Low density approach to the Kondo-lattice model

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We propose a new approach to the (ferromagnetic) Kondo-lattice model in the low density region, where the model is thought to give a reasonable frame work for manganites with perovskite structure exhibiting the "colossal magnetoresistance" -effect. Results for the temperature- dependent quasiparticle density of states are presented. Typical features can be interpreted in terms of elementary spin-exchange processes between itinerant conduction electrons and localized moments. The approach is exact in the zero bandwidth limit for all temperatures and at \( T = 0 \) for arbitrary bandwidths, fulfills exact high-energy expansions and reproduces correctly second order perturbation theory in the exchange coupling.

I. INTRODUCTION

The Kondo-lattice model (KLM) [1] describes the interplay of itinerant electrons in a partially filled energy band with quantum mechanical spins (magnetic moments), localized at certain lattice sites. Characteristic model properties result from an interband interaction between the two subsystems.

On the one hand, the energy bandstructure is modified by the magnetic state of the spin system (temperature dependences, band splittings, band deformations), while, on the other, the magnetic state of the spin system is even provoked by the itinerant electrons because the KLM does not incorporate a direct exchange between the moments. The model-Hamiltonian consists of two parts

\[
H = H_s + H_{sf}
\]  
(1)

\( H_s \) is the kinetic energy of itinerant band electrons,

\[
H_s = \sum_{\mathbf{i}, \mathbf{j}, \sigma} T_{\mathbf{i} \mathbf{j}} c^\dagger_{\mathbf{i} \sigma} c_{\mathbf{j} \sigma}
\]  
(2)

where \( c^\dagger_{\mathbf{i} \sigma}(c_{\mathbf{i} \sigma}) \) is the creation (annihilation) operator of a band electron specified by the lower indices. \( T_{\mathbf{i} \mathbf{j}} \) are the hopping integrals. The second term in (1) is an interband exchange term with coupling strength \( J \), written as an intra-atomic interaction between the conduction electron spin \( \sigma_i \) and the localized magnetic moment represented by the spin operator \( \mathbf{S}_i \):

\[
H_{sf} = -J \sum_i \sigma_i \cdot \mathbf{S}_i.
\]  
(3)

According to the sign of the exchange coupling \( J \), a parallel \((J > 0)\) or an antiparallel \((J < 0)\) alignment of itinerant and localized spin is favoured with remarkable differences in the physical properties. The parallel \((J > 0)\) orientation is often referred to as "ferromagnetic Kondo-lattice model" (FKLM); alternatively known as "s-f or s-d model". The applications of the KLM are rather manifold.

A. Magnetic semiconductors:

Prototypes are the Europium chalcogenides EuX (X = O, S, Se, Te) [2] which are known to exhibit a spectacular temperature dependence of the band states. The "red shift" of the optical absorption edge upon cooling from \( T = T_c \) to \( T = 0K \) [2, 3] is due to a corresponding shift of the lower conduction band edge. There is clear evidence that in these materials the exchange \( J \) is positive, typically of order some tenth of eV. The coupling can therefore be classified as weak to intermediate.

B. Semimagnetic semiconductors:

In systems like \( \text{Cd}_{1-x}\text{Mn}_x\text{Te} \) and \( \text{Hg}_{1-x}\text{Fe}_x\text{Se} \) randomly distributed \( \text{Mn}^{2+} \) or \( \text{Fe}^{2+} \) ions provide localized magnetic moments which influence, via the exchange mechanism \( J \), the band states of the II-VI semiconductors CdTe and HgSe. For moderate doping \( x \), the moments do not order collectively so that a striking temperature dependence, as that of the magnetic semiconductors (EuX), cannot be expected. However, an anomalous magnetic field dependence of optical transitions and therewith of the bandstructure is observed [4] ("giant Zeeman splitting"). From respective experimental data, \( J > 0 \) can be concluded. The coupling must be classified as weak.

C. Local-moment metals:

In ferromagnetic metals such as the Rare Earth element Gd, the magnetism is due to strictly localized 4f electrons while the conductivity properties are determined by itinerant (5d, 6s) electrons. The \( T = 0 \)-moment of Gd is found to be 7.63\( \mu_B \) [5], \( 7\mu_B \) stem from the exactly half-filled 4f shell. The excess-moment of 0.63\( \mu_B \) originates from an induced spin polarization of the "a priori" non-magnetic conduction bands, indicating a weak or intermediate coupling \( J > 0 \) [6]. Many of the recent
research activities have been focussed on the temperature dependence of the induced exchange splitting. Is it collapsing for $T \to T_c$ or does it persist even in the paramagnetic phase [6, 7]? The $J$-induced correlation and quasi particle effects in the valence and conduction bands of Gd (or equivalently Dy, Tb) lead to highly complex and therefore controversially discussed photoemission data [8, 9], the interpretation of which is far from settled (see review in [7]). While the magnetic ordering of the semiconductors and insulators (class 1) has to be explained via special superexchange mechanisms, which is beyond the field of application of the FKLM, it is commonly accepted that the collective magnetism of the "local moment" metals is caused by the RKKY interaction. The latter is also based on the exchange interaction $J$. The FKLM therefore provides, at least in a qualitative manner, a selfconsistent description of magnetic and electronic properties of materials such as Gd [6, 10].

