Uniform hopping approach to the FM Kondo Model at finite temperature

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(Dated: November 28, 2002)

We study the ferromagnetic Kondo model with classical corespins via unbiased Monte-Carlo simulations and derive a simplified model for the treatment of the corespins at any temperature. Our simplified model captures the main aspects of the Kondo model and can easily be evaluated both numerically and analytically. It provides a better qualitative understanding of the physical features of the Kondo model and rationalizes the Monte-Carlo results including the spectral density $A(k)$ of a 1D chain with nearest neighbor Coulomb repulsion. By calculating the specific heat and the susceptibility of systems up to size $16^4$, we determine the Curie temperature of the 3D one-orbital double-exchange model, which agrees with experimental values.

PACS numbers: 71.10.-w, 75.10.-b, 75.30.Kz

I. INTRODUCTION

Manganese oxides such as La$_{1-x}$Sr$_x$MnO$_3$ and La$_{1-x}$Ca$_x$MnO$_3$ have been attracting considerable attention since the discovery of colossal magnetoresistance (CMR). These materials crystalize in the perovskite-type lattice structure where the crystal field breaks the symmetry of the atomic wave function of the manganese $d$-electrons. The energetically lower $t_{2g}$ levels are occupied by three localized electrons. Due to a strong Hund coupling their spins are aligned, forming a localized corespin with $S = 3/2$. The electron configuration of the Mn$^{3+}$ ion is $t_{2g}^3 e_g^1$, whereas for Mn$^{4+}$ ions the $e_g$ electron is missing. Due to a hybridization of the $e_g$ wave function with the oxygen $2p$ orbitals, the $e_g$ electrons are itinerant and can move from an Mn$^{3+}$ ion to a neighboring Mn$^{4+}$ via a bridging $O^{2-}$. The interplay of various physical ingredients such as the strong Hund coupling of the itinerant electrons to localized corespins, Coulomb correlations, and electron-phonon coupling leads to a rich phase diagram including antiferromagnetic insulating, ferromagnetic metallic and charge ordered domains. The carriers moving in the spin and orbital background show remarkable dynamical features.

Since full many-body calculations for a realistic model, including all degrees of freedom, are not possible yet, several approximate studies of simplified models have been performed in order to unravel individual pieces of the rich phase diagram of the manganites. The electronic degree of freedom are generally treated by a Kondo lattice model, which in the strong Hund coupling limit is commonly referred to as the double-exchange (DE) model, a term introduced by Zener. In addition, the correlation of the itinerant $e_g$ electrons is well described by a nearest neighbor (n.n.) Coulomb interaction. The on-site Hubbard term merely renormalizes the already strong Hund coupling. For the Kondo model with quantum spins, it is still impossible to derive rigorous numerical and analytical results. If the $S=3/2$ corespins are treated classically, however, the model can be treated by unbiased Monte Carlo techniques. The impact of quantum spins on the electronic properties has been studied in Ref. It appears that quantum effects are important for $S=1/2$ corespins or at $T = 0$. For finite temperature and $S=3/2$, classical spins present a reasonable approximation.

Elaborate Monte Carlo (MC) simulations for the FM Kondo model with classical corespins have been performed by Dagotto et al. and Yi et al. and by Furukawa et al. Static and dynamical properties of the model have been determined. These studies revealed features which have been interpreted as signatures of phase-separation (PS). PS has also been reported from computations based on a dynamical mean field treatment of the DE model at $T = 0$. A phase diagram and critical exponents of the DE model have been determined with a Hybrid MC algorithm.

In the manganites, the Hund coupling $J_H$ is much stronger than the kinetic energy. Consequently, configurations are very unlikely in which the electronic spin is antiparallel to the local corespin. It is therefore common practise to use $J_H = \infty$ and to ignore antiparallel spin arrangements altogether. This approximation yields reasonable results in the ferromagnetic regime. Close to half-filling, however, a finite ferromagnetic Hund coupling even enhances the antiferromagnetic ordering of the corespins. In a previous paper, we have proposed an effective spinless fermion (ESF) model that takes effects of antiparallel $t_{2g} - e_g$ spin configurations into account via virtual excitations. It has been demonstrated that the results of the ESF model are in excellent agreement with those of the original Kondo model even for moderate values of $J_H$.

In Ref. we also introduced the uniform hopping approach (UHA), which replaces the influence of the random corespins on the $e_g$ electron dynamics by an effective uniform hopping process. In that work, the hopping parameter was determined by minimization of the ground-state energy. Essential physical features of the original model could be described even quantitatively by UHA, while the configuration space, and hence the numerical effort, was reduced by several orders of magnitude. Besides the numerical advantage, UHA also allows the derivation of analytical results in some limiting cases.

