Quantum effects in the quasiparticle structure of the ferromagnetic Kondo lattice model

D. Meyer†, C. Santos and W. Nolting
Lehrstuhl Festkörpertheorie, Institut für Physik, Humboldt-Universität zu Berlin, Invalidenstr. 110, 10115 Berlin, Germany

Abstract. A new “Dynamical Mean-field theory” based approach for the Kondo lattice model with quantum spins is introduced. The inspection of exactly solvable limiting cases and several known approximation methods, namely the second-order perturbation theory, the self-consistent CPA and finally a moment-conserving decoupling of the equations of motion help in evaluating the new approach. This comprehensive investigation gives some certainty to our results: Whereas our method is somewhat limited in the investigation of the $J < 0$-model, the results for $J > 0$ reveal important aspects of the physics of the model: The energetically lowest states are not completely spin-polarized. A band splitting, which occurs already for relatively low interaction strengths, can be related to distinct elementary excitations, namely magnon emission (absorption) and the formation of magnetic polarons. We demonstrate the properties of the ferromagnetic Kondo lattice model in terms of spectral densities and quasiparticle densities of states.

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1. Introduction

The Kondo model and its periodic extension, the Kondo lattice model (KLM), which describe spin-exchange interaction between a localized spin or a system of localized spins, respectively, and a band of itinerant electrons, has been subject of intense theoretical studies in the past [1, 2, 3, 4, 5, 6]. This model has been applied to a variety of different problems in solid-state physics using both a ferromagnetic and antiferromagnetic coupling constant $J$.

The model with $J < 0$ is the one originally known as Kondo lattice model or simply Kondo model in its non-periodic form with a single impurity spin in the system. It was used by Kondo to explain the unusual temperature behavior of the resistivity of magnetic impurities in non-magnetic hosts [4]. The negative spin-exchange interaction can be derived from the hybridization of a correlated “atomic” level with a conduction band, the situation described by the Anderson model [7, 8]. In the limit of a low-lying half-filled atomic level and strong correlations, the Anderson model can be mapped onto the Kondo model with a negative exchange constant $J$. The Kondo lattice model is still subject to much theoretical work, the main objective is the understanding of the unusual physical behavior found in Heavy-Fermion materials [8].

† present Address: Department of Mathematics, Imperial College, London, United Kingdom
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A model with identical operator structure in the Hamiltonian, but with positive exchange constant has been known in the literature for a long time by many different names (double exchange model, s-d model, s-f model, . . . ) [1, 2, 3, 4]. For clarity, we will refer to this model in the following as ferromagnetic Kondo lattice model. The model with ferromagnetic exchange has to be understood as an effective one. The origins of the exchange with \(J > 0\) are found in the interband Coulomb correlations [3]. This situation is believed to dominate the physical properties of important systems such as the magnetic semiconductors [10] (EuX; X = O, S, Se, Te), the diluted magnetic semiconductors [11] (Cd\(_{1-x}\)Mn\(_x\)Te, Hg\(_{1-x}\)Fe\(_x\)Se), and the "local moment" metals [12] (Gd, Dy, Tb). To these problems, the ferromagnetic KLM was successfully applied [13, 14, 15]. Recently, this variant of the KLM has gained a lot of interest with the discovery of the colossal magnetoresistance (CMR) materials [10, 17]. In these materials, typically manganese oxides with perovskite structure (La\(_{1-x}\)(Ca,Sr)\(_x\)MnO\(_3\)), the double-exchange model [1, 2] has been successfully applied to explain the origin of ferromagnetic order and is expected to be a good starting point to investigate the resistivity anomalies [14]. This double-exchange model, however, is nothing else than the Kondo lattice model with ferromagnetic (positive) exchange constant in the strong coupling limit. In the CMR materials, the localized \(S = \frac{3}{2}\)-spin of the model represents the more or less localized manganese 3\(d\)-\(t_{2g}\) electrons, whereas the conduction band is formed by the \(e_g\) electrons. The interband-exchange interaction is nothing else but the intra-shell Hund's rule coupling. Since the 3\(d\)-\(e_g\) electrons of the manganese form a relatively narrow band (theoretical results from band-structure calculations: 1–2 eV [19, 20, 21] and experimental estimates: 3–4 eV [22, 23]) and Hund's coupling is assumed to be large, the model has to be taken in the intermediate to strong coupling regime. There are few estimates about the value of the interaction constant in the literature, e.g. \(J \approx 1\) eV [19, 24], but these are challenged as to be too small [25]. Most theoretical papers of the last years concerned with colossal magnetoresistance assume classical spins \(S \to \infty\) [26]. Although it is true that the important energy scale is \(J S\), there are much more implications of \(S \to \infty\) that are not justified in the strong-coupling limit for a \(S = \frac{3}{2}\) system. In several papers, it was stated that "... the \(e_g\) electrons are oriented parallel to the \(t_{2g}\) spins." [28] or equivalently "... so one only need consider configurations with \(e_g\) electrons parallel to core spins." [25]. We will show below using exact results as well as several well-defined approximation methods, that for \(S = \frac{3}{2}\), there is a considerable amount of spin-\(\downarrow\) spectral weight located in the main region of the spin-\(\uparrow\) states even for large interaction strengths. The assumption of a half-metallic state [30], made in the two citations above can therefore never be met in the KLM with quantum spins and is merely an effect of the (unphysical) limit of "classical" spins. The recently discussed half-metallic behaviour of the manganites [31] must have a different origin.

However, for the opposite sign of \(J\), exactly the assumed effect happens in the strong-coupling limit: the lowest-lying excitations in the conduction band density of states will be purely spin-\(\downarrow\). This already implies that results for the Kondo lattice model with \(J > 0\) and \(J < 0\) cannot simply be reverted into the respective other case. The change of sign changes the whole physics of the system. For \(J < 0\) an antiparallel ("antiferromagnetic") alignment of the conduction band spin and the localized spin lowers the internal energy. For a sufficient band filling, this tends to a screening of the local moments by conduction electrons, well-known from the Kondo effect that
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refers to a single magnetic impurity in a conduction electron sea. From this, the name “Kondo lattice model” was originally derived for the $J < 0$ case.

We will further show that already for comparatively low interaction strengths the spin-exchange interaction alone leads to an opening of a gap in the density of states. This extraordinary correlation effect could give hints to the explanation of a recently discovered pseudogap in the manegese oxides [32].

To prove our claims already laid out so far, we will first review two important non-trivial exactly solvable limiting cases of the Kondo lattice model in Sec. 2. The first is the zero-bandwidth limit (“atomic limit”) where the bandwidth of the conduction band is set to $W = 0$ [33]. The second exactly solvable limiting case is the so-called ferromagnetically saturated semiconductor [34, 35, 36, 37, 38, 39, 40, 41, 42, 13, 14]. This is essentially the zero-temperature limit of the model with vanishing electron density and fully aligned spin system. In this limit, striking correlation effects can be observed and discussed. These limiting cases will already give clear evidence to our propositions made above. In Sec. 3 we will present a new dynamical mean-field theory (DMFT)-based approach for the KLM with $S = \frac{1}{2}$ spins. To circumstantiate our theory, we will introduce three more approximation schemes which also keep the spin as a quantum variable, not relying on the classical spin limit. The first will be a second-order perturbation theory (SOPT) for the KLM based on the projector operator formalism [43, 44]. The self-consistent CPA (coherent potential approximation) is a straightforward extension to the well-known CPA for the KLM [45, 6, 46, 47, 48]. It starts from the zero-bandwidth limit discussed before. The third approximation method is a moment-conserving decoupling procedure for the equation of motion of the single-electron Green function. This approximation scheme continuously evolves from the exactly solvable limit of the ferromagnetically saturated semiconductor. It will be called Moment-Conserving Decoupling Approximation (MCDA). The comparison of the results obtained by these three methods and our DMFT scheme, each of which starts from a different limit allows to evaluate the range of applicability of the new approach, and to select the most trustworthy common features of all methods to gain a reliable picture of the physics of the ferromagnetic KLM.