D. Manganites-perovskites

Since the discovery of the "colossal magnetoresistance (CMR)" [11, 12], the manganese oxides with perovskite structures $T_{1-x}D_x MnO_3$ ($T =$ La, Pr, Nd ; $D =$ Sr, Ca, Ba, Pb) have attracted high scientific interest. The prototypes $La_{1-x} (Ca, Sr)_x MnO_3$ are since long the protagonists of the "double exchange" mechanism [13]. Replacing, in $La^{3+} Mn^{3+} O_3$, a trivalent $La^{3+}$ ion by a divalent earth-alkali ion ($Ca^{2+}$, $Sr^{2+}$) requires an additional electron from the manganese for the binding. The result is a homogenous valence mixture of the manganese ion ($Mn^{2+}_{1-x} Mn^{3+}_x$). The three $3d - t_{2g}$ electrons of $Mn^{4+}$ are considered as more or less localized forming a local $S = 3/2$ spin. The fourth electron in $Mn^{3+}$ is of $3d - e_g$ type and is itinerant. It is assumed that it interacts via intra-shell Hund's rule coupling ("double exchange model" [14]) with the $S = 3/2$ spins. The manganites are bad electrical conductors. It has therefore to be assumed that the intraatomic coupling $J > 0$ is much stronger than the hopping-matrix element $|t|$ ($J \gg |t|$). Theoretical estimates for the bandwidth yield $W = 1 - 2 eV$ [15-17], experimental data propose $W = 3 - 4 eV$ [18, 19]. The exchange coupling $J$ is not very well known, the $J = 1 eV$ of refs. [15, 20] are sometimes questioned as being too small [21]. In any case, the manganites belong to the strongly coupled FKLM which cannot be treated perturbatively with respect to $J$. The FKLM will certainly be overcharged to reproduce all the details of the rich phase diagram of $La_{1-x}Ca_x MnO_3$, e.g., according to which the ground state is antiferromagnetic for $x = 0$ and 1, ferromagnetic for $x \approx 0.2 - 0.4$, with paramagnetic regions and phase separations in between [12]. Nevertheless, the FKLM is thought to give a reasonable frame work for an at least qualitative understanding of the interesting physics of the manganites [22, 23].

E. Heavy Fermions

The above subclasses are all characterized by a ferromagnetic exchange interaction $J > 0$. The original Kondo-lattice model [24], however, refers to $J < 0$, favouring an antiparallel alignment of conduction electron spin and localized spin. This situation is obviously realized in the Heavy-Fermion systems, which are to be found especially among Ce-compounds and which have provoked intensive research activities because of their extraordinary physical properties. Doniach [24] was the first to point out that there should be a phase transition from a magnetic state for small $|J|$ to a non-magnetic Kondo state for large $|J|$ characterized by a screening of the local moments by the conduction electron spins. The magnetic state is due to the RKKY-interaction, which as an effect of second order ($\sim J^2$) is independent of the sign of $J$. However, the Kondo screening is of course absent for $J > 0$, i.e., for all the above discussed subclasses. For most of the Heavy-Fermion systems, the RKKY coupling favours an antiferromagnetic ordering of the local moments. In $CeCu_{6-x}Au_x$ the competitive behaviour of the RKKY and the Kondo screening tendencies can impressively be observed by varying the concentration $x$ [25]. $CeCu_6 (x = 0)$ is non-magnetic because of perfect Kondo screening, while for $x > 0.1$ the RKKY component dominates taking care for an antiferromagnetic ordering up to $x = 1$ ($CeCu_5 Au$) with increasing Neel-temperature $TN$ for increasing $x$.

$J < 0$ does not necessarily lead to antiferromagnetism. The compound $CeSi_x$ is ferromagnetic for $1.6 \leq x \leq 1.85$ [26] with a strongly reduced magnetic moment. The Curie temperature of the ferromagnetic Kondo system ($J < 0$) $CeNi_x Pt_{1-x}$ first increases in between $x = 0$ and $x = 0.5$ from 5.8K ($x = 0$) to about 8.6K ($x = 0.5$) in order to decrease then rapidly and disappearing eventually at $x = 0.55$ [27]. The magnetic moment per Ce ion diminishes steadily with $x$ because of increasing Kondo screening and disappears completely at $x = 0.95$.

The above-presented list documents the rich variety of applications for the KLM. Since the many-body problem of the Hamiltonian (1) could not be solved exactly up to now, approximations must be tolerated. Most of the recent theoretical papers, aiming at the CMR-materials, assume classical spins $S \to \infty$ [28-30], mainly in order to be able to apply "dynamical mean field theory" (DMFT) to the FKLM problem. The merits of DMFT, e. g., with respect to the Hubbard model, are indisputable, but the assumption of classical spins in the KLM appears very problematic. Several important features, as, e.g., the magnon emission and absorption by the itinerant electrons, are excluded from the very beginning. The importance of such effects has been discussed in detail in ref. [10]. Conclusions such as, that at $T = 0$ the spins of the $e_g$ electrons are oriented parallel to the $t_{2g}$-spins [30], are correct only for $S \to \infty$. For any finite spin, there is a considerable amount of $\downarrow - \text{spectral weight overlapping with } \uparrow - \text{states even for very large } J$. Recently, a
DMFT-based approach to the KLM with quantum spins has been proposed [31] which uses a fermionization of the local spin operators. The theory is restricted to \( S = 1/2 \) but retains the quantum nature of the spins. A band splitting, which occurs already for relatively low interaction strengths, can be related to distinct elementary excitations, namely magnon emission and absorption by the itinerant electron and the formation of magnetic polarons. The results, which are in remarkable agreement with those from the "moment conserving decoupling approach" (MCDA) in ref. [10], confirm the importance of the quantum nature of the spins.