In the present paper we extend the UHA to finite
temperature. Thermal fluctuations of the corespins are mapped to fluctuations of the uniform hopping parameter. In order to include entropy effects correctly, we have to determine the density $\Gamma(u)$ of corespin states for a given hopping parameter $u$. The reliability of the finite-temperature UHA is scrutinized by a detailed comparison of the results for various properties of the one-orbital DE model with unbiased MC data.

So far, in most MC simulations the Coulomb interaction of the $e_g$ electrons has been neglected due to its additional computational burden. It should, however, have an important impact, particularly on phase separation. Moreover, at quarter filling the n.n. repulsion leads to the charge ordering (CO) phase. We have performed MC simulations for the Kondo model including a Hubbard-like Coulomb interaction. In these simulations, for each classical corespin configuration, the electronic degrees of freedom are treated by Lanczos exact diagonalization. We find that also in this case UHA yields reliable results while reducing the computational complexity by orders of magnitude. An excerpt of the results is given here, while a thorough discussion will be provided elsewhere.

Moreover, at quarter filling the n.n. repulsion leads to an important impact, particularly on phase separation. For strong Hund coupling $J_H \gg t$, the electronic density of states (DOS) essentially consists of two sub-bands, a lower- and an upper 'Kondo band', split by approximately $2J_H$. In the lower band the itinerant $e_g$ electrons move such that their spins are predominantly parallel to the $t_{2g}$ corespins, while the opposite is true for the upper band. Throughout this paper, the electronic density $n$ (number of electrons per orbital) will be restricted to $0 \leq n \leq 1$, i.e. only the lower Kondo band is involved.

II. MODEL HAMILTONIAN AND UNBIASED MONTE CARLO

In this paper, we will concentrate on properties of the itinerant $e_g$ electrons interacting with the local $t_{2g}$ corespins. It is commonly believed that the electronic degrees of freedom are well described by a multi-orbital Kondo lattice model

$$
\hat{H} = - \sum_{i,\alpha,\beta} t_{i\alpha,j\beta} a_{i\alpha\sigma}^\dagger a_{j\beta\sigma} + J_H \sum_{i,\alpha} \hat{\sigma}_{i\alpha} \hat{S}_i + \sum_{i,j,\alpha,\beta} V_{ia,j\beta} \hat{n}_{ia} \hat{n}_{j\beta} + J' \sum_{<ij>} \mathbf{S}_i \cdot \mathbf{S}_j .
$$

As proposed by de Gennes, Dagotto et al., and Furukawa the $t_{2g}$ spins $\mathbf{S}_i$ are treated classically, which is equivalent to the limit $S \to \infty$. The spin degrees of freedom are thus replaced by unit vectors $\mathbf{S}_i$, parameterized by polar and azimuthal angles $\theta_i$ and $\phi_i$, respectively. The magnitude of both corespins and $g$-spins is absorbed into the exchange couplings.

Equation (1) consists of a kinetic term for the itinerant $e_g$ electrons with transfer integrals $t_{i\alpha,j\beta}$, where $i(j)$ are site indices, $\alpha(\beta)$ orbital indices, and $\sigma(\sigma')$ spin indices. The transfer integrals, which are restricted to n.n. sites, are given as matrices in the orbital indices $\alpha, \beta = 1(2)$ for $x^2-y^2$ ($3z^2-r^2$) orbitals (see e.g. Ref. 22).

$$
t_{i,i+\hat{z}} = t \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad t_{i,i+\hat{z}/\hat{y}} = t \begin{pmatrix} 3/4 & \mp \sqrt{3}/4 \\ \mp \sqrt{3}/4 & 1/4 \end{pmatrix} .
$$

The overall hopping strength $t$, which will be used as unit of energy, by setting $t = 1$. The operators $a_{i\alpha\sigma}^\dagger (a_{i\alpha\sigma})$ create (annihilate) $e_g$ electrons at site $x_i$ in orbital $\alpha$ with spin $\sigma$. The second term of the Hamiltonian describes the Hund coupling with exchange integral $J_H$, where $\hat{\sigma}_{i\alpha}$ stands for the spin of the electron at site $i$ in orbital $\alpha$. The spin-resolved occupation number operator is denoted by $\hat{n}_{i\alpha\sigma}$. The third term describes a Coulomb repulsion, with $\hat{n}_{ia}$ being the spin-integrated density operator. The local Hubbard interaction is excluded from the sum, i.e. $V_{ia,ia} = 0$, as it effectively merely modifies the Hund coupling $J_H$. Finally, Eq. (1) contains a superexchange term. The value of the exchange coupling is $J' \approx 0.022$ accounting for the weak antiferromagnetic coupling of the $t_{2g}$ electrons.