2. The Kondo lattice model and its many-body problem

2.1. Hamiltonian

The Kondo-lattice model (or $s$-$f$ model) traces back the characteristic features of the underlying physical system to an interband exchange coupling of itinerant conduction electrons to (quasi-) localized magnetic moments described by the following model Hamiltonian [3, 3]

$$H = H_s + H_{sf} + (H_U + H_{ff}) =$$

$$= \sum_{ij\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} - J \sum_i \sigma_i \cdot S_i + \left( \frac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} - \sum_{i,j} \hat{J}_{ij} S_i \cdot S_j \right)$$

$c_{i\sigma}^\dagger$ ($= \frac{1}{\sqrt{\mathcal{N}}} \sum_k c_{k\sigma}^\dagger e^{-i k \cdot R_i}$) and $c_{i\sigma}$ are, respectively, creation and annihilation operators of a band electron being specified by the lower indices. The hopping integrals $T_{ij}$ are connected by Fourier transformation to the single-electron Bloch energies $T_{ij} = \frac{1}{\mathcal{N}} \sum_k \epsilon(k) e^{i k \cdot (R_j - R_i)}$. 


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The interband (sf) exchange with coupling strength $J$ is taken as an intra-atomic interaction between the conduction electron spin $\sigma_i$ and the localized magnetic moment represented by the spin operator $S_m$. For practical reasons it is sometimes convenient to use the second quantization representation of the band electron spin $\sigma_i$ which leads to the following form of the interband-interaction term:

$$H_{sf} = -\frac{1}{2}J \sum_{i,\sigma} \left( z_\sigma S_\sigma^z n_{i\sigma} + S_\sigma^z c_{i \sigma}^\dagger c_{i \sigma}^\dagger \right)$$ (2)

Here we have used the abbreviations $n_{i\sigma} = c_{i \sigma}^\dagger c_{i \sigma}$, $z_{\sigma(\pm)} = +1(-1)$ and $S_\sigma^z = S_\sigma^z + iz_\sigma S_\sigma^y$. The first term in (2) describes an Ising-like interaction between the z-components of the spin-operators, while the second term incorporates spin exchange processes between the localized and the itinerant system.

The last two terms are an extension to the original model: $H_{ff}$ leads to the 'correlated Kondo lattice model', it introduces correlations between the conduction electrons in form of a 'Hubbard-type' interaction. We will include this term in some parts of the discussion below. The second term, $H_{ff}$ represents a direct spin-exchange between localized moments on different lattice sites. Although the sf exchange can lead to an effective RKKY interaction between the spins for non-vanishing band occupation, a "superexchange"could also be included. In case of an empty conduction band, this term becomes essential as source of magnetic order. $J_{ij}$ are the superexchange integrals. We state once more that the original Kondo-lattice model (or sf-model) is defined by $H = H_s + H_{sf}$, only. The additional terms in Eq. (3) are used as soon as physical requirements do not allow to neglect them.

If we are mainly interested in the conduction electron properties then the single-electron Green function $G_{ij\sigma}(E) = \langle \langle c_{i\sigma}; c_{j\sigma}^\dagger \rangle \rangle_E$ is of primary interest. Its equation of motion reads for the correlated KLM

$$\sum_m \left( E \delta_{im} - T_{im} \right) G_{m\sigma\sigma}(E) = \hbar \delta_{ij} - \frac{1}{2} J \left( z_\sigma I_{ii,j\sigma}(E) + F_{ii,j\sigma}(E) \right) + UT_{iii,j\sigma}(E)$$ (3)

The two types of interaction terms in (3) let appear the “spinflip function” $F_{im,j\sigma}(E) = \langle \langle S_i^z \sigma_m \sigma_i; c_{j\sigma}^\dagger \rangle \rangle_E$ and the “Ising function” $I_{im,j\sigma}(E) = \langle \langle S_i^z \sigma_m \sigma_i; c_{j\sigma}^\dagger \rangle \rangle_E$, while the “Hubbard-function” $\Gamma_{im,j\sigma}(E) = \langle \langle c_{j\sigma}^\dagger \sigma_m \sigma_i; c_{j\sigma}^\dagger \rangle \rangle_E$ comes into play only when the “Hubbard-interaction” (last term in Eq. (3)) is switched on.

The three “higher” Green functions on the right-hand side of Eq. (3) prevent a direct solution of the equation of motion. A formal solution for the Fourier-transformed single-electron Green function,

$$G_{k\sigma}(E) = \langle \langle c_{k\sigma}^\dagger; c_{k\sigma}^\dagger \rangle \rangle_E = \frac{\hbar}{E - \epsilon(k) - \Sigma_{k\sigma}(E)}$$ (4)

defines the electronic selfenergy $\Sigma_{k\sigma}(E)$ by the ansatz $\langle \langle [c_{k\sigma}; H - H_s]_{-}; c_{k\sigma}^\dagger \rangle \rangle_E = \Sigma_{k\sigma}(E)G_{k\sigma}(E)$ For the general case $\Sigma_{k\sigma}(E)$ cannot be determined rigorously.

Before introducing some approaches to the not exactly solvable many-body problem of the KLM let us discuss in the next sections two rather illustrative limiting cases which can help to test the unavoidable approximations.

2.2. The zero-bandwidth limit

Let us assume that the arbitrarily filled conduction band is shrinked to an $N$-fold degenerate level $T_0$: $\epsilon(k) \rightarrow T_0 \forall k$. Nevertheless, we consider the f-spin system as
collectively ordered for \( T < T_c \) by any direct or indirect exchange interaction. In this case, the hierarchy of equations of motion decouples exactly and can rigorously be solved [33]. The resulting energies and respective spectral weights are

\[
\begin{align*}
E_1 &= T_0 - \frac{1}{2} JS \quad \alpha_{1\sigma} = \frac{1}{2S+1} \{ S + 1 + z_\sigma \langle S^2 \rangle + \gamma_{-\sigma} - z_\sigma \Delta_{-\sigma} - \langle S + 1 \rangle \langle n_{-\sigma} \rangle \} \\
E_2 &= T_0 + \frac{1}{2} J(S + 1) \quad \alpha_{2\sigma} = \frac{1}{2S+1} \{ S - z_\sigma \langle S^2 \rangle - \gamma_{-\sigma} + z_\sigma \Delta_{-\sigma} - S \langle n_{-\sigma} \rangle \} \\
E_3 &= T_0 + U - \frac{1}{2} J(S + 1) \quad \alpha_{3\sigma} = \frac{1}{2S+1} \{ S \langle n_{-\sigma} \rangle - \gamma_{-\sigma} + z_\sigma \Delta_{-\sigma} \} \\
E_4 &= T_0 + U + \frac{1}{2} JS \quad \alpha_{4\sigma} = \frac{1}{2S+1} \{ (S + 1) \langle n_{-\sigma} \rangle + \gamma_{-\sigma} - z_\sigma \Delta_{-\sigma} \}
\end{align*}
\]

The “Hubbard-U” in \( E_3 \) and \( E_4 \) indicates that these excitations are bound to a double occupancy of the respective lattice site. \( E_1 \) and \( E_2 \) appear when our “test electron” enters an empty site. If it orients its spin parallel to the local spin-saturated semiconductor [34, 35, 36, 37, 38, 39, 40, 41, 42, 13, 14]. In this case, the energy \( E_1 \) is needed. In case of an antiparallel spin orientation a triplet or a singlet state is formed. The first requires the energy \( E_2 \), the second \( E_2 \). The latter is therefore two-fold degenerate. The spectral weights are, contrary to the energy levels, strongly dependent on the magnetization state of the \( f \)-system and the band filling. For a complete solution one needs the average occupation number \( \langle n_{-\sigma} \rangle \) and the mixed correlation functions \( \gamma_{\sigma} = \langle S^\tau c_{i-\sigma}^\dagger \rangle \) and \( \Delta_{-\sigma} = \langle S^\tau n_{i\sigma} \rangle \). The evaluation can selfconsistently be done by use of the spectral theorem for the Green functions \( G_{i\sigma}(E) \), \( L_{i\sigma}(E) \) and \( F_{i\sigma}(E) \) (cf. Ref. [33]). It is interesting to observe that in any case from the four poles only three do appear. For less than half-filled bands and \( J > 0 \) (\( J < 0 \)) \( \alpha_{3\sigma} \) \( (\alpha_{4\sigma}) \) vanishes, and for more than half-filled \( \alpha_{3\sigma} \) \( (\alpha_{1\sigma}) \) does. It should be mentioned that the spectral weights \( \alpha_{i\sigma} \) do not explicitly depend on the coupling constants \( J \) and \( U \). That means, on the one side, that even for \( U = 0 \) the \( s-f \) interaction produces a splitting into four not coinciding quasiparticle levels. On the other hand, there is a striking dependence of \( \Delta_{-\sigma} \) and \( \langle n_{-\sigma} \rangle \) on the sign of the \( s-f \) coupling. That transfers to the spectral weights giving them some indirect dependence on \( J/J \). For \( J > 0 \) and \( J < 0 \) the order of the energy levels is different resulting via the spectral theorem in different correlation functions. Note that the mentioned dependence on \( J \) concerns only the sign of \( J \). The spectral weights are not influenced by the absolute value \( |J| \).