Due to some reasons, the above-mentioned theories [10, 31] are best justified for weak and intermediate couplings \( J \). In this paper, we propose an approximate scheme which mainly aims at the strong coupling regime \([10, 31]\) are best justified for weak and intermediate couplings \( J \). We use the abbreviations:

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If we are mainly interested in the conduction electron properties, then the single-electron Green function,

is of primary interest. Its equation of motion reads:

where the two types of interaction terms in (4) lead to the "spinflip function",

and the "Ising function":

The two "higher" Green functions on the right-hand side of (7) predict a direct solution of the equation of motion. A formal solution for the Fourier-transformed single-electron Green function,


defines the in general complex self-energy \( \Sigma_{k\sigma}(E) \) by the ansatz

\( \epsilon(k) \) are the Bloch energies:

An illustrative quantity which we are going to discuss in the following is the quasiparticle density of states (QDOS):

For the general case neither \( \Sigma_{k\sigma}(E) \) nor \( G_{k\sigma}(E) \) can be determined exactly. However, some rigorous statements are possible and shall now be listed up.

### II. THEORY

#### A. The many body problem

The model-Hamiltonian (1) defines a non-trivial many-body problem, the exact solution of which is known only for a small number of special cases. For practical reasons, it is sometimes more convenient to use the second quantized form of the exchange interaction (3):

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#### B. Zero-bandwidth limit

The final goal of our study is to arrive at a self-energy formula being credible first of all in the strong coupling limit \( JS >> W \). That means, in particular, that our approach has to fulfill the exactly solvable zero-bandwidth case [32]:

\( T_{ij} \to T_{0}\delta_{ij} \); \( \epsilon(k) \to T_{0} \forall k \).

The conduction band is shrunk to an N-fold degenerate level \( T_{0} \). The localized spin system, however, is furthoren
considered as collectively ordered for \( T < T_c \) by any direct or indirect exchange interaction. The latter is not a part of the KLM. The localized magnetization \( \langle S^z \rangle \) Therefore enters the calculation as external parameter. With (14), the hierarchy of equations of motion for the single-electron Green function \( G_{ij}(E) \), following from eq. (7), decouples exactly [32]. The result is a four-pole function:

\[
G_{i\sigma}^{(W=0)}(E) = \sum_{j=1}^{4} \frac{\alpha_{ij\sigma}}{E - E_{j\sigma}}
\]

with spin-independent poles at

\[
E_{1\sigma} = T_0 - \frac{1}{2}JS; \quad E_{2\sigma} = T_0 + \frac{1}{2}J(S + 1).
\]

\[
E_{3\sigma} = T_0 - \frac{1}{2}J(S + 1); \quad E_{4\sigma} = T_0 + \frac{1}{2}JS
\]

The \( j = 1,2 \)-excitations (Eq. (16)) refer to singly occupied sites; more strictly, they appear when the test electron is brought to a site, where no other "conduction" electron is present. It then orients its spin parallel (\( E_{1\sigma} \)) or antiparallel (\( E_{2\sigma} \)) to the local spin. These excitations are bound to spin-dependent spectral weights:

\[
\alpha_{1\sigma} = \frac{1}{2S + 1} \{ S + 1 + m_\sigma + \Delta_{-\sigma} \}
\]

\[
\alpha_{2\sigma} = \frac{1}{2S + 1} \{ S - m_\sigma - \Delta_{-\sigma} - S \langle n_{-\sigma} \rangle \}.\]

Here we have abbreviated:

\[
m_\sigma = z_\sigma \langle S^z \rangle
\]

\[
\Delta_{\sigma} = \langle S_i^z c_i^{\dagger} c_\sigma \rangle + z_\sigma \langle S_i^z n_{i\sigma} \rangle
\]

The "mixed" correlation function \( \Delta_{\sigma} \) can be derived via the spectral theorem from the Ising- and the spinflip-functions (8 and 9). Exploiting the equation of motion (7), this can even be expressed in terms of the single-electron Green function:

\[
\Delta_{\sigma} = \frac{1}{\pi h N} \sum_k \int_{-\infty}^{+\infty} dE f_-(E) (E - \epsilon(k)) ImG_{k\sigma}(E)
\]

\[
\langle n_{\sigma} \rangle = \frac{1}{\pi h N} \sum_k \int_{-\infty}^{+\infty} dE f_-(E) ImG_{k\sigma}(E).
\]

The expectation values in the spectral weights \( \alpha_{1,2\sigma} \) are, therefore, all selfconsistently determinable by the required single-electron Green function itself.

