Correlation effects in the valence bands of ferromagnetic semiconductor EuS

A. Sharma*1 and W. Nolting1

1 Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr.15, 12489, Berlin, Germany.

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We present a many body analysis of the multi-band Kondo lattice model. The study is then combined with the first principles TB-LMTO band structure calculations, in order to investigate the temperature dependent correlation effects in the 3p valence bands of the ferromagnetic semiconductor EuS. Some of the physical properties of interest like the quasi-particle density of states (Q-DOS), spectral density (SD) and quasi-particle band structure (Q-BS) are calculated and discussed. Therewith, we propose a spin resolved ARPES of the valence bands of EuS to be performed.

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1 INTRODUCTION

The europium chalcogenides EuX, with X=O,S,Se and Te, formed the subject of many studies for more than forty years. They are magnetic semiconductors and one of the early motivation was the hope of using these materials as magneto-optical memories in the computers and magneto-optical modulators. Moreover, the europium monochalcogenides are face centered cubic materials that are ideal examples of Heisenberg exchange model and thus formed good exemplary substances for studying magnetism. In such a motivated background experiments were performed to study their properties and use them for practical purposes. Though apart from various dopings and substitutions, it turned out that the ordering temperature could not be raised up to room temperature. Also, these materials were found difficult to prepare. But, despite such difficulties, the studies on these materials attracted attention from a more academic point of view as it highlighted many interesting physical properties. For example [1, 2], a metal-insulator transition in Eu-rich EuO has been observed while red-shift of the absorption edge, Faraday rotation, circular dichroism and spin polarization explained magnetic and magneto-optical effects. Such interesting properties have not only provided the motivation for theoretical and experimental investigations on these materials, but further studies on them permit a better understanding on more complex systems like the Diluted Magnetic Semiconductors (DMS) which are believed to be one of the essential materials behind the technology called spintronics [3, 4].

The motivation behind such a study is to combine many body theoretical analysis with bandstructure calculations for real materials. The goal is to study the temperature dependent electronic correlation effects in the valence bands of EuS. A similar study has been carried out earlier for the conduction bands of EuS [5] but under a different kind of a theoretical approach. The chalcogenide, EuS, was under a lot of experimental and theoretical investigation to study its magnetic and electronic properties, starting from early 1960s which reported nuclear magnetic resonance [6] till the latest being on EuS thin films [7] while the list remains extensive.

This paper is organized as follows. In section 2, we formulate the complete multi-band Hamiltonian.

* Corresponding author: e-mail: anand@physik.hu-berlin.de

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A self energy ansatz, reliable for low carrier densities, is used to solve the model Hamiltonian. The temperature and spin dependent density of states (DOS) are presented for two weakly hybridized bands in a simple cubic lattice with coupling strength, hybridization and magnetization being the parameters for the model study. The results are then compared with one of the exact limiting cases of the model, namely the ferromagnetically saturated semiconductor and are found to be coinciding. In section 3, such a many body model is combined with first principles T=0 band-structure calculation, tight binding linear muffin-tin orbital (TB-LMTO), in order to calculate some of the physical properties like quasi-particle density of states (Q-DOS), spectral density (SD) and quasi-particle band structure (Q-BS) for realistic ferromagnetic semiconducting material EuS. The final section 4, concludes with the proposition of a spin resolved ARPES experiment to be performed in order to examine our results.

2 THEORY AND MODEL CALCULATION

The multi-band Kondo lattice model (KLM) Hamiltonian reads as follows;

\[ H = H_{\text{kin}} + H_{\text{int}} \]  \hspace{1cm} (1)

where

\[ H_{\text{kin}} = \sum_{i,j,\alpha,\beta,\sigma} T_{ij}^{\alpha\beta} c_{i,\alpha,\sigma}^{\dagger} c_{j,\beta,\sigma} \]  \hspace{1cm} (2)

and

\[ H_{\text{int}} = -\frac{J}{2} \sum_{i,\alpha,\sigma} (z_{\sigma} S_{i,\sigma} c_{i,\alpha,\sigma}^{\dagger} c_{i,\alpha,\sigma} + S_{i,\sigma}^{\dagger} c_{i,\alpha,-\sigma}^{\dagger} c_{i,\alpha,\sigma}) \]  \hspace{1cm} (3)