2.3. The ferromagnetically saturated semiconductor

There is another very instructive limiting case that can be treated rigorously. It concerns the situation of a single electron in an otherwise empty conduction band at \( T = 0 \), when the local moment system is ferromagnetically saturated. In this case the Coulomb interaction is meaningless, the “Hubbard-function” \( \Gamma_{i\sigma,j\sigma}(E) \) is identical to zero. In the zero-bandwidth limit, discussed in the last section, for the \( \uparrow \)-spectrum all spectral weights disappear except for \( \alpha_{1\uparrow} = 1 \), while for the \( \downarrow \)-spectrum the levels \( E_1 \) and \( E_2 \) survive with \( \alpha_{1\downarrow} = \frac{1}{2S+1} \) and \( \alpha_{2\downarrow} = \frac{2S+1}{2S+1} \).

For finite bandwidth the mentioned special case is that of a ferromagnetically saturated semiconductor [33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 13, 14]. In this case, the spin-\( \uparrow \) quasiparticle density of states \( \rho_\uparrow(E) \) is only rigidly shifted compared to the “free” Bloch density of states.

\[
\rho_\uparrow(E) \xrightarrow{T=0; n=0} \rho_0(E + \frac{1}{2} JS)
\]
Consequently, the quasiparticle dispersion is undeformed with respect to the Bloch energies, $E_\uparrow(k) \rightarrow \epsilon(k) - \frac{1}{2}JS$. The $\downarrow$-spectrum is more complicated because a $\downarrow$-electron has several possibilities to exchange its spin with the antiparallel $f$ spins. Therefore, the $\sigma = \downarrow$-spinflip function is not at all trivial. However, its equation of motion decouples exactly, producing a closed system of equations which can be solved after Fourier transformation for the single-electron Green function. The corresponding selfenergy $\Sigma_{k\downarrow}(E)$ reads:

$$\Sigma_{k\downarrow}(E) = \frac{1}{2}JS \left( \frac{1 + \frac{1}{2}JB_k(E)}{1 - \frac{1}{2}JB_k(E)} \right)$$

$$B_k(E) = \frac{\hbar}{N} \sum_q \left( E - \epsilon(k - q) + \frac{1}{2}JS - \hbar\omega(q) \right)^{-1}$$

Figure 1. Spin-$\downarrow$ spectral densities (quasiparticle bandstructures) of the ferromagnetically saturated semiconductor for $S = \frac{1}{2}$ and $J$ as indicated along several symmetry directions. The left (right) column displays the $J < 0$ ($J > 0$) case, the top-most picture shows the interaction-free spectral density.
\( \hbar \omega(q) \) are the spin wave energies following from the Heisenberg exchange \( H_{ff} \) (cf. Eq. (6)), \( \hbar \omega(q) = 2S \left( \hat{J}(q = 0) - \hat{J}(q) \right) \). \( \hat{J}(q) \) is the Fourier transform of the exchange integral \( \hat{J}_{ij} \). Usually the spin wave energies will be smaller by about two orders of magnitude than other typical energies of the system as the exchange constant \( J \) or the Bloch bandwidth \( W \). As a general result the spectral density \( S_{k\downarrow}(E) \) consists of two structures corresponding to special elementary excitation processes of the \( \downarrow \) electron. There is a rather broad structure built up by “scattering states” which result from magnon emission by the original \( \downarrow \) electron. Thereby the excited electron reverses its spin becoming a \( \uparrow \) electron. Such a process is possible only if there are \( \uparrow \) band states within reach for the original \( \downarrow \) electron to land after the spinflip. The scattering states therefore occupy the same energy region as the \( \uparrow \)-DOS (6).

There is another possibility for the \( \downarrow \) electron to flip its spin. It can also be done by a repeated emission and reabsorption of a magnon by the conduction electron resulting in a “dressed” particle propagating through the lattice accompanied by a virtual cloud of magnons. For not too small positive (negative) \( J \) the energy of this “dressed” particle lies above (below) the scattering spectrum giving even rise to a bound state, i.e. to a quasiparticle with infinite lifetime which we call the “magnetic polaron.” Outside the scattering region the polaron peak manifests itself as a \( \delta \)-function. As soon as the peak dips into the scattering part the polaron gets a finite lifetime after which it decays into a \( \uparrow \) electron plus magnon. Figure 1 shows the down-spin quasiparticle bandstructure as derived from the respective spectral density as a density plot. The degree of blackening is a measure of the spectral density magnitude. Sharp dark lines refer to pronounced peaks in the spectral density representing quasiparticles with long life-time. For weak coupling \( |JS| < 0.1 \) scattering processes smear out a little bit the “free” dispersion but do not lead to strong deformations. However, already for moderate couplings \( |JS| \gtrsim 0.2 \) one recognizes for some \( k \) vectors the appearance of a sharp polaron dispersion. For \( J > 0 \) (right column) the magnetic polaron is stable on the high-energy side of the \( \uparrow \) spectrum, for \( J < 0 \) on the low-energy side. In addition the scattering spectrum is clearly visible taking away a great part of the total spectral weight. In the antiferromagnetic KLM the magnetic polaron represents the ground state configuration \( \uparrow \) (3). For still rather moderate couplings of \( |JS| \gtrsim 0.3 \) the polaron dispersion has split off over the full Brillouin zone. The magnetic polaron has an infinite lifetime. It is surprising that even the broad scattering structure is obviously bunched together as if it were a rather stable quasiparticle. It is noteworthy to repeat that the results of Fig. 1 are exact and free of any uncontrollable approximation. So we have to expect these quasiparticle effects in real systems, too. This holds also for the quasiparticle density of states (QDOS) plotted in Fig. 2 for several exchange couplings \( |J| \). According to Eq. (6) the \( \uparrow \)-QDOS is only rigidly shifted to higher (lower) energies for \( J < 0 \) (\( J > 0 \)). Correlation effects appear exclusively in the \( \downarrow \) spectrum. For \( |JS| \gtrsim 0.25 \) a band splitting sets in. One of the subbands occupies the same energy region as \( \rho_{\uparrow}(E) \) being therefore built up by the mentioned scattering states. In the ferromagnetic (\( J > 0 \)) KLM it is the low energy part of the spectrum containing a considerable amount of \( \downarrow \)-spectral weight. This is not a specialty of the \( S = \frac{1}{2} \) case or of weak and moderate couplings exhibited in Fig. 2 but holds equivalently, e.g., for \( S = \frac{3}{2} \) and in the strong coupling region (\( |JS| \gtrsim 1.0 \), see last row in Fig. 2). After the band splitting has set in the weights of the two spin-\( \downarrow \) subbands are close to the zero-bandwidth values \( \frac{1}{2S + 1} \) for the lower, and \( \frac{2S}{2S + 1} \) for the upper part (\( J > 0 \)), i.e. independent of \( J \). The very often used assumption, when the KLM is applied
Figure 2. Spin-↑ (↓) density of states of the ferromagnetically saturated semiconductor as function of energy as solid (dotted) line. The upper three figures of each column show the DOS for a $S = \frac{1}{2}$ system with interaction strengths $|J| \in \{0.1; 0.5; 1.0\}$ corresponding to the spectral densities of Fig. 1. The respective lowest figure shows a $S = \frac{3}{2}$ system with $|J| = 1.0$. The left (right) column corresponds to $J < 0$ ($J > 0$).