The two other poles \( E_{3\sigma} \) and \( E_{4\sigma} \) are bound to double occupancies of the lattice site. The test electron enters a site which is already occupied by another electron with opposite spin. The corresponding spectral weights,

\[
\alpha_{3\sigma} = \frac{1}{2S + 1} \{ S \langle n_{-\sigma} \rangle - \Delta_{-\sigma} \}
\]

\[
\alpha_{4\sigma} = \frac{1}{2S + 1} \{ (S + 1) \langle n_{-\sigma} \rangle + \Delta_{-\sigma} \}
\]

vanish in the limit of zero band occupation. It may be considered a shortcoming of the KLM that the excitation energies (17) do not contain the Coulomb interaction energy. Switching on a Hubbard interaction \( U \) leads to an additive term \( U \) in \( E_{3\sigma} \) as well as in \( E_{4\sigma} \) [32], shifting these excitations to higher energies. While the Hubbard-U is of course the exact ansatz in the zero-bandwidth limit, it is not so obvious by which type of Coulomb interaction the KLM should be extended ("correlated KLM" [30]) when aiming at one of the subclasses described in the Introduction. To avoid this ambiguity we restrict our following considerations to the low-density limit \( n \rightarrow 0 \), where the selfenergy of the zero-bandwidth KLM reads according to eqs. (16)-(19):

\[
\Sigma_{(W=0)}^{(\sigma)}(E) \rightarrow 0 \frac{J^2S(S + 1) - \frac{1}{2}Jm_\sigma(E - T_0)}{E - T_0 - \frac{1}{2}J(m_\sigma + 1)}.
\]

This rigorous result will be exploited later for testing our approximate theory.

### C. Ferromagnetically saturated semiconductor

There is another very instructive limiting case that can be treated exactly. It concerns a single electron in an otherwise empty conduction band interacting with a ferromagnetically saturated local moment system (\( T = 0 \)). In the zero-bandwidth limit (Sect. II.2) for the \( \uparrow \)-spectrum, all the spectral weights (19), (24) and (25) disappear, except for \( \alpha_{1\uparrow} = 1 \). In the \( \downarrow \)-spectrum the levels \( E_{1\downarrow} \) and \( E_{2\downarrow} \) survive with the weights \( \alpha_{1\downarrow} = \frac{1}{2S+1} \) and \( \alpha_{2\downarrow} = \frac{2S}{2S+1} \).

For finite bandwidth, the mentioned special case is that of a ferromagnetically saturated semiconductor (EuO at \( T = 0 \)) [10, 31, 33-35]. In this situation, an \( \uparrow \)-electron has no chance for a spin-flip, the corresponding quasi-particle density of states, \( \rho_{\uparrow}(E) \), is therefore only rigidly shifted compared to the "free" DOS [10] and the self-energy is a constant:

\[
\Sigma_{k\uparrow}^{(T=0,n=0)}(E) = \Sigma_{k\downarrow}^{(T=0,n=0)}(E) = \frac{1}{2}JS.
\]
The $\downarrow$-spectrum is more complicated since a $\downarrow$-electron has several possibilities to exchange its spin with the antiparallel, localized spins. The spinflip function (8) does not at all vanish as in the $\uparrow$-case. Nevertheless, the problem is exactly solvable resulting in a wave-vector independent self-energy:

$$\Sigma^{(T=0,n=0)}(E) = \frac{1}{2}JS \left( 1 + \frac{JG_0(E + \frac{1}{2}JS)}{1 - \frac{1}{2}JG_0(E + \frac{1}{2}JS)} \right).$$

(28)

$G_\sigma(E)$ is the "free" propagator:

$$G_0(E) = \frac{1}{N} \sum_k G^{(0)}_{k\sigma}(E) = \frac{1}{N} \sum_k \frac{1}{E - \epsilon(k)}.$$  

(29)

The reason for the wave-vector independence of the self-energy can be traced back [10] to the lack of a direct (Heisenberg) exchange term in the model-Hamiltonian (1). Therefore $\Sigma^{(T=0,n=0)}(E)$ does not contain magnon energies $\hbar \omega(q)$ which come into play when the excited $\downarrow$-electron flips its spin by magnon emission. Neglecting the exchange between the local-moment spins $S_i$ may be considered as the $\hbar \omega(q) \equiv 0$ case. As a consequence, the electronic self-energy becomes wave-vector independent. There does not arise any problem in calculating the limit ($n = 0$, $T = 0$) with the inclusion of a Heisenberg exchange ($\sim J_\delta S_i \cdot S_j$). Then the wave-vector dependence of the selfenergy reappears [10].

D. Second-order perturbation theory

Conventional diagrammatic perturbation theory for the Kondo-lattice model does not work because of the lack of Wick’s theorem. A fertile alternative is the Mori-Formalism [36, 37], which allows for a systematic expansions of the electronic selfenergy of the KLM with respect to the powers of $J$. That has successfully been done previously for the weakly coupled Hubbard model by the use of the modified perturbation theory of [38, 39]. In the case of the KLM, the first order term is just the mean-field result $\frac{1}{2}Jm_\sigma$, while in the second order, one finds (Eq. (3.12) in ref. 39):

$$\Sigma^{(2)}_{k\sigma}(E) \rightarrow \frac{J^2}{4N^2} \sum_q \left\langle \left( \left\langle S_{-q}^z S_q^z \right\rangle^{(1)} \right\rangle G^{(0)}_{k+q} \left( E - \frac{1}{2}Jm_\sigma \right) \right.$$  

$$+ \left\langle \left\langle \delta S_{-q}^z \cdot \delta S_q^z \right\rangle^{(1)} \right\rangle G^{(0)}_{k+q} \left( E + \frac{1}{2}Jm_\sigma \right) \right\rangle.$$  

(30)