The term \( H_{\text{kin}} \) denotes the kinetic energy of the valence band electrons, 3p orbital in case of EuS, with \( c_{i,\alpha,\sigma}^{\dagger} \) and \( c_{i,\alpha,\sigma} \) being the fermionic creation and annihilation operators, respectively, at lattice site \( R_i \). The latin letters \( (i,j,...) \) as subscripts, symbolize the crystal lattice indices while the band indices are depicted as superscripts in Greek letters \( (\alpha,\beta,...) \) and the spin is denoted as \( \sigma (=\uparrow,\downarrow) \). Such a notation is used throughout the text. The multi-band hopping term, \( T_{ij}^{\alpha\beta} \), is connected by Fourier transformation to the free Bloch energies \( \epsilon^{\alpha\beta}(k) \)

\[ T_{ij}^{\alpha\beta} = \frac{1}{N} \sum_{k} \epsilon^{\alpha\beta}(k) e^{-ik(R_i-R_j)} \]  \hspace{1cm} (4)

\( H_{\text{int}} \) is an intra-atomic exchange interaction term being further split into two subterms. The first describes the Ising type interaction between the z-component of the localized and itinerant carrier spins while the other comprises spin exchange processes which are responsible for many of the KLM properties. \( J \) is the exchange coupling strength which we assume to be \( k \)-independent and \( S_{i,\sigma}^{\alpha} \) refers to the localized spin at site \( R_i \)

\[ S_{i,\sigma}^{\alpha} = \sum_{\alpha} \frac{z_{\alpha} S_{i,\alpha,\sigma} + S_{i,\alpha,\sigma}^{\dagger} c_{i,\alpha,-\sigma}^{\dagger} c_{i,\alpha,\sigma}}{} \]  \hspace{1cm} (5)

The Hamiltonian in eq. (1) provokes a nontrivial many body problem that cannot be solved exactly. Approximations must be considered. We proceed to solve the problem by the equation of motion method using double-time retarded Green function [8]

\[ G_{\mu\nu}(E) = \langle \langle c_{\mu,\sigma}^{\dagger} c_{\mu,\nu,\sigma} \rangle \rangle E \]  \hspace{1cm} (6)
where $l,m$ and $\mu,\nu$ are the lattice and band indices respectively. The equation of motion reads as follows

$$E G_{lm\sigma}^{\mu\nu}(E) = \hbar \delta_{lm} \delta_{\mu\nu} + \sum_{j,\gamma} T_{lj}^{\mu\gamma} G_{j\mu\sigma}^{\gamma\nu}(E) - \frac{J}{2} [\Gamma_{lm\sigma}^{\mu\nu}(E) + F_{lm\sigma}^{\mu\nu}(E)] \tag{7}$$

where we use the following notations

$$\Gamma_{lm\sigma}^{\mu\nu}(E) = \langle \langle S_l^z c_{\mu\sigma}; c_{m\nu\sigma}^\dagger \rangle \rangle_E \tag{8a}$$

$$F_{lm\sigma}^{\mu\nu}(E) = \langle \langle S_l^{-\sigma} c_{\mu-\sigma}; c_{m\nu\sigma}^\dagger \rangle \rangle_E \tag{8b}$$

We find that eq.(8a) and eq.(8b) are higher order Green functions blocking the direct solution of the equation of motion as they can’t be decoupled into the forms of the original Green function. But, a rather formal solution can be stated as

$$\hat{G}_{k\sigma}(E) = \frac{\hbar}{\hat{I}} [(E + i0^+) \hat{I} - \hat{c}(k) - \hat{\Sigma}_{k\sigma}(E)]^{-1} \tag{9}$$

where we exclude the band indices by representing the terms in a generalized matrix form on symbolizing a hat over it

$$\hat{G}_{l\sigma}(E) = \frac{1}{N} \sum_k \hat{G}_{k\sigma}(E) \ e^{-i k \cdot (R_l - R_m)} \tag{10}$$