3. Dynamical mean-field theory

3.1. Mapping onto an impurity model

It is not possible to directly apply the methods of the dynamical mean-field theory [50] to the KLM. One exception is the case of the classical-spin limit ($S \to \infty$) [26, 27], thus removing the quantum nature of the spins. The effect of quantum mechanics is strongest for $S = \frac{1}{2}$, but also for $S = \frac{3}{2}$, they dramatically influence the spectrum [13, 14]. The assumption of classical spins for $S = \frac{3}{2}$, as done in Refs. [25, 28], needs therefore careful analysis of the neglected effects.

Another possibility to derive a dynamical mean-field theory for the Kondo lattice model is the fermionization of the localized spin operators as suggested in [51]. This approach is, however limited to $S = \frac{1}{2}$ systems (see also [32, 33, 34]). The first part of our approach will closely follow Ref. [51], but as discussed below, will then differ from the cited reference.
The localized spins in the Hamiltonian (1) can be expressed in terms of auxiliary fermion operators \( f_{i\sigma} \) (\( f_{i\sigma}^\dagger \)) [11]:

\[
S_i \rightarrow S_i^{(f)} = \sum_{\sigma,\sigma'} f_{i\sigma}^{\dagger} \tau_{\sigma\sigma'} f_{i\sigma'}
\]  

(9)

Here, \( \tau_{\sigma\sigma'} \) represents the Pauli matrices. This is the same transformation that led to (2) where it was applied to the conduction electron spin \( \sigma \). The “fermionization” according to Eq. (9) implies the introduction of the constraint:

\[
Q_i = \sum_{\sigma} n_{i\sigma}^{(f)} = \sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} = 1 \quad \forall i
\]  

(10)

The inclusion of this constraint via a Lagrange formalism corresponds to the addition of a Hubbard-like interaction term for the \( f \)-fermions to the Hamiltonian with the interaction constant \( U^{(f)} \rightarrow \infty \). The one-particle energy of the \( f \)-fermions is located at \( -\frac{U^{(f)}}{2} \). The “fermionized KLM” takes the form:

\[
H^{\text{ferm.}} = \sum_{k,\sigma} \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma} - \frac{J}{2} \sum_i \sigma_i \cdot S_i^{(f)} - \frac{U^{(f)}}{2} \sum_{\sigma} f_{i\sigma}^{\dagger} f_{i\sigma} + \frac{U^{(f)}}{2} \sum_{\sigma} n_{i\sigma}^{(f)} n_{i^{-}\sigma}^{(f)}
\]  

(11)

This Hamiltonian describes a system of two different kinds of \( S = \frac{1}{2} \) fermions coupled by a local spin-exchange interaction. The \( f \)-fermions are additionally correlated via the Hubbard-type of interaction to prevent double-occupancy. This Hamiltonian resembles the periodic Anderson model (PAM) [8] in some way. In fact the only difference in the operator structure is the “coupling” between conduction band and \( f \) state. In the PAM, this is simply a kinetic-energy term (“hybridization”), whereas here, the two subsystems are coupled by the spin exchange. Essentially, the “fermionized KLM” is a rudimentary version of the general multi-band Hubbard model with (local) inter-band interaction. For this model, the DMFT is discussed by [50]. It is straightforward to apply the standard methods of the DMFT to map model (11) onto an appropriate impurity model with the corresponding self-consistency condition to determine the parameters of the impurity model. This leads to the following Hamiltonian for the impurity model (single-site Kondo model, SSKM) with fermionized \( f \)-spins:

\[
H_{\text{SSKM}}^{\text{ferm.}} = \sum_{k,\sigma} \eta(k) c_{k\sigma}^\dagger c_{k\sigma} - \frac{J}{2} \sigma_0 \cdot S^{(f)} - \frac{U^{(f)}}{2} \sum_{\sigma} f_{\sigma}^{\dagger} f_{\sigma} + \frac{U^{(f)}}{2} \sum_{\sigma} n_{\sigma}^{(f)} n_{\sigma^{-}}^{(f)}
\]  

(12)

with only one “impurity” site for the \( f \)-fermions. The spin-exchange interaction acts only at this single site denoted by the site-index 0. It is advisable to express the conduction band part of Hamiltonian (12) in local space and single out the operators referring to the impurity site 0:

\[
\sum_{k,\sigma} \eta(k) c_{k\sigma}^\dagger c_{k\sigma} = \sum_{i,j,\sigma} T_{ij} c_{i\sigma}^\dagger c_{j\sigma} =
\]  

(13)

\[
\sum_{\sigma} T_{00} c_{0\sigma}^\dagger c_{0\sigma} + \sum_{i \neq 0} T_{0i} \left( c_{i\sigma}^\dagger c_{i\sigma} + c_{i\sigma}^\dagger c_{0\sigma} + c_{0\sigma}^\dagger c_{i\sigma} \right) + \sum_{i,j \neq 0} T_{ij} c_{i\sigma}^\dagger c_{j\sigma}
\]

For better readability, we will denote the construction operators at the site 0 with the symbol \( d_{\sigma} \) (\( d_{\sigma}^\dagger \)), the on-site energy will be denoted \( T_{00} \rightarrow \epsilon_d \). Finally we introduce a unitary transformation which diagonalizes the last term of the second line in Eq. (13). The transformed fermion operators will be denoted \( a_{k\sigma} \) (\( a_{k\sigma}^\dagger \)), the hopping \( T_{0i} \rightarrow V_{kd} \)
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and finally \( T_{ij} \rightarrow \tilde{\eta}(k) \) for \( i \neq j \). In the context of the DMFT, one does not need to know the explicit structure of this unitary transformation since \( \tilde{\eta}(k) \) and \( V_{kd} \) need not be known explicitly either. The parameters of the single-site Kondo model will be determined by the self-consistency condition of the DMFT (see below).

A direct solution of model (12) is, to our knowledge not possible. However, it can be further simplified: The Hubbard term originating from the constraint (10) can be eliminated by simply reversing the “fermionization” procedure which led from Hamiltonian (1) to (11). The auxiliary fermion operators get replaced by a local spin-\( \frac{1}{2} \) operator at the impurity site, and the constraint (10) can be dropped. This leads to the final version of the single-site Kondo model:

\[
H_{SSKM} = \sum_{k,\sigma} \tilde{\eta}(k) a_k^{\dagger} a_{k\sigma} + e_d \sum_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + \sum_{k,\sigma} V_{kd} \left( d_{\sigma}^{\dagger} a_{k\sigma} + a_{k\sigma}^{\dagger} d_{\sigma} \right) - \frac{J}{2} \sigma^{(d)} \cdot S \tag{14}
\]

This last step, which could be called “de-fermionization”, distinguishes our approach from the one used in Ref. [51] and others. This “de-fermionization” ensures the exact fulfillment of the constraint (10), which could for example only be kept on average (\( \sum_{\sigma} n_{\sigma}^{(f)} = 1 \) instead of \( \sum_{\sigma} n_{\sigma}^{(f)} = 1 \)) in [51].

The parameters determining the conduction band in the Hamiltonian (14), namely \( \tilde{\eta}(k) \) and \( V_{kd} \) have to be specified according to the DMFT self-consistency condition: The local conduction band Green function (cf. (4)) should be equivalent to the \( d \)-operator Green function of the single-site model, \( \langle \langle d_{\sigma}^{\dagger} d_{\sigma} \rangle \rangle = G^{(d)}_{\sigma}(E) \):

\[
\frac{1}{N} \sum_{k} G_{k\sigma}(E) = G^{(d)}_{\sigma}(E) = \frac{\hbar}{E - e_d - \Delta_{\sigma}(E) - \Sigma^{(d)}_{\sigma}(E)} \tag{15}
\]

where the right equation follows from the formal solution of the equation of motion of \( G^{(d)}_{\sigma}(E) \). So instead of the usual definition for the hybridization function, \( \Delta(E) = \sum_{k} \frac{V_{kd}^{2}}{\tilde{\eta}(k)} \), it has to be determined so that Eq. (15) holds. One will see below that the knowledge of \( \Delta_{\sigma}(E) \), which can become spin-dependent through this procedure, is sufficient to solve the single-site Kondo model (14). Its dispersion \( \tilde{\eta}(k) \) and the hybridization parameter \( V_{kd} \) need not to be determined explicitly.