$< \cdots >^{(1)}$ means mean-field averaging, while the q-dependent spin operator is defined as usual,

$$S^\alpha_q = \sum_i S_i^\alpha e^{-i\mathbf{q} \cdot \mathbf{R}_i} \quad (\alpha = +, -, z).$$

(31)

$\delta S^z_q$ is a short-hand notation:

$$\delta S^z_q = S^z_q - \left\langle S^z_q \right\rangle^{(1)}.$$  

(32)

In the following we are interested in the local self-energy $\Sigma^\sigma(E) = \frac{1}{2} \sum_k \Sigma_{k\sigma}(E)$ only, for which we find with (30) up to order $J^2$ in the limit $n \to 0$ to be:

$$\Sigma^\sigma(E) = -\frac{1}{2} Jm_\sigma + \frac{1}{4} J^2 \{ S(S + 1) - m_\sigma(m_\sigma + 1) \} G_0(E) + O(J^3).$$  

(33)

E. High-energy expansions

For controlling unavoidable approximations, the spectral moments $M_{k\sigma}^{(n)}$ of the spectral density $S_{k\sigma}(E)$

$$S_{k\sigma}(E) = -\frac{1}{\pi} \text{Im} G_{k\sigma}(E)$$

are of great importance:

$$M_{k\sigma}^{(n)} = \frac{1}{\hbar} \int_{-\infty}^{+\infty} dE \cdot E^n \cdot S_{k\sigma}(E).$$  

(35)

In principle, they can be calculated rigorously via the equivalent expression

$$M_{k\sigma}^{(n)} = \left\langle \left[ \cdots [c_{-\sigma}, H]_{-\sigma}, \cdots, c_{-\sigma}]_{-\sigma} \right]^{+}_{n-fold} \right\rangle.$$  

(36)

There is a close connection between the spectral moments and the high-energy behaviour of the Green function:

$$G_{k\sigma}(E) = \int_{-\infty}^{+\infty} dE' \frac{S_{k\sigma}(E')}{E - E'}$$  

$$= \frac{1}{E} \sum_{n=0}^{\infty} \int_{-\infty}^{+\infty} dE' \left( \frac{E'}{E} \right)^n S_{k\sigma}(E').$$  

(37)

Because of the Dyson equation,

$$EG_{k\sigma}(E) = \hbar + \left( \epsilon(k) + \Sigma_{k\sigma}(E) \right) G_{k\sigma}(E)$$

an analogous expansion holds for the selfenergy:

$$\Sigma_{k\sigma}(E) = \sum_{m=0}^{\infty} \frac{C_{k\sigma}^{(m)}}{E^m}.$$  

(39)

The coefficients $C_{k\sigma}^{(m)}$ turn out to be simple functions of the moments up to order $m + 1$:

$$C_{k\sigma}^{(0)} = M_{k\sigma}^{(1)} - \epsilon(k)$$  

(40)
Using the definition (36), the moments of the KLM can be explicitly calculated by the use of the model-Hamiltonian (1). After tedious but straightforward manipulations, one finds in the low-density limit (\(n \to 0\)), for the first four moments:

\[ M_{k\sigma}^{(0)} = 1 \]  
\[ M_{k\sigma}^{(1)} = \epsilon(k) - \frac{1}{2} J m_\sigma \]  
\[ M_{k\sigma}^{(2)} = \epsilon^2(k) - J m_\sigma \epsilon(k) + \frac{1}{4} J^2 (S(S + 1) - m_\sigma) \]  
\[ M_{k\sigma}^{(3)} = \epsilon^3(k) - \frac{3}{2} J m_\sigma \epsilon^2(k) + \frac{1}{4} J^2 \{ A_\sigma(k) + B(k) + 2 \epsilon(k)(S(S + 1) - m_\sigma) \} + \frac{1}{8} J^3 \{ S(S + 1)(1 - m_\sigma) - m_\sigma \}. \]

\( A_\sigma(k) \) and \( B(k) \) are related to spin-correlation functions:

\[ A_\sigma(k) = \frac{1}{N} \sum_{i,j} e^{ik(R_i - R_j)} T_{ij} \langle S_i^{- \sigma} \cdot S_j^{\sigma} \rangle \]  
\[ B(k) = \frac{1}{N} \sum_{i,j} e^{ik(R_i - R_j)} T_{ij} \langle S_i^{\sigma} \cdot S_j^{- \sigma} \rangle. \]

Inserting these expressions into eqs. (40-42) we get for the first three selfenergy coefficients:

\[ C_{k\sigma}^{(0)} = -\frac{1}{2} J m_\sigma \]  
\[ C_{k\sigma}^{(1)} = -\frac{1}{4} J^2 (S(S + 1) - m_\sigma(m_\sigma + 1)) \]  
\[ C_{k\sigma}^{(2)} = -\frac{1}{4} J^2 (A_\sigma(k) + B(k) - \epsilon(k)m_\sigma^2) + \frac{1}{8} J^3 (1 + m_\sigma)(S(S + 1) - m_\sigma(m_\sigma + 1)). \]

They determine the high-energy behaviour of the selfenergy (39).