The terms in eq. (9) are explained as follows : $\hat{I}$ is an identity matrix and $\hat{c}(k)$ is a hopping matrix with the diagonal terms of the matrix exemplifying the intra-band hopping and the off-diagonal terms denoting the inter-band hopping. The self energy, $\Sigma_{l\sigma}(E)$, containing all the influences of the different interactions being of fundamental importance can be understood as

$$\langle \langle [H_{int}, c_{l\mu\sigma}] - c_{m\nu\sigma}^\dagger \rangle \rangle = \sum_{p,\gamma} \Sigma_{lp\sigma}^{\mu\gamma}(E) G_{p\mu\sigma}^{\gamma\nu}(E) \tag{11}$$

Now, we are left with a problem of finding a multi-band self energy ansatz, in order to compute the Green function matrix and thereby calculate some of the physical quantities of interest like the quasi-particle spectral density (SD)

$$A_{k\sigma}(E) = -\frac{1}{\pi} \text{Im} \text{Tr} \hat{G}_{k\sigma}(E) \tag{12}$$

and the quasi-particle density of states (Q-DOS)

$$\rho_{\sigma}(E) = \frac{1}{N\hbar} \sum_k A_{k\sigma}(E) \tag{13}$$

As observed from our many body theoretical model, we are only interested in the influence of inter-band exchange on the valence band states in order to study the electronic correlations and not aimed at calculating the magnetic properties via self consistent calculation of the localized magnetization. For this purpose, we neglect the exchange interaction between the localized spins, $S_i^\sigma$, in our model. Furthermore, since we consider fully occupied valence bands, the Coulomb interaction is unimportant and this can further reduce the complexity in formulating the self energy ansatz. Actually, in case of realistic calculations of EuS, the Coulomb interaction is implicitly taken in the LSDA bandstructure calculations. So, the single particle excitation energies contain the Coulomb interactions and need not be taken into account in the self energy ansatz. Thus, the criterion required by our multi-band electronic self energy is that it should be accurately defined in the low carrier density regime and weak coupling strength, which is the case for the
study of magnetic semiconductors.

It is known that the above statements can be satisfied by the interpolating self energy ansatz (ISA) being proposed for a single band model [9]. Such an ansatz is considered to work for all coupling strengths and band occupations. Various exactly known limiting cases like the weak and strong coupling behavior, zero bandwidth limit [10], etc. are shown to be satisfied by the single-band ISA. Though it is not self-evident in case of multi-band situation that these confining cases would hold true, nevertheless we propose to replace the single particle Green function for the multi-band case by the respective matrix Green function. As seen in theoretical analysis given in Appendix A, the important case of ferromagnetically saturated semiconductor gives the same self-energy ansatz as in the single band case (eq.(26) and eq.(27) in Ref. 9) which strongly supports our ansatz. With the help of such analysis, we put forward for the multi-band self-energy (ISA);

$$\mathbf{\tilde{\Sigma}}_{\sigma}(E) = \frac{J}{2} M_{-\sigma} \mathbf{\tilde{T}} + \frac{J^2}{4} a_{-\sigma} \mathbf{\tilde{G}}_{-\sigma}(E + \frac{J}{2} M_{-\sigma}) \left[ \mathbf{\tilde{T}} - \frac{J}{2} \mathbf{\tilde{G}}_{-\sigma}(E + \frac{J}{2} M_{-\sigma}) \right]^{-1}$$

(14)

where

$$M_{\sigma} = z_{\sigma} \langle S^z \rangle; \quad a_{\sigma} = S(S + 1) + M_{\sigma}(M_{\sigma} + 1).$$

and the bare Green function matrix is defined as :

$$\mathbf{\tilde{G}}_{\sigma}(E) = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{(E + i0^+) \mathbf{\tilde{T}} - \mathbf{\tilde{\epsilon}}(\mathbf{k})}$$

It retains the formerly proposed ISA structure in the single band case. As seen in eq. (14), we are interested only in the local self energy

$$\mathbf{\tilde{\Sigma}}_{\sigma}(E) = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{\tilde{\Sigma}}_{\mathbf{k}\sigma}(E)$$

The physical reason for the wave-vector dependence of the self energy is mainly due to the magnon energies $\hbar \omega(\mathbf{k})$ appearing at finite temperature. But, as stated earlier, we neglect a direct Heisenberg exchange between the localized spins and this can be interpreted as the $\hbar \omega(\mathbf{k}) \to 0$ limit. The localized magnetization $\langle S^z \rangle$ shall be considered as an external parameter being responsible for the induced temperature dependence of the band states.