The DMFT, i.e. the mapping of the KLM onto the single-site model is, except for the limit of infinite spatial dimensions, an approximation, equivalent to the local approximation. In the exactly solvable case of the ferromagnetic semiconductor (cf. Sec. 2.3) this is equivalent to neglecting the magnon energies which are assumed to be at least one order of magnitude smaller than the energy scales under consideration here, e.g. bandwidth or \( J \).

Next, we will introduce an approximative method to solve the single-site Kondo model defined by Hamiltonian (14) for an arbitrary hybridization function \( \Delta_{\sigma}(E) \).

3.2. Hybridization approximation

In the following section, we derive an equation of motion-based method to solve the single-site Kondo model (14). Since in this section we deal only with this model, we suppress all subscripts distinguishing between quantities in the lattice and the single-site model.

Starting point is the equation of motion for the \( d \)-Green function:

\[
EG^{(d)}_{\sigma}(E) = \hbar + e_d G^{(d)}_{\sigma}(E) + \sum_{k} V_{kd} \langle \langle a_{k\sigma}^{\dagger} d_{\sigma} \rangle \rangle - \frac{J}{2} \sum_{\sigma} (z_{\sigma} I_{\sigma}(E) + F_{\sigma}(E)) \tag{16}
\]
where the higher Green functions $I_{\sigma}(E) = \langle \langle d_{\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle$ and $F_{\sigma}(E) = \langle \langle d_{-\sigma} S^{-\sigma} ; d^\dagger_{\sigma} \rangle \rangle$, corresponding to the Green functions $I_{im,j\sigma}(E)$ and $F_{im,j\sigma}(E)$ for the lattice case, are introduced. The “mixed” Green function $\langle \langle a_{k\sigma} ; d^\dagger_{\sigma} \rangle \rangle$ can be eliminated by investigating its equation of motion:

$$
\sum_k V_{kd} \langle \langle a_{k\sigma} ; d^\dagger_{\sigma} \rangle \rangle = \sum_k \frac{V^2_{kd}}{E - \eta(k)} G_{\sigma}^{(d)}(E) = \Delta(E) G_{\sigma}^{(d)}(E) \tag{17}
$$

thereby defining the hybridization function $\Delta(E) = \sum_k \frac{V^2_{kd}}{E - \eta(k)}$. This yields the final equation of motion:

$$(E - (e_d + \Delta(E))) G_{\sigma}^{(d)}(E) = \hbar - \frac{J}{2} \sum_{\sigma} (z_{\sigma} I_{\sigma}(E) + F_{\sigma}(E)) \tag{18}
$$

Eq. (18) looks, except for the $\Delta(E)$ in the prefactor of $G_{\sigma}^{(d)}(E)$, like the equation of motion of the zero-bandwidth limit. The hybridization function $\Delta(E)$ is due to the $V_{kd}$-term in the Hamiltonian. This term prohibits an exact solution. In fact, the “hybridization” via $V_{kd}$ is nothing else than the inter-site hopping which was neglected in the zero-bandwidth limit. This term will force us to make certain approximations in the determination of the higher Green functions on the right-hand side of Eq. (18).

We will exemplify this using the $I_{\sigma}(E)$-function. Its equation of motion reads

$$(E - e_d) I_{\sigma}(E) = \hbar \langle S^z \rangle + \sum_k V_{kd} \langle \langle a_{k\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle - \frac{J}{2} \left( z_{\sigma} \langle \langle d_{\sigma} S^z S^z ; d^\dagger_{\sigma} \rangle \rangle + \langle \langle d_{-\sigma} S^{-\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle - z_{\sigma} \langle \langle d_{\sigma} d^\dagger_{\sigma} d_{-\sigma} S^{-\sigma} ; d^\dagger_{\sigma} \rangle \rangle \right) \tag{19}
$$

where on the one hand, higher “impurity-site” Green functions are introduced, but on the other hand also a higher “mixed” Green function, $\langle \langle a_{k\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle$. In analogy to the one-particle mixed Green function, Eq. (17), we use the following substitution:

$$
\sum_k V_{kd} \langle \langle a_{k\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle \rightarrow \Delta(E) \langle \langle d_{\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle = \Delta(E) I_{\sigma}(E) \tag{20}
$$

The justification of this procedure can be found in analogy to the “self-energy substitution” known from other approximation methods for the KLM (see e.g. [14]) by inspecting the spectral representations of the relevant Green functions. This reveals that all of them have the same single-particle poles, they differ only in the respective weights given by matrix elements of the type $\langle E_n|A|E_m \rangle$. Here $|E_n \rangle$ are the energy eigenstates and $A$ represents one of the relevant operators: $d_{\sigma}$, $a_{k\sigma}$, $d_{\sigma} S^z$ or $a_{k\sigma} S^z$. From Eq. (17) follows that the hybridization function accounts for the differences of the matrix elements of the first two operators ($d_{\sigma}$ and $a_{k\sigma}$). Assuming that these differences are almost equal to those of the matrix elements built up by the latter two operators leads to the hybridization approximation.

This is the only approximation necessary to decouple the hierarchy of equations of motion. In the case of $S = \frac{1}{2}$ spins, there are only 6 different “impurity-site” Green functions, whose equations of motion form a closed set of equations. Besides the already introduced Green functions $G_{\sigma}^{(d)}(E)$, $I_{\sigma}(E)$ and $F_{\sigma}(E)$, these are

$$
F_{\sigma}^{(1)}(E) = \langle \langle d_{-\sigma} d^\dagger_{-\sigma} d_{\sigma} S^z ; d^\dagger_{\sigma} \rangle \rangle \\
F_{\sigma}^{(2)}(E) = \langle \langle d_{-\sigma} d^\dagger_{\sigma} d_{-\sigma} S^{-\sigma} ; d^\dagger_{\sigma} \rangle \rangle \\
D_{\sigma}(E) = \langle \langle d_{-\sigma} d^\dagger_{-\sigma} d_{\sigma} ; d^\dagger_{\sigma} \rangle \rangle \tag{21}
$$
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Several expectation values, introduced into the theory via the inhomogeneities of the equations of motion can be expressed in terms of the above-mentioned Green functions, a self-consistent solution has to be found.

At this point, let us comment on the reliability of this approximation. Although only one approximation enters our decoupling procedure (cf. Eq. (20)), it still has to be seen as an uncontrollable approximation meaning that there is no true small parameter. There are two non-trivial limiting cases where the replacement (20) becomes exact: The first is the limit $V_{kd} \to 0$, representing the zero-bandwidth KLM of Sec. 2.2. But already a small, but finite bandwidth in the KLM could lead to any (unknown) expression for $\Delta(E)$ implying that we can not necessarily assume $V_{kd}$ to be small any more. The second limit is the “classical spin” limit where the “spin variable” $S$ has no operator properties any more. Here, the replacement of Eq. (20) reduces to (17). However since we are interested in the general case with finite $S$ and bandwidth, we have to confirm the trustworthiness of this approximation by a comparison with other well-tested methods.

4. Other approximation methods

We are now going to introduce three further approximation methods for the KLM. These are known from literature, their strengths and weaknesses have been identified. The three methods differ substantially with respect to the theoretical assumptions made for an approximate solution of the KLM. Common features following from these procedures and the above-introduced DMFT scheme should then give some credit of reliability, in particular when they additionally fit the exact limiting cases discussed in Sec. 3.

4.1. Second-order perturbation theory

An application of the usual diagrammatic perturbation theory to the Kondo model cannot be performed due to the absence of Wick’s theorem. Only for low temperatures (spin-wave approximation) [55] or in the classical-spin limit [56], this method is applicable. The projection operator formalism of Mori [43, 44] is better suited for the Kondo model. It has been used successfully to describe correlation effects in the Hubbard model in the weak coupling regime [57]. The general formula for the second-order contribution $\Sigma^{(2)}(E)$ can be found there (Eq. (3.12) in Ref. [57]). To allow for a better comparison with the other approximations in this paper, we further approximate the self-energy taking only $k$ averaged occupation numbers into account (local approximation).