**F. Interpolation formula**

We want to construct an approximate expression for the electronic selfenergy of the low-density KLM, which fulfills the zero-bandwidth limit (26) for all temperatures \(T\) and arbitrary coupling strengths \(J\), as well as the exact \(T = 0\)-result (27) and (28) for arbitrary bandwidths and couplings. Furthermore, it should reproduce the correct high-energy (strong coupling) behaviour (39) and in addition also the weak-coupling result (33). Guided by the non-trivial \((n = 0, T = 0)\)-result (28), we start with the following ansatz for the local selfenergy:

\[ \Sigma_\sigma(E) = -\frac{1}{2} J m_\sigma + \frac{1}{4} J^2 a_\sigma G_0(E - \frac{1}{2} J m_\sigma) + \frac{1}{4} J^2 b_\sigma G_0(E - \frac{1}{2} J m_\sigma). \]

\(a_\sigma\) and \(b_\sigma\) are at first unknown parameters. It is easy to recognize that this ansatz reproduces the exact limit (27) and (28) of ferromagnetic saturation, if \(T = 0, n = 0\),

\[ a_\sigma = (1 - z_\sigma)S \quad b_\downarrow = \frac{1}{2} J \quad b_\uparrow \text{ arbitrary} \]

and the zero-bandwidth limit (26), if

\[ \epsilon(k) \to 0 \quad \forall k \]

\[ a_\sigma = S(S + 1) - m_\sigma(m_\sigma + 1) \]

\[ b_\sigma = b_{- \sigma} = \frac{1}{2} J \]

We note that (54) agrees with (53) for \(T=0\)!

By (52), we concentrate ourselves from the very beginning on the local part of the selfenergy. As already stated above, the wave-vector dependence of the selfenergy is mainly due to magnon energies \(\hbar \omega(q)\) appearing at finite temperature in magnon emission and absorption processes by the band electron. However, the neglect of a direct Heisenberg exchange between the localized spins in the KLM can be interpreted as the \(\hbar \omega(q) \to 0\) limit.

We fix the parameters \(a_\sigma\) and \(b_\sigma\) in the ansatz (52), by equating the high-energy expansion (39). For this purpose, we first develop (52) in terms of powers of the inverse energy. That requires the respective high-energy expression of the mean-field propagator \(G_0(E - \frac{1}{2} J m_\sigma)\), which is exactly known:

\[ G_0 \left( E - \frac{1}{2} J m_\sigma \right) = \sum_{n=0}^{\infty} \frac{M_\sigma^{(n)}}{E^{n+1}} \]

\[ M_\sigma^{(n)} = \frac{1}{N} \sum_k \left( \epsilon(k) + \frac{1}{2} J m_\sigma \right)^n. \]

From (52) it then follows:

\[ G_0 \left( E - \frac{1}{2} J m_\sigma \right) = \sum_{n=0}^{\infty} \frac{M_\sigma^{(n)}}{E^{n+1}} \]

\[ M_\sigma^{(n)} = \frac{1}{N} \sum_k \left( \epsilon(k) + \frac{1}{2} J m_\sigma \right)^n. \]
\[ \Sigma_{\sigma}(E) = -\frac{J m_{\sigma}}{2} + \frac{J^2 a_{\sigma}}{4} \sum_{m=0}^{\infty} \frac{M_{\sigma}^{(m)}}{E_{m+1}} \sum_{p=0}^{\infty} \left[ b_p \sum_{n=0}^{\infty} \frac{\hat{M}_{\sigma}^{(n)}}{E_{n+1}} \right]^p \]

\[ = -\frac{1}{2} J m_{\sigma} + \frac{1}{E} \left\{ \frac{1}{4} J^2 \hat{M}_{\sigma}^{(0)} \right\} a_{\sigma} + \frac{1}{E^2} \left\{ \frac{1}{4} J^2 a_{\sigma} \times \left( \hat{M}_{\sigma}^{(1)} + b_{\sigma} \left( \hat{M}_{\sigma}^{(0)} \right)^2 \right) \right\} + O \left( \frac{1}{E^3} \right). \] (57)

The so-derived local selfenergy coefficients,

\[ C_{\sigma}^{(m)} = \frac{1}{N} \sum_{k} C_{k,\sigma}^{(m)} \] (58)

\[ C_{\sigma}^{(0)} = \frac{1}{2} J m_{\sigma} \] (59)

\[ C_{\sigma}^{(1)} = \frac{1}{4} J^2 a_{\sigma} \] (60)

\[ C_{\sigma}^{(2)} = \frac{1}{4} J^2 a_{\sigma} \left( T_0 + \frac{1}{2} J m_{\sigma} + b_{\sigma} \right) \] (61)

\[ (\sigma = e) \]

can be compared to the exact expressions following from (49)-(51):

\[ C_{\sigma}^{(0)} = -\frac{1}{2} J m_{\sigma} \] (62)

\[ C_{\sigma}^{(1)} = \frac{1}{4} J^2 (S(S+1) - m_{\sigma}(m_{\sigma}+1)) \] (63)

\[ C_{\sigma}^{(2)} = \frac{1}{4} J^2 \left( T_0 + \frac{1}{2} J (1 + m_{\sigma}) \right) (S(S+1) - m_{\sigma}(m_{\sigma}+1)). \] (64)

\[ C_{\sigma}^{(0)} \] is identically fulfilled. Agreement for the two other coefficients is achieved by setting

\[ a_{\sigma} = S(S+1) - m_{\sigma}(m_{\sigma}+1) \] (65)

\[ b_{\sigma} = \frac{1}{2} J = b_{-\sigma}. \] (66)

These are the same expressions as found in (54) for the special zero-bandwidth limit.