In principle, apart from the above discussed proposal one could also consider other alternative approaches for the many body analysis like the dynamical mean field theory (DMFT) in order to study the correlation effects. But, it is known [11] that the methods of DMFT can not be directly applied to the Kondo lattice model. One exception is the case of the classical spin limit, thus removing the quantum nature of the spins. While there is another possibility to derive a DMFT for Kondo lattice model, based on the fermionization of the localized spin operators as suggested in [12], but it is limited to $S=\frac{1}{2}$. Recently, in an article [13], the correlation effects were discussed by introducing DMFT based approaches but for a single band Kondo lattice model and with an evaluation compared with the exactly solvable limiting cases and several other known approximate methods.

Considering our multi-band electronic self energy ansatz, we proceed to perform a model calculation of two weakly hybridized bands on a simple cubic (sc) lattice where the terms in the (2 x 2) hopping matrix, $\mathbf{\tilde{\epsilon}}(\mathbf{k})$, are taken using the sc Bloch density of states (DOS) in the tight binding approximation [14]. We assume the bandwidth (W) of both the bands, i.e intra-band transfer energy to be 1.0 eV while that for inter-band to be 0.10 eV. The center of gravity of one of the free Bloch band is chosen to be energy zero while for the other it is taken as 0.25 eV.

In order to study the electronic correlations, one examines the effect of a test electron by creating (or annihilating) it in an empty (or filled) band. In our case, we first annihilate an electron from the completely...
filled band. Thus, removal of ↓(↑) electron will create a ↑(↓) hole which will give insight into the study. The correlation effects are studied by calculating the electronic self energy. But, apart from electronic sub-system, we also have the magnetic sub-system. The exchange coupling between the itinerant electron and localized spins adds up to the correlation effects as they produce spin-flip transitions and Ising like interactions in addition to the kinetic energy.

Fig. 1 describes the weak coupling behavior, JS ≪ W. The calculated density of states (DOS) are shown for the parameters: J=0.2 eV, S=1.5 and different values of magnetization, \( \langle S^z \rangle \) = 1.0, 2/3, 1/3 and 0.0 which are represented as thick solid line, dotted line, broken line and double-dotted broken line, respectively. The exact solution, ferromagnetically saturated semiconductor, is represented as stars and it is found to coincide with results of \( \langle S^z \rangle = S \).

Fig. 2 The same as Fig. 1 except for J=0.5.

Fig. 3 The same as Fig. 1 except for J=1.0.

At T=0 K and fully occupied bands, the removal of a ↓ electron (i.e. creation of a ↑ hole) produces a stable quasi-particle since the ↑ hole has no chance to flip its spin with the ferromagnetically saturated spin (⇑) sub-system. The imaginary part of the self energy vanishes indicating infinite lifetimes. The situation is different for the removal of an ↑ electron (i.e, creation of ↓ hole) as the ↓ hole can exchange its spin with the ferromagnetically saturated spin sub-system and have finite lifetime. It can emit a magnon and become a ↑ hole provided there exist ↑ hole states which can be occupied after spin-flip process. These
are the scattering states which occupy the same energy regions as of the $\uparrow$ spectrum. The scattering states become more distinct with increasing coupling strength as seen in Fig. 2 and Fig. 3. The other possibility for the $\downarrow$ hole to exchange its spin could be by repeated emission and absorption of magnons, thus forming a quasi-particle called magnetic polaron.

However, at finite temperatures, the spin sub-system is no longer perfectly aligned. There are magnons in the system that can be absorbed by the itinerant charge carriers. As seen from the figures, at finite temperatures the spectral weight gets redistributed due to spin flip term in the exchange interaction with deformations in the density of states. In the limit $T \to T_c (\langle S^2 \rangle \to 0)$ the induced spin asymmetry is removed.

3 PHYSICAL PROPERTIES : EuS

In this section, we study the electronic correlations in the $3p$ valence bands of ferromagnetic semiconductor EuS by combining the multi-band self energy ansatz for the many body part along with the first principles TB-LMTO bandstructure calculations.