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A. Effective Spinless Fermions

It is expedient to use the individual $t_{2g}$ spin directions $\vec{S}_i$ as the local quantization axes for the spin of the itinerant $e_g$ electrons at the respective sites. This representation is particularly useful for the $J_H \to \infty$ limit, but also for the projection technique, which takes into account virtual processes for finite Hund coupling. The transformation in the electronic spin is described by a local unitary $2 \times 2$ matrix $U(S_i)$ with

$$\vec{a}^\dagger_{i\alpha} = U(S_i) \vec{c}^\dagger_{i\alpha}, \quad \vec{c}^\dagger_{i\alpha} = U^\dagger(S_i) \vec{a}^\dagger_{i\alpha},$$

where $\vec{a}^\dagger_{i\alpha}$ is a column vector with entries $a_{i\alpha\uparrow}$ and $a_{i\alpha\downarrow}$, respectively. The transformed annihilation operators in local quantization are represented by $\vec{c}^\dagger_{i\alpha}$. For the creation operators we have

$$\vec{a}^\dagger_{i\alpha} = \vec{c}^\dagger_{i\alpha} U(S_i), \quad \vec{c}^\dagger_{i\alpha} = \vec{a}^\dagger_{i\alpha} U(S_i).$$

The unitary matrix $U(S_i)$ depends upon $S_i$ and is chosen such that it diagonalizes the individual contributions to the Kondo exchange

$$\vec{a}_{i\alpha} \vec{S}_i = \vec{a}^\dagger_{i\alpha} \left( \vec{S}_i \right) \vec{a}_{i\alpha} = \vec{c}^\dagger_{i\alpha} \left( U^\dagger(S_i) \left( \vec{S}_i \right) U(S_i) \right) \vec{c}_{i\alpha},$$

(5)

with $\vec{S}$ being the vector of Pauli matrices. The eigenvalues of of $(\vec{S}_i)$ are $\pm 1$ and the matrix of eigenvectors is given by

$$U(S_i) = \left( \begin{array}{cc} c_i & s_i e^{-i\phi_i} \\ s_i e^{i\phi_i} & -c_i \end{array} \right),$$

(6)

with the abbreviations $c_j = \cos(\theta_j/2)$ and $s_j = \sin(\theta_j/2)$ and the restriction $0 \leq \theta_j \leq \pi$. The Kondo exchange term in Eq. (3) in the new representation reads

$$\vec{a}_{i\alpha} \vec{S}_i = \hat{n}_{i\alpha\uparrow} - \hat{n}_{i\alpha\downarrow}.$$  

(7)

The spin-integrated density operators $\hat{n}_{i\alpha}$ are unaffected by the unitary transformation. The entire Kondo Hamiltonian becomes

$$\hat{H} = - \sum_{ij\alpha,\beta} t^\sigma_{ij,\alpha}\beta c^\dagger_{i\sigma\alpha} c_{j\beta\sigma} + 2J_H \sum_{i\alpha} \hat{n}_{i\alpha\downarrow} + \sum_{ij\alpha,\beta} V_{ij,\alpha}\beta \hat{n}_{i\alpha} \hat{n}_{j\beta} + J' \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j.$$  

(8)

We have added an additional term $\hat{H}_c = J_H \vec{N}$ proportional to the $e_g$-electron number $N$, equivalent to a trivial shift of the chemical potential.

The prize to be paid for the simple structure of the Hund term is that the modified hopping integrals $t^\sigma_{ij,\alpha}\beta$ now depend upon the $t_{2g}$ corespins:

$$t^\sigma_{ij,\alpha}\beta = t_{\alpha,\beta} \left( U^\dagger(S_i) U(S_j) \right)_{\sigma,\sigma'} = t_{ij,\alpha}\beta u^\sigma_{ij},$$

(9)

The relative orientation of the $t_{2g}$ corespins at site $i$ and $j$ enters via

$$u^\sigma_{ij} = e^{i\phi_{ij}} = \cos(\theta_{ij}/2) e^{i\psi_{ij}},$$

$$u_{ij}^{\sigma,\sigma'} = \sigma(c_j s_i e^{-i\phi_{ij}} - c_j s_i e^{-i\phi_{ij}}) = \sin(\theta_{ij}/2) e^{i\chi_{ij}}.$$  

(10)

These factors depend on the relative angle $\theta_{ij}$ of corespins $\vec{S}_i$ and $\vec{S}_j$ and on some complex phases $\psi_{ij}$ and $\chi_{ij}$. It should be noticed that the modified hopping part of the Hamiltonian is still Hermitian, because $u^\sigma_{ij} = \left( u^{\sigma'}_{ij} \right)^\ast$.

