3}$ eV, using $m^* =$ free electron mass and $M \sim 50 \times 10^{-24}$ g.

Equation (4.4) is obtained under slow electron approximation. Thus we see that even at the absolute zero of temperature for the up spin electron energy is lowered by the phonons. For low doping (very low fermi energy of conduction electron.) in EuO the relaxation effects involving optical phonons will not be important at $T = 0$.

Unlike in the up spin case, the down spin conduction electrons will be affected by both electron-phonon and electron-magnon interactions.

$$(i) = \sum \frac{I_m^2}{(E \downarrow - \epsilon_{k-\lambda} - E_{\lambda}^m - A(E \downarrow, k - \lambda \uparrow))} \quad (4.5)$$

is the renormalization arising from electron-magnon interaction corrected by $A(E \downarrow, k - \lambda \uparrow)$ due to the presence of phonons. Taking $E_{\lambda}^m = D\lambda^2$, where $D = 2JSa^2$ with $J = \frac{k_B \theta_c}{2S}$, k_B being the Boltzman constant and θ_c Curie temperature (for EuO, $\theta_c \sim 70\text{K}$ (Methfessel Mattis 1967)), and $E \downarrow \approx \epsilon_{k \downarrow}$, we get $E \downarrow - \epsilon_{k-\lambda \uparrow} \approx IS$ and $IS \gg D\lambda^2$, for all values of λ including λ_{\max} . Further, we estimate that $A(E, k - \lambda \uparrow) \simeq 4 \times 10^{-3}$ eV and $B(E, k - q \downarrow) \simeq 1.2 \times 10^{-2}$ eV $\approx 10^{-2}$ eVt. Accordingly, equation (4.5) reduces to $I/16 \approx 1.2 \times 10^{-2}$ eV. Let us now consider

$$(ii) = \sum_q \frac{P_q^2}{E \downarrow - \epsilon_{k-q \downarrow} - E_q^p - B(E, k - q \downarrow)} \quad (4.6)$$

Except for the presence of $B(E, k - q \downarrow)$ the calculations are exactly similar to that for the up spin case. Hence, (ii) is estimated to be of the order of -10^{-2} eV.

For

$$(iii) = P_q^2 I_m^2 (\dots),$$

the last expression of equation (3.8) is taken into account. This will reduce to

$$\approx - \frac{a^2 F^2 m^*}{384 SM\omega_q \hbar} \approx - 2.4 \times 10^{-4} \text{ eV.}$$

(The presence of $B(E, k - q \downarrow)$ is taken into account. This is of the order of -10^{-3} eV, if ω_0 is between 10^{13} and 10^{14} c/s).

When we add all these contributions from (i) to (iii) we get the total reduction in electron energy to be -10^{-3} eV.

At this stage we do not consider relaxation effects in that they will not be important at $T = 0$ K.

5. Conclusions

The main results of our calculations are summarised as follows:

(a) There is a possibility of polaron formation for up spin electron even at $T=0$ K.

(b) The simultaneous consideration of electron-magnon and electron-phonon interaction effects suggest new features concerning energy renormalisation and mass enhancement of conduction electrons. For the spin down conduction electrons the effects of electron-magnon and electron-phonon interactions (*i.e.*, the terms (i) and (ii) tend to compensate each other. Accordingly, if only these terms were to be considered there will be slight enhancement or lowering in effective mass. The interference term (iii) thus plays an important role.

Acknowledgement

The authors would like to thank G Baskaran for discussions. One of us (SSS) is grateful to the Centre for Theoretical Studies, Indian Institute of Science, Bangalore, for hospitality and financial support during the final stage of the work.

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