EuS crystallizes in a rocksalt structure with lattice constant, $a=5.95 \text{ Å}$. Each Eu$^{2+}$ ion has twelve nearest and six next nearest Eu-neighbors and they occupy lattice sites of a fcc structure. The magnetism in EuS is due to the half-filled $4f$ shell of Eu$^{2+}$ and its magnetic properties are well described using the Heisenberg model with the ferromagnetic transition temperature, $T_c=16.54 \text{ K}$. In this material, the nearest neighbor exchange interaction is ferromagnetic while the next nearest neighbor is anti-ferromagnetic.

In order to have the single particle excitation energies, i.e the hopping matrices, and all the interactions which are not directly included in our Hamiltonian, we perform the TB-LMTO bandstructure calculations using the program of Anderson [15, 16].

Fig. 4 shows the spin-dependent bandstructure (LSDA) of the valence bands of EuS. In TB-LMTO, the original Hamiltonian is transformed to a tight-binding Hamiltonian containing only the nearest neighbor correlations. The evaluation is restricted only to $3p$ bands. There are some difficulties which arise due to the strongly localized character of $4f$ levels and in order to avoid such difficulties, we consider the seven $4f$ electrons as core electrons, since these electrons enter our model only as localized moments.

The LDA-density of states is displayed in Fig. 5. Assuming that the LDA treatment of the ferromagnetism is quite compatible with the Stoner (mean field) picture, the $T=0$ splitting amounts to $\Delta E=JS$. On taking the centers of gravity of the DOS for both the spins and along with the above assumption, the exchange splitting amounts to $\Delta E=0.1512 \text{ eV}$ which results in the value for the exchange coupling strength as $J=0.0432 \text{ eV}$ where the spin value, $S=3.5$. One can also calculate the exchange coupling by taking the energy difference of the upper edge shift between both the spins which gives $J=0.0253 \text{ eV}$ or calculate the mean value of the spin polarized energy difference taken along each k-points in the first Brillouin zone which gives $J=0.0529 \text{ eV}$. It was found that the coupling strength obtained by center of gravity approach, reflects more correlation effects as was shown in the previous work [5] for the conduction bands of EuS.

The single particle output obtained from the bandstructure calculations are in the form of Hamiltonian
and overlap matrix, posing a generalized eigenvalue problem to be solved. In order to employ such matrices as an input for the many body calculations, one has to perform a Cholesky decomposition so as to reduce the generalized problem to an eigenvalue problem. Using such an approach, one can factorize the Hamiltonian matrices and then obtain new Hamiltonian matrices using overlap matrices, which can be used directly as hopping integrals, \( \hat{\epsilon}(\mathbf{k}) \). We use the multi-band self energy ansatz eq. (14) to compute the Green function eq. (6) and therewith calculate the spectral densities eq. (12) and densities of states eq. (13).

Fig. 6 represents the quasi-particle band-structure for some high-symmetry directions in the first Brillouin zone. The degree of blackening measures the magnitude of the spectral function. Correlation effects are clearly visible along many parts, especially along the center of the valence band. As seen in the ↑

\[ \langle S_z \rangle \]

\[ \hat{\epsilon}(\mathbf{k}) \]

\[ \text{Fig. 5} \] Spin-dependent density of states of 3\( p \) bands of EuS. Using the center of gravity of the bands, the exchange splitting amounts to \( \Delta E = 0.1512 \) eV.

\[ \text{Fig. 6} \] Spin-dependent quasi-particle bandstructure of 3\( p \) valence bands of EuS for different values of magnetization \( \langle S_z \rangle \).
spectrum even at $T=0$ K ($\langle S_z \rangle = 1$), parts of the dispersions are washed out showing lifetime effects due to correlation in terms of magnon emission and re-absorption with simultaneous spin-flips as explained earlier. But at the same temperature, the $\downarrow$ spectrum shows sharp lines indicating infinite lifetime as expected. While at finite temperature ($\langle S_z \rangle = 0.5$), the finite lifetimes appear in case of both the spin spectra as the ferromagnetically saturated spin system is not perfectly aligned giving rise to magnons which can be absorbed by the itinerant charge carriers. At transition temperature ($\langle S_z \rangle = 0.0$), the spin asymmetry is removed. Strong temperature dependent correlation effects are seen mainly along the W-L directions.