4.2. Self-consistent CPA

Next, we want to introduce a modification of the well-known “coherent potential approximation” (CPA) [58] for the KLM. The CPA is a standard many-body approach that starts from a fictitious alloy in analogy to the interacting particle system. Starting point may be the zero bandwidth limit of Sec. 2.2. We think of a four-component alloy each constituent of which is characterized by one of the energy levels $E_i$ in Eq. (5). The spectral weights $\alpha_v$ in (3) are then to be interpreted as the “concentrations” of the alloy components as seen by a propagating $\sigma$-electron. The fictitious alloy for a
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\[ \sigma \text{-electron is built up by the local moments and by the frozen } (-\sigma) \text{ electrons. The CPA-selfenergy of the } \sigma \text{-electron is found by the well-known formula} \]

\[ 0 = \sum_{p=1}^{4} \alpha_{p\sigma} \left( \frac{E_p - \Sigma_{\sigma}(E) - T_0}{1 - G_{t\sigma}(E)(E_p - \Sigma_{\sigma}(E) - T_0)} \right) \] (22)

As a consequence of the single-site aspect of the CPA the resulting selfenergy is wave-vector independent. According to Eq. (5) the “concentrations” \( \alpha_{i\sigma} \) depend on a sum of the “higher” correlation functions \( I_{ii,i\sigma}(E) \) and \( F_{ii,i\sigma}(E) \), which can rigorously be expressed by the single-electron Green function.

\[ \gamma_\sigma + z_\sigma \Delta_\sigma = \frac{-1}{\hbar \pi N} \sum_k \int_{-\infty}^{+\infty} dE f_-(E) (E - \epsilon(k)) \text{Im} G_{k\sigma}(E) \] (23)

The shortcomings of the CPA-procedure lie on hand. The one is the same as that in the conventional alloy analogy of the Hubbard model, namely the assumption of frozen \((-\sigma)\) electrons. This is partially removed by our proposed modification of the standard CPA procedure for the KLM, namely the selfconsistent calculation of the higher correlation functions \( \gamma_\sigma \) and \( \Delta_\sigma \) via Eq. (23) as well as the band-occupation \( \langle n_{-\sigma} \rangle \) via the spectral theorem for the one-electron Green function. Maybe even more serious in the case of the KLM is the blocking of repeated spin exchange with the local moment system. Magnon emission or absorption is not involved. So we cannot expect that the CPA-treatment correctly reproduces the exact limiting case of Sec. 2.3. However, some general information about the quasiparticle bandstructure might be possible, in particular in the strong coupling (“split band”) regime. By construction the method yields the correct zero-bandwidth limit.

4.3. The moment-conserving decoupling approach (MCDA)

A Green function method which takes the spin dynamics correctly into account has been proposed in Ref. [14]. For details about this approach, we refer the reader to the cited paper, here we summarize the result shortly.

This decoupling approach yields finally a selfenergy of the following structure:

\[ \Sigma_{k\sigma}(E) = -\frac{1}{2} J z_\sigma \langle S^z \rangle + \frac{1}{4} J^2 D_{k\sigma}(E) \] (24)

The first term is linear in the coupling \( J \) and proportional to the \( 4f \) magnetization \( \langle S^z \rangle \). It just represents the result of a mean-field approximation being correct in the weak-coupling limit. The second term in (24) contains all the spin exchange processes which may happen. It is a complicated functional of the selfenergy itself. So (24) is not at all an analytical solution but an implicit equation for the selfenergy. We do not present here the lengthy expression for \( D_{k\sigma}(E) \) referring the reader for further details to Ref. [14]. It should be mentioned, however, that \( D_{k\sigma}(E) \) contains several expectation values which must be fixed to get a self-consistent solution. No problems arise with the mixed correlation functions \( \gamma_\sigma = \langle S_i^z c_{i-\sigma}^\dagger c_{i\sigma} \rangle \) and \( \Delta_\sigma = \langle S_i^z n_{i\sigma} \rangle \). They can rigorously be expressed by the spin flip function \( F_{ii,i\sigma}(E) \) and the Ising function \( I_{ii,i\sigma}(E) \) defined previously. Both functions are already involved in the procedure, so that no further approximations are necessary to fix \( \gamma_\sigma \) and \( \Delta_\sigma \). For pure local-moment correlations such as \( \langle S_i^z \rangle, \langle S_i^z S_i^\pm \rangle, \ldots \), however, a special treatment is necessary, e.g. as described in Ref. [14].
5. Results

In the following section, we discuss the results obtained for the DMFT and the three approximation schemes of Sec. I for the ferromagnetic Kondo lattice model with \( S = \frac{1}{2} \). Since we are interested in the reaction of the conduction band due to the magnetic order of the spin system, we have not calculated the latter self-consistently. Instead, we have simulated the magnetic order by determining \( \langle S_z \rangle \) using a Brillouin function. Temperatures are given in units of \( T_c \). Within the CPA, our choice of \( \langle S_z \rangle \) can lead to unphysical results. Namely in the case of \( \langle S_z \rangle \to S \), some of the weights \( \langle 1 - n - \sigma \rangle \) can become negative. There is an upper bound for \( \langle S_z \rangle \) \( \langle 0.33 \rangle \). We therefore had to limit \( \langle S_z \rangle \) to \( \langle S_z \rangle \lesssim 0.33 \) for some of the CPA calculations. Within the DMFT calculations, we experienced severe numerical problems which forced us to introduce a further approximation: “mean-field”-decoupling the \( F^{(1)}_\sigma(E) \) and \( F^{(2)}_\sigma(E) \) functions simplifies the system of equations of motion:

\[
F^{(1)}_\sigma(E) \approx (1 - \langle n - \sigma \rangle) \Gamma_\sigma(E) + \langle S^z \rangle D_\sigma(E) + \langle (1 - n - \sigma) S^z \rangle G^{(d)}(E)
\]

\[
F^{(2)}_\sigma(E) \approx \langle n_\sigma \rangle F_\sigma(E) - \langle S^- d_\sigma d^- \rangle G^{(d)}(E)
\]

All DMFT-results presented below were obtained using the hybridization approximation in combination with this unrestricted-mean-field decoupling of \( F^{(1)}_\sigma(E) \) and \( F^{(2)}_\sigma(E) \).

In all calculations, the conduction band is described by a tight-binding DOS for a simple-cubic lattice structure \([59]\) of unit width (\( W = 1 eV \)). The Curie temperature is taken as \( T_c = 250 K \).
The quasiparticle densities of states (DOS) for quarter-filling and different values of $J$ are plotted in Figs. 3 and 4 for $T = 0$ and $T = T_c$, respectively. As indicated, the columns correspond to DMFT, MCDA, CPA and SOPT, respectively (from left to right).

We will begin the discussion with the DMFT results shown in the left column of Fig. 3. A small value of $J$ leads to a spin-dependent shift of the spin-$\uparrow$ and $\downarrow$ DOS, as one would obtain by a simple mean-field decoupling, i.e. by replacing $S_z$ by its mean value $\langle S_z \rangle$ in Hamiltonian (1). With increasing $J$, the DOS show some striking correlation effects: first a broadening, later the onset of a splitting of the band can be observed. Whereas in general, the correlation effects are stronger for spin $\downarrow$ (indicated by a stronger quasiparticle damping), the splitting is, in contrast to the other two methods, more pronounced in the spin-$\uparrow$ DOS. However, here the split-of (upper) peak has much less spectral weight than the original peak which, except for a band-narrowing still resembles strongly the free conduction band DOS.

The picture is very similar in the MCDA. Again, a mean-field like spin-dependent bandshift is observed for small $J$. On increasing $J$, the spin-$\downarrow$ DOS broadens, and a two-peak structure emerges. The spin-$\uparrow$ DOS remains, except for a small tail at its upper edge, unchanged. This behavior can easily be understood by comparing with the special case of the ferromagnetically saturated semiconductor as discussion in Sec. 2.3 since the MCDA develops continuously into this special case for $n \to 0$ and $T \to 0$. The spin-$\downarrow$ DOS splits into a scattering part (low energies) and the polaron-like part at higher energies above the conduction band. Unlike the $n = 0$ case, however, there are some, but weak modification in the $\uparrow$ DOS, namely the above mentioned tail at its upper edge. This can be interpreted as a scattering contribution for spin-$\uparrow$ electrons. The origin of this is the finite number of spin-$\downarrow$ electrons.