Inserting (65) and (66) into (52) yields a self-energy result, which is exact for \( T = 0 \) (\( m_{\sigma} = z_{\sigma} S \)) but arbitrary bandwidths \( W \) and exchange couplings \( J \). It fulfills the zero-bandwidth limit for all couplings \( J \) and all temperatures \( T \). It obeys the high-energy behaviour which is important for the strong-coupling regime. Furthermore, the comparison with (33) shows that the approach fits second-order perturbation theory, thus being reliable in the weak-coupling regime, too. We believe that (52) together with (65) and (66) represents a trustworthy approach to the low-density self-energy of the Kondo-lattice model. In the next Section we present a numerical evaluation.

### III. RESULTS

We have evaluated our theory for an sc lattice using the respective Bloch-density of states (B-DOS) in tight-binding approximation [40]. The center of gravity \( T_0 \) of the Bloch-band is chosen as energy zero. Fig. 1 shows the temperature-dependent quasiparticle density of states (Q-DOS) \( \rho_{\sigma}(E) \) for a strongly coupled system \( J = 2.0 \text{ eV}, S = 7/2, W = 1 \text{ eV} \). The electronic spectrum gets its temperature-dependence exclusively through the local-moment magnetization \( m = |m_{\sigma}| = |(S^z)| \), which must be considered as an external parameter. \( m = 3.5 \) means \( T = 0K \) (ferromagnetic saturation), while \( m = 0 \) belongs to \( T = T_c \). The Q-DOS for each spin direction consists of two subbands separated by an energy of the order \( \frac{1}{2} J (2S + 1) \). They originate from the two atomic levels \( E_{1\sigma} \) and \( E_{2\sigma} \) in the zero-bandwidth limit (16).

A special case is the ferromagnetic saturation, for which the ↑-spectrum consists only of the undeformed low-energy band \( \rho_\uparrow(E) = \rho_\downarrow E = \rho_\downarrow (E + \frac{1}{2}JS) \). The ↑-electron has no chance to exchange its spin with the perfectly aligned local-spin system. The spinflip terms in the exchange interaction (4) therefore do not work, only the Ising-like part (first term in (4)) takes care for a rigid shift of the excitation spectrum. The ↓-spectrum is more complicated because a ↓-electron can, even at \( T = 0K \), exchange its spin with the ferromagnetically saturated spin system. One possibility is to emit a magnon, therewith reversing its own spin and becoming a ↑-electron. Such a spinflip-excitation is of course
possible only if there are ↑ states within reach on which the original ↓ electron can land after the spinflip. That is the reason why the low-energy ↓ subband occupies the same energy region as the ↑ band.

For $T > 0$ ($m < 3.5$) the ↑ spectrum too, becomes more structured because the localized spin system is no longer perfectly aligned. The system now contains magnons which can be absorbed by the ↑ electron. Even polaron formation becomes possible. The spectral weight of the upper ↑ quasiparticle subband raises with increasing temperature, i.e., increasing magnon density. Fig.1 illustrates that the temperature-dependence of the Q-DOS mainly affects the spectral weights of the subbands and not so much their positions. This is a typical feature of the strong coupling regime $JS >> W$. In such a situation, the band electron mobility is rather poor, it stays for a relatively long time at the same lattice site. The actual quantization axis is then the localized spin ($S = 3/2$), to which the electron can orient its spin parallel ("spin up" in the local frame) or antiparallel ("spin down" in the local frame). The excitation energy for a parallel alignment roughly amounts to $-\frac{1}{2}JS$, and for an antiferromagnetic alignment, to $+\frac{1}{2}J(S + 1)$. The lower quasiparticle subband consists of states belonging to the situation where the band electron appears in the local frame as "spin up" electron. This may happen directly or after emitting/absorbing a magnon. In the upper subband the electron has entered the local frame with an enlarged vertical scale.

FIG. 2: Same as in figure 1 but with enlarged vertical scale.

FIG. 3: Quasi-particle density of states (in the positive half of the frame) and imaginary part of the selfenergy (in the negative half of the frame) as a function of energy for various values of magnetization. Full line for spin up and dotted line for spin down. $J = 2$, $S = 3/2$ and $W = 1$.

FIG. 4: Quasi-particle density of states as a function of energy for various values of magnetization. Full line for spin up and dotted line for spin down. $J = 2$, $S = 3/2$ and $W = 1$.

The ↓ electron has another possibility to exchange its spin with the ferromagnetically saturated moment system by a repeated magnon emission and reabsorption. In a c lattice rametation of laron” upper that p in the quasip change
frame as "spin down" electron. This is impossible for a \( \uparrow - \downarrow \) electron at \( T = 0 \)K, when all localized spins are parallelly aligned \( (m = S) \). While the excitation energies are almost temperature-independent, the probability for the electron to be in the local frame as a "spin up" or as a "spin down" particle strongly depends on temperature. That manifests itself in the spectral weight of the respective quasiparticle subband, which therefore is temperature- and spin-dependent. There remains a small probability that the band electron is not trapped by the localized spin, but rather propagates with high mobility through the spin lattice. In such a case the effective quantization axis is no longer the local spin but rather the direction of the global magnetization \( \langle S^z \rangle \). Fig.2 shows the Q-DOS for the same parameters as in Fig. 1 but on a finer scale. One recognizes two tiny satellites which emerge from the two main peaks with increasing temperature (decreasing magnetization \( m \)). The \( \downarrow \)-satellite has a lower energy than the \( \uparrow - \) satellite. This can be understood as follows: The original \( \downarrow \) electron, for entering the low energy part of the spectrum, will predominantly do this by emitting a magnon thereby reversing its own spin. In case of being not trapped by a local spin, it then moves as a \( \downarrow \) electron through the spin lattice. On the other hand, an original \( \uparrow \) electron has to absorb a magnon in order to enter the high-energy part of the spectrum and propagating then as \( \downarrow \) electron. With decreasing magnetization the two satellites collapse mean field-like. In the strong coupling region (\( JS \gg W \)), pictured in Figs. 1 and 2, the satellites have only very small spectral weights, nevertheless representing interesting physics.