In order to have a closer look at the correlations, the spin and $k$-dependent spectral densities are plotted at some high-symmetry points (W,L,X) in the first Brillouin zone. It can be compared with the angle-resolved photoemission experiments and for this purpose we propose that an experiment be performed.

As seen in Fig. 7, well defined quasi-particle peaks appear with an additional spin split below $T_c$. The exchange splitting collapses for $T \rightarrow T_c$ and the quasi-particle damping increases with increasing temperature. Similar explanations hold for the other high-symmetry points (Fig. 8 and Fig. 9). The correlations are clearly observed at the W-point. With increasing temperature, there’s a strong damping as seen along the energy spectrum. Interestingly, the same W-point remains the point of discussion in case of the conduction band calculations of EuS [5].

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{X_point.png}
\caption{Spectral density at X - point.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{W_point.png}
\caption{Spectral density at W - point.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{L_point.png}
\caption{Spectral density at L - point.}
\end{figure}
The quasi-particle density of states (Q-DOS) is plotted in Fig. 10. As observed, due to weaker exchange coupling, the appearance of polaronlike quasi-particle branches are less likely in the real material calculation. The temperature influence on the spectrum is seen in terms of strong deformations, mostly at the center, and in terms of shifts. While the $k$-dependent spectral densities refers to the angle resolved photoemission, the Q-DOS can be considered as the angle integrated part.

![Fig. 10 Quasi-particle density of states (Q-DOS) of the 3p valence bands of EuS.](image)

4 SUMMARY and CONCLUSION

In this paper, we have studied the effects of electronic correlation on the 3p valence bands of the ferromagnetic semiconductor EuS. We started with multi-band Kondo lattice Hamiltonian which is sufficient enough to explain the necessary physics. Using Green function approach, we try to evaluate the Hamiltonian. We put forward an Interpolating Self energy Ansatz (ISA) for the multi-band situation and obtain the solution, i.e the required Green function, to predict some physical properties. In order to test the theory, we perform model calculations and interesting features are highlighted. For two weakly hybridized bands assuming free Bloch densities of states on a simple cubic lattice, polaron-like and scattering states are observed for intermediate and strong coupling strengths. Strong temperature dependent correlation effects are noticed in the form of deformations and shifts in the energy spectrum. A non-trivial exactly solvable limiting case of the model is correctly reproduced thus confirming the proposed multi-band self energy ansatz.

Such a self energy ansatz, which amounts to the many body interactions, is later on combined with the first principles TB-LMTO bandstructure calculations for calculating the properties of real materials. The bandstructure output in the form of hamiltonian and overlap matrices of the 3p valence band electrons of EuS, serve as an input in the form of hopping integrals for the many body calculations. The exchange coupling strength is obtained from the LDA bandstructure calculations as a result of energy difference in the center of gravities of the spin polarized density of states. With these parameter inputs, physical properties like quasi-particle spectral densities (Q-SD) and densities of states (Q-DOS) are estimated for different values of magnetization. One can also obtain other interesting physical quantities like the lifetime or the effective mass of the quasi-particles but it is not planned for the present article. While, in one of the previous work [17], emphasis was laid upon calculating the spin flip probabilities which exhibit the lifetime effects. These quantities were calculated using the time-dependent spectral density which were used to express the spin polarization of the field emitted electrons thus highlighting the issue of spin filter effects of the europium chalcogenides. Eventually, as a consequence of our present calculations, the temperature dependent correlation effects are observed at the center of band and mainly in the W-L direction. For the
sake of comparison, we propose and spin-dependent ARPES to be performed on the valence bands of EuS.

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A Case of ferromagnetically saturated semiconductor

In the main text of this paper, we mentioned one limiting approach of the multi-band model namely the ferromagnetically saturated semiconductor which exhibits the quasi-particle called magnetic polaron. It is that quasi-particle where a bare electron (or hole) is dressed by a virtual cloud of magnons. In this section, we present the analytical result of it. We are interested in finding a solution for the model at T=0 with ferromagnetically saturated spin sub-system ($\langle S^z \rangle = S$) and for fully occupied bands and $\sigma = \uparrow, \downarrow$.