Also the CPA DOS show a remarkably similar picture as the previously discussed theories. Again, there is the mean-field shift for small $J$. For larger values of $J$, the
splitting of the spin-$\downarrow$ DOS sets in similarly to the other two methods. Here, this can be contributed to the two single-occupancy quasiparticle energies $E_1$ and $E_2$ known from the zero-bandwidth limit (cf. Sec. 2.2). For $n \neq 0$ a third quasiparticle energy carries non-vanishing weight, namely the $E_4$ peak. This is located between the two other peaks since we switched off the conduction band Coulomb interaction $U$ (cf. Eq. (1)). For $J = 0.4$, the appearance of this third peak in between the two main peaks is vaguely visible. A remarkable difference to the DMFT and MCDA results is the fact, that the spin-$\uparrow$ and scattering part of the spin-$\downarrow$ DOS do not cover the same energy range. This shortcoming of the CPA is due to the neglection of spin-dynamics (magnons) as mentioned in Sec. 4.2 (cf. Ref. [40]).

The SOPT results are, for the plotted values of $J$ in the weak- and intermediate coupling regime, not too far away from the other results. For small $J$, where the SOPT becomes by definition reliable, the mean-field shift as in the other methods is clearly observable. Similar to the other methods, the deformation of the spin-$\downarrow$ DOS is much stronger than that of the spin-$\uparrow$ DOS. However, for larger $J$, the SOPT never shows a true band splitting, its range of validity is certainly restricted.

For $T = T_c$, where spin-symmetry is re-established, the DMFT, MCDA and CPA give a similar overall picture. The resulting DOS shows, already for $J \gtrsim 0.3$, a two-peak structure (DMFT and MCDA), in the CPA a third peak is dimly noticeable. The most remarkable observation is the near-coincidence of the DMFT and MCDA results for all $J$ values. The transition from the (clearly distinct) $T = 0$ DOS to the (resembling) $T = T_c$ DOS is continuous for both theories. The SOPT, however, has to be seen as a complete failure for a paramagnetic system already for relatively small $J \approx 0.3$. This can already be read of the formula for calculating the self-energy, which is more or less trivial. The corresponding results cannot be connected to any of the exactly solvable limiting cases (cf. Sec. 4.1).

A sound-standing interpretation of the observations is not difficult since the MCDA can be traced back to the exactly solved limiting case of the ferromagnetically saturated semiconductor (cf. Sec. 2.3) and the CPA to that of the zero-bandwidth limit discussed in Sec. 2.2. The SOPT, of course, becomes reliable for small $J$. Although all four presented methods are of approximate nature and their results do, at least for intermediate-to-large values of $J$, differ, some common properties emerge: For small $J$, the behavior is genuine mean-field like, a bandshift proportional to $\pm J \langle S^z \rangle$ is observed. For larger $J$, the onset of a band splitting occurs. At $T = 0$ this primarily affects the spin-$\downarrow$ DOS. This fact is understandable by examination of the ferromagnetically saturated semiconductor where the band splitting was discussed in terms of a scattering band and the magnetic polaron. In that case the spin-$\uparrow$ DOS remains, except for a simple shift, unaffected by the interaction simply because spin-flip of spin-$\uparrow$ electrons is suppressed in this case. Now for finite $n$, this is only approximately true. The spin-$\downarrow$ DOS still shows strong correlation effects, but also the spin-$\uparrow$ DOS is affected due to the finite number of spin-$\downarrow$ electrons in the system. This manifests itself differently in the various methods: in the MCDA, a tail is seen at the upper edge of the spin-$\uparrow$ DOS, in the CPA, a shoulder develops, and in the DMFT approach, a band splitting is observable. From this we conclude that correlation effects are much more pronounced in the DMFT than in the other two theories. At $T = T_c$, the dip indicating the onset of the band splitting is still existing for all but the SOPT method. In CPA, MCDA and the DMFT results this splitting is of similar size, which can easily be read off the CPA where it is simply given by the difference of the respective energies from the zero-bandwidth limit (see Eq. (5)). The two most
pronounced peaks correspond to the single-occupancy quasiparticle energies $E_1$ and $E_2$, the band splitting is therefore approximately $\Delta E = J(S + \frac{1}{2})$.

This is in contrast to the results obtained by dynamical mean-field theory for the $S \to \infty$ KLM (KLM with classical spins). The emerging picture for classical spins is the following [25]. At $T = 0$, the DOS is characterized by a mean-field like “Zeeman” splitting between the bands of both spin directions. With increasing temperature, at each of the respective spin-$\uparrow$ or $\downarrow$ band, spectral weight of the opposite spin direction appears, until finally at $T = T_c$, the system becomes paramagnetic. The splitting into two subbands separated by $\Delta E = JS$ stays constant. Comparing our results with the $S \to \infty$ ones, phenomenologically the DOS’s show completely different characteristics at $T = 0$, especially in the spin-$\downarrow$ band. For $T = T_c$, the DOS’s look quite similar. However, the physics behind the scenes turn out to be completely different as can be seen, e.g., by the inconsistent size of the band splitting $\Delta E$. Whereas in the classical-spin limit, the splitting is always due to a mean-field like “on-site Zeeman splitting”, in the case of quantum spins, the various elementary excitations as discussed in the case of the ferromagnetically saturated semiconductor, are responsible for the sub-band structure. For the ferromagnetically saturated system, the neglect of spin-flip processes and magnons in the $S \to \infty$ calculation lead to the picture of a half-metal [26]. This does not apply for any finite value of $S$ and is therefore clearly an artifact of the $S \to \infty$ limit.

Let us shortly remark on the situation with anti-ferromagnetic coupling ($J < 0$) [60]. All four approximation methods presented here do not show any signs of Kondo screening. An investigation of the special low-temperature physics of the model with $J < 0$ is therefore not possible. However, some remarks about the behavior of the model for $T > T_K$ can be made: In general the excitation spectra are broader than in the $J > 0$ case. The resulting exchange splitting of $\Delta E \approx JS$ is also larger than for $J > 0$ which can already be seen in the zero-bandwidth limit. This is again in sharp contrast to the $S = \infty$ results, where the size of the splitting is independent of the sign of $J$.

6. Conclusions

In this paper, we investigated the Kondo lattice model (KLM) focusing on the model with positive (ferromagnetic) exchange constant $J$. We discussed two exactly solvable, but nevertheless non-trivial limiting cases as well as four different approximation methods. The results obtained by these methods, maybe except for the perturbation theory, compare generally reasonably well. Sometimes even nearly perfect matches occur (cf. Fig. 4). In general, the differences between the methods are smaller for the paramagnetic than the ferromagnetic system.

From the comparison of common features of these approximation methods in combination with the exact results, the following picture emerges for the quasiparticle structure of the ferromagnetic Kondo lattice model: For small $|J|$, a mean-field like shift of $\uparrow$ and $\downarrow$ DOS is visible. Already for intermediate coupling strengths, a band splitting of size $\Delta E = J(S + \frac{1}{2})$ occurs. The relevant energy scale for the splitting is $JS \approx 0.3$. In the case of ferromagnetic saturation ($T = 0$), the splitting is more pronounced in the $\downarrow$ than in the $\uparrow$ DOS. This band-splitting should not be confused with the splitting found in the limit of “classical spins” ($S \to \infty$). There, the splitting is simply due to a mean-field like Zeeman-splitting and therefore of the size $\Delta E = JS$. Contrary to that, our results clearly show that the two emerging subbands
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can be traced back to the two elementary excitations known from the limit of the ferromagnetically saturated semiconductor (see above). The magnetic saturation of the spin-system suppresses these processes for spin-↑ electrons which explains the stronger footprint of the correlations in the spin-↓ DOS. For finite temperatures, the magnetic polaron generally remains a well defined quasiparticle, represented by a rather sharp Lorentzian peak in the spectral density. Now the spin-↑ electrons can also participate in spin-exchange processes since the localized spins are not fully aligned any more. The spin-symmetric DOS at $T \gtrsim T_c$ also show the characteristic splitting. Our results also confirm the fundamental differences between the $J > 0$ and the $J < 0$ case of the Kondo lattice model: It can be read of both exactly solvable limiting cases that the ground state will be different depending on the sign of $J$. The approximative approaches of Secs. 3 and 4 do not allow a deeper investigation of the model with $J < 0$ due to the inability to reproduce the special low-temperature properties of that model (“Kondo physics”). Another important conclusion from our calculations can be drawn: There is always finite spin-↓ spectral weight in the region of the spin-↑ DOS. This spectral weight does not disappear in the limit $J \to \infty$ but only in the limit $S \to \infty$ (“classical spins”). For the ferromagnetic KLM ($J > 0$), this implies that the KLM for $S = \frac{3}{2}$ and large $J$, corresponding to the situation found in manganites, will not be a half-metal for $T = 0$, contrary to the predictions of $S \to \infty$ calculations.