The parameters used in Figs. 3, 4 and 5 (\( J = 2 \)eV, \( W = 1 \)eV, \( S = 3/2 \)) should be typical for the manganites. It is sometimes claimed \([21,30]\) that because of the strong coupling \( JS \), the itinerant electron \( (e_g) \) spin is oriented at \( T = 0 \)K in any case parallel to the localized \( (t_{2g}) \) spin. According to the exact \( m = S = 3/2 \)-part of Fig.3, this can strictly be ruled out for the FKLM. In the mentioned papers the assumption of full polarization is an artefact due to the restriction to classical spins \( (S \to \infty) \). The temperature-dependence of the Q-DOS is of course very similar to the \( S = 7/2 \) case in Fig. 1. Even the satellites, which describe the "free" electron propagation after emitting/absorbing a magnon, do appear (Fig. 4). However, because of the smaller distance between the two main peaks \( (\approx \frac{1}{2} J(2S + 1)) \) the mean-field shift of the satellites is not so clearly visible as for the higher spin in Fig. 1.

The imaginary part of the self-energy is directly related to quasiparticle damping and lifetime, respectively. Fig. 3 demonstrates that the polaron states (upper part of the spectrum) represent quasiparticles with almost infinite lifetimes since \( \text{Im} \Sigma_\sigma (E) \) is zero in this region. For \( T = 0 \)K, this is an exact result. In ferromagnetic saturation the whole \( \uparrow - \downarrow \) spectrum consists of stable states. It turns out that, in the here discussed strong coupling regime, even for finite temperatures, only the states of the mean-field satellites are getting finite lifetimes. The sharp peak of \( \text{Im} \Sigma_\sigma (E) \) falls always into the bandgap, which is provoked by a divergence of the real part of the selfenergy (Fig. 5). It has therefore no direct influence on the lifetime of quasiparticles.

Up to now we have only discussed the FKLM in the strong coupling regime. As demonstrated in Sect. II.D, our interpolating approach is correct in the weak-coupling region, too. Fig. 6 shows, as an example, the Q-DOS for \( J = 0.2 \)eV, \( W = 1 \)eV and \( S = 3/2 \). The tendency to the two-subband structure can be recognized for weak couplings, too. The physical interpretation of the responsible elementary processes is the same as in the above-discussed strong coupling case. For \( T = 0 \) all \( \uparrow \) states represent stable quasiparticles, the respective imaginary part of the selfenergy vanishes. With increasing demagnetization of the local moment system, \( \text{Im} \Sigma_\uparrow (E) \) becomes finite indicating finite lifetimes of \( \uparrow - \) quasiparticles due to magnon absorption, which is impossible at \( T = 0 \) because of ferromagnetic saturation. Magnon emission by \( \downarrow \) electrons, however, is always possible. It should be pointed out that the upper part of the \( \downarrow \) spectrum obviously consists, at low temperature, of stable polaron states.

It is surprising that already very small couplings are sufficient to create a pseudo gap in the quasiparticle...
FIG. 6: Quasi-particle density of states (in the positive half of the frame) and imaginary part of the selfenergy (in the negative half of the frame) as a function of energy for different values of magnetization. Full line for spin up and dotted line for spin down. Imaginary selfenergy is multiplied by a factor of 5 for better clarity. \( J = 0.2 \), \( S = 3/2 \) and \( W = 1 \).

FIG. 7: Quasi-particle density of states as a function of energy for different values of coupling constant \( J \). Full line for spin up and dotted line for spin down. \( m = 1.5 \) (ferromagnetic saturation), \( S = 3/2 \) and \( W = 1 \).

spectrum. According to Fig. 7, which shows the exact \( T = 0 - \rho_\sigma(E) \) for various exchange couplings \( J \), the gap opens already for \( J = 0.4eV \). Our results for the weakly coupled FKLM are very similar to those presented in ref. 10.

IV. CONCLUSIONS

We have presented an approach to the ferromagnetic Kondo-lattice model in the low-density limit \( (n \to 0) \). The theory uses an interpolation formula for the electronic selfenergy which fulfills a maximum number of limiting cases. It reproduces the non-trivial rigorous special case of a single electron in an otherwise empty conduction band at \( T = 0 \) (ferromagnetically saturated semiconductor), and that for arbitrary bandwidths and coupling constants. It is exact in the zero-bandwidth limit for all temperatures and all exchange couplings. It obeys the high-energy expansion of the selfenergy, guaranteeing therewith the right strong-coupling behaviour, as well as perturbation theory of second order (\( \propto J^2 \)) for the weak-coupling magnet reparation

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