In such situation, the Ising-like higher order Green function eq. (8a) becomes;

$$\Gamma_{lm\sigma}^{\mu\nu}(E) = S\Gamma_{lm\sigma}^{\mu\nu}(E)$$

(15)

Now, let us consider: a) $\sigma = \uparrow$ and b) $\sigma = \downarrow$ and try to evaluate the self energy in both the cases.

a) For $\sigma = \uparrow$, the equation of motion for the spin-flip function

$$F_{lm\sigma}^{\mu\nu}(E) = \langle \langle S_{l^{-}}^{\downarrow} c_{l\mu\sigma}; c_{lm\sigma}^{\dagger} \rangle \rangle_E$$

reads as follows,

$$E F_{lm\downarrow}^{\mu\nu}(E) = \langle \langle S_{l^{-}}^{\downarrow} c_{l\mu\downarrow}; H \rangle \rangle_E$$

which takes the form as given below yielding higher order Green functions,

$$EF_{lm\sigma}^{\mu\nu}(E) = \sum_{p\gamma} T_{lp\gamma}^{\mu\nu} \langle \langle S_{l^{-}}^{\downarrow} c_{p\gamma\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E - \frac{J}{2} \{ \langle \langle S_{l^{-}}^{\downarrow} S_{l^{-}}^{\dagger} c_{l\mu\uparrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E - \langle \langle S_{l^{-}}^{\downarrow} S_{l^{-}}^{\dagger} c_{l\mu\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E \}
\sum_{\lambda} \{ \langle \langle S_{l^{-}}^{\downarrow} c_{l\lambda\sigma} c_{l\lambda\sigma} c_{l\mu\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E \} - 2 \{ \langle \langle S_{l^{-}}^{\downarrow} c_{l\lambda\uparrow} c_{l\lambda\uparrow} c_{l\mu\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E \}$$

The higher order Green functions resulting from the spin-flip equation of motion can be evaluated exactly for the case of fully occupied bands and at T=0,

$$\langle \langle S_{l^{-}}^{\downarrow} S_{l^{-}}^{\dagger} c_{l\mu\sigma}; c_{lm\sigma}^{\dagger} \rangle \rangle_E = 0$$

(16a)

$$\langle \langle S_{l^{-}}^{\downarrow} S_{l^{-}}^{\dagger} c_{l\mu\downarrow}; c_{lm\uparrow}^{\dagger} \rangle \rangle_E = SF_{lm\uparrow}^{\mu\nu}(E)$$

(16b)

$$\langle \langle S_{l^{-}}^{\downarrow} (c_{l\lambda\uparrow} c_{l\lambda\uparrow} - c_{l\lambda\downarrow} c_{l\lambda\downarrow}) c_{l\mu\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E = \delta_{\mu\lambda} F_{lm\downarrow}^{\mu\nu}(E)$$

(16c)

$$\langle \langle S_{l^{-}}^{\downarrow} c_{l\lambda\downarrow} c_{l\lambda\sigma} c_{l\mu\downarrow}; c_{lm\sigma}^{\dagger} \rangle \rangle_E = -\delta_{\mu\lambda} S G_{lm\downarrow}^{\mu\nu}(E)$$

(16d)

On substituting the eq. (16) in the spin-flip equation of motion and taking the Fourier transform we get;

$$E \frac{J S}{2} F_{k,k',q,q'}^{\mu\nu}(E) = \sum_{\lambda} \epsilon^{\lambda\lambda} (k\cdot q) F_{k,k',q,q'}^{\lambda\lambda}(E) - \frac{J}{2N} \sum_{t} F_{k,k',t,t}^{\mu\nu}(E) - \frac{J S}{\sqrt{N}} \hat{G}_{k}^{\mu\nu}(E)$$

and in the matrix form, it can be written as follows

$$[E - \frac{J S}{2} \hat{I} - \hat{c}(k\cdot q)] \hat{F}_{k,k',q,q'}^{\mu\nu}(E) = -\frac{J}{2N} \sum_{t} \hat{F}_{k,k',t,t}^{\mu\nu}(E) - \frac{J S}{\sqrt{N}} \hat{G}_{k}^{\mu\nu}(E)$$