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[1] C. Zener, Phys. Rev. 81(4), 440 1951.
[2] P. W. Anderson and H. Hasegawa, Phys. Rev. 100(2), 675 1955.
[3] T. Kasuya, Prog. Theor. Phys. 16(1), 45 1956.
[4] J. Kondo, Prog. Theor. Phys. 32, 37 1964.
[5] E. L. Nagaev, phys. stat. sol. (b) 65, 11 1974.
[6] W. Nolting, phys. stat. sol. (b) 96, 11 1979.
[7] P. W. Anderson, Phys. Rev. 124(1), 41 1961.
[8] A. C. Hewson, The Kondo Problem to Heavy Fermions, Cambridge University Press 1993.
[9] J. R. Schrieffer and P. A. Wolff, Phys. Rev. 149(2), 491 1966.
[10] P. Wachter, In K. A. Gschneidner and L. Eyring, editors, Handbook on the Physics and Chemistry of Rare Earth volume 2 page 507. Elsevier Science Publishers Amsterdam 1979.
[11] J. Kossut, phys. stat. sol. (b) 78, 537 1976.
[12] S. Legfuld, In E. P. Wohlfarth, editor, Ferromagnetic Materials volume 1 chapter 3. North Holland Amsterdam 1980.
[13] W. Nolting, S. Mathi Jaya, and S. Rex, Phys. Rev. B 54(20), 14455 1996.
[14] W. Nolting, S. Rex, and S. Mathi Jaya, J. Phys.: Condens. Matter 9, 1301 1997.
[15] S. Rex, V. Eyert, and W. Nolting, J. Magn. Magn. Mat. 192, 529 1999.
[16] S. Jin, T. H. Tiefel, M. McCormack, R. A. Fastnacht, R. Ramesh, and L. H. Chen, Science 264, 413 1994.
[17] A. P. Ramirez, J. Phys.: Condens. Matter 9, 8171 1997.
[18] E. Dagotto, S. Yunoki, A. L. Malvezzi, A. Moreo, J. Hu, S. Capponi, D. Poilblanc, and N. Furukawa, Phys. Rev. B 58(10), 6414 1998.
[19] S. Satpathy, Z. S. Popović, and F. R. Vukajlović, Phys. Rev. Lett. 76(6), 960 1996.
[20] W. Pickett and D. J. Singh, Phys. Rev. B 53(3), 1146 1996.
[21] D. J. Singh and W. E. Pickett, Phys. Rev. B 57(1), 88 1998.
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[22] J.-H. Park, C. T. Chen, S.-W. Cheong, W. Bao, G. Meigs, V. Chakarian, and Y. U. Idzerda, Phys. Rev. Lett. 76(22), 4215 1996.
[23] T. Saitoh, A. Sekiyama, K. Kobayashi, T. Mizokawa, A. Fujimori, D. D. Sarma, Y. Takeda, and M. Takano, Phys. Rev. B 56(14), 8836 1997.
[24] Y. Okimoto, T. Katsufuji, T. Ishikawa, A. Urushibara, T. Arima, and Y. Tokura, Phys. Rev. Lett. 75(1), 109 1995.
[25] A. J. Millis, R. Mueller, and B. I. Shraiman, Phys. Rev. B 54(8), 5405 1996.
[26] N. Furukawa, cond-mat/9812066.
[27] A. J. Millis, P. B. Littlewood, and B. I. Shraiman, Phys. Rev. Lett. 74(22), 5168 2000.
[28] K. Held and D. Vollhardt, Phys. Rev. Lett. 84(22), 5168 2000.
[29] A. Chattopadhyay, A. J. Millis, and S. Das Sarma, cond-mat/0004151.
[30] R. R. P. Singh, W. E. Pickett, D. W. Hone, and D. J. Scalapino, cond-mat/0007086 2000.
[31] Y. Okimoto, T. Katsufuji, T. Ishikawa, A. Urushibara, T. Arima, and Y. Tokura, Phys. Rev. Lett. 75(1), 109 1995.
[32] A. J. Millis, P. B. Littlewood, and B. I. Shraiman, Phys. Rev. Lett. 74(22), 5168 2000.
[33] W. Nolting and M. Matlak, phys. stat. sol. (b) 123, 155 1984.
[34] S. Methfessel and D. C. Mattis, Handb. Phys. 18, Springer-Berlin 1968, p. 389.
[35] Y. A. Izyumov and M. V. Medvedev, Sov. Phys. – JETP 32, 109 1971.
[36] P. Richmond, J. Phys. C 3, 2402 1970.
[37] B. S. Shastry and D. C. Mattis, Phys. Rev. B 24, 5340 1981.
[38] S. R. Allan and D. M. Edwars, J. Phys. C 15, 2151 1982.
[39] M. I. Auslender, V. Yu. Irkhin, and M. I. Katsnelson, J. Phys. C 17, 669 1984.
[40] W. Nolting, U. Dubil, and M. Matlak, J. Phys. C 18, 3533 1985.
[41] W. Nolting, U. Dubil, and M. Matlak, J. Phys. C 18, 3687 1985.
[42] W. Nolting and U. Dubil, phys. stat. sol. (b) 130, 561 1985.
[43] H. Mori, Prog. Theor. Phys. 33, 423 1965.
[44] H. Mori, Prog. Theor. Phys. 34, 399 1966.
[45] K. Kubo, J. Phys. Soc. Japan 36(1), 32 1974.
[46] W. Nolting, Viel-Teilchen-Theorie volume 7 of Grundkurs: Theoretische Physik, Friedr. Vieweg & Sohn Verlagsgesellschaft mbH Braunschweig/Wiesbaden 4 edition 1997.
[47] D.M. Edwards, A. C. M. Green, and K. Kubo, J. Phys.: Condens. Matter 11, 2791 1999.
[48] A. C. M. Green and D. M. Edwars, J. Phys.: Condens. Matter 11, 10511 1999.
[49] H. Tszurugi, M. Sgrist, and K. Ueda, Rev. Mod. Phys. 69(3), 809 1997.
[50] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68(1), 13 1996.
[51] N. Matsumoto and F. Okhawa, Phys. Rev. B 51(7), 4110 1995.
[52] T. Pruschke, B. Steininger, and J. Keller, Physica B 206&207, 154 1995.
[53] M. Jarrell, H. Pang, D.L. Cox, and K.H. Luk, Phys. Rev. Lett. 77(8), 1612 1996.
[54] T. Schork, S. Blawid, and J. Igarashi, Phys. Rev. B 59(15), 9888 1999.
[55] R. B. Woolsey and R. M. White, Phys. Rev. B 1(11), 4474 1970.
[56] F. Ry, J. Helman, and W. Baltensperger, Phys. kondens. Materie 6, 105 1967.
[57] G. Bulk and R. J. Helman, Phys. Rev. B 41, 413 1990.
[58] B. Velicky, S. Kirkpatrick, and H. Ehrenreich, Phys. Rev. 175, 747 1968.
[59] R. J. Helman, J. Phys. Chem. Solids 30, 609 1969.
[60] D. Meyer, Electron Correlation effects in ferromagnetic local-moment and intermediate-valence systems, Dissertation Humboldt-Universität zu Berlin 2001.