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Let us now define the effective Green function,
\[ \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) = \frac{1}{N} \sum_{\mathbf{q}} \left( (E - \frac{JS}{2}) \hat{I} - \hat{c}(\mathbf{k} - \mathbf{q}) \right)^{-1} \]
which upon substituting in the matrix form of the spin-flip equation of motion implies,
\[ \frac{1}{\sqrt{N}} \sum_{\mathbf{q}} \hat{F}_{\mathbf{k}, \mathbf{k}-\mathbf{q}, \sigma}(E) = -JS \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \hat{I} + \frac{J}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \right)^{-1} \hat{G}_{\uparrow}(E) \]
(17)

Now, if we consider the Fourier transform of eq. (7) and substitute eq. (17) and eq. (15) in it, we get the result for the Green function as
\[ [(E + \frac{JS}{2}) \hat{I} - \hat{c}(\mathbf{k})] \hat{G}_{\mathbf{k}}(E) = \hbar \hat{I} + \frac{J}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \hat{I} + \frac{J}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \right)^{-1} \hat{G}_{\uparrow}(E) \]
i.e.,
\[ \hat{G}_{\mathbf{k}}(E) = \hbar \hat{I}[(E + i0^+) \hat{I} - \hat{c}(\mathbf{k})] + \frac{JS}{2} \hat{I} - \frac{J^2}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \hat{I} + \frac{J}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \right)^{-1} \hat{G}_{\uparrow}(E) \]
(18)
On comparing eq. (9) and eq. (18) we get the self energy ansatz as
\[ \hat{\Sigma}_{\uparrow}(E) = -JS \hat{I} \hat{G}_{\mathbf{k}}(E) = \frac{JS}{2} \hat{I} + \frac{JS}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \hat{I} + \frac{J}{2} \hat{G}_{\uparrow}^{\text{eff}}(E - \frac{JS}{2}) \right)^{-1} \hat{G}_{\uparrow}(E) \]
(19)
b) For \( \sigma = \downarrow \), the spin-flip function vanishes;
\[ F_{\mu\nu}^{\sigma\sigma}(E) = \langle \langle S_{\downarrow}^{\sigma} c_{\mu\sigma}; c_{\nu\sigma}^{\dagger} \rangle \rangle E = 0 \]
The equation of motion for the Green function, i.e. eq. (7) reduces to,
\[ (E - \frac{JS}{2}) G_{\mu\nu}^{\sigma\sigma}(E) = \hbar \delta_{\mu\nu} + \sum_{\gamma} T_{\mu\gamma}^{\sigma\sigma} \hat{G}_{\gamma\nu}^{\sigma\sigma}(E) \]
And upon taking Fourier transform we have,
\[ (E - \frac{JS}{2}) \hat{G}_{\mathbf{k}\downarrow}(E) = \hbar \delta_{\mu\nu} + \sum_{\gamma} e^{\gamma\mathbf{k}}(\mathbf{E}) \hat{G}_{\gamma\nu}^{\sigma\sigma}(E) \]
which can be written in matrix form
\[ \hat{G}_{\mathbf{k}}(E) = \hbar \hat{I}[(E - \frac{JS}{2}) \hat{I} - \hat{c}(\mathbf{k})]^{-1} \]
(20)
Thus, the self energy becomes;
\[ \hat{\Sigma}_{\downarrow}(E) = -\frac{JS}{2} \hat{I} \]
(21)
As seen, eq. (19) and eq. (21) give the spin-dependent form of the self energy which for the case of fully occupied bands and ferromagnetically saturated spin sub-system can be written down as follows;
\[ \hat{\Sigma}_{\sigma}(E) = -\frac{JS_{\sigma} \sigma}{2} \hat{I} + \frac{JS_{\sigma}(z_{\sigma} + 1)}{4} \hat{G}_{\sigma}^{\text{eff}}(E - \frac{JS_{\sigma}}{2}) \hat{I} + \frac{J}{2} \hat{G}_{\sigma}^{\text{eff}}(E - \frac{JS_{\sigma}}{2}) \right)^{-1} \hat{G}_{\sigma}(E) \]
(22)

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