The advantage of the local quantization is, as described in Ref. 13, that the energetically unfavorable states with $e_g$ electrons antiparallel to the local $t_{2g}$ corespins can be integrated out. This leads to the effective spinless fermion model

$$\hat{H}_p = - \sum_{ij,\alpha,\beta} t^{\uparrow\uparrow}_{ij,\alpha,\beta} c^\dagger_{i\alpha} c_{j\beta} - \sum_{ij,\alpha,\beta,\alpha'} t^{\uparrow\uparrow}_{ij,\alpha,\beta} t^{\uparrow\uparrow}_{ij,\alpha',\beta} \frac{1}{2J_H} c^\dagger_{i\alpha} c_{i\alpha} + \sum_{ij,\alpha,\beta} V_{ij,\alpha}\beta \hat{n}_{i\alpha} \hat{n}_{j\beta} + J' \sum_{<ij>} \vec{S}_i \cdot \vec{S}_j.$$  

(11)

The spin index has therefore been omitted. With respect
to a global spin-quantization axis, the ESF model \([\text{11}\] still contains contributions from both spin-up and spin-down electrons. The V-dependent contributions in the energy denominator have been ignored, since \( |V_{\alpha \beta} | \ll |J_{\mu}| \). In principle, the effective Hamiltonian also contains “three-site” hopping processes. It has been shown \([\text{12}\) that the three-site term has negligible impact, and it has been ignored here.

Since each eigenvector can have an arbitrary phase, the unitary matrix in Eq. (6) is not unique. This implies that

\[
U(S_i) = \begin{pmatrix} c_i & s_i e^{-i\phi_i} \\ s_i e^{i\phi_i} & -c_i \end{pmatrix} \begin{pmatrix} e^{i\theta(i)} & 0 \\ 0 & e^{i\theta(j)} \end{pmatrix}
\]

also diagonalizes the Kondo term. The additional phase factors modify the hopping integrals of the spin-up channel as

\[
\begin{align*}
\alpha_{ij}^{\uparrow} &= (c_i c_j + s_i s_j e^{i(\phi_j - \phi_i)}) \int d\theta / 2 e^{i(\phi_j + \phi_i)/2} \\
&= \cos(\theta_{ij}/2) e^{i(\phi_j + \phi_i)/2}.
\end{align*}
\]

Consequently, in the one-dimensional case and with open boundaries, we can choose the local phase factors such that the n.n. hopping integrals are simply given by the real numbers \( \cos(\theta_{ij}/2) \).

**B. Grand Canonical Treatment**

Our model contains classical (corespins) and quantum mechanical \( (e_g\text{-electrons}) \) degrees of freedom. The appropriate way to cope with this situation in statistical mechanics is to define the grand canonical partition function as

\[
Z = \int \mathcal{D}[S] \ e^{-\beta (H(\theta, \phi) - \mu N)}
\]

\[
\int \mathcal{D}[S] = \prod_{i=1}^{L} \left( \int_0^\pi d\theta_i \sin \theta_i \int_0^{2\pi} d\phi_i \right),
\]

where \( \text{tr}_e \) indicates the trace over fermionic degrees of freedom at inverse temperature \( \beta \), \( N \) is the operator for the total number of \( e_g \) electrons, \( L \) is the number of lattice sites, and \( \mu \) stands for the chemical potential. Upon integrating out the fermionic degrees of freedom, we obtain the statistical weight of a corespin configuration \( S \)

\[
w(S) = \frac{\text{tr}_e e^{-\beta (H(S) - \mu N)} Z}{Z}.
\]

Equation (13) is the starting point of Monte Carlo simulations for the Kondo model \([\text{13}\) where the sum over the classical spins is performed via importance sampling. The spin configurations \( S \) enter the Markov chain according to the weight factor \( w(S) \) that is computed via exact diagonalization of the corresponding Hamiltonian in Eq. (6). In the 1D case we have performed MC simulations in which spins in domains of random lengths were rotated. We have performed MC runs with 1000 measurements. The skip between subsequent measurements was chosen to be some hundreds of lattice sweeps reducing autocorrelations to a negligible level.

Apart from quantities that can be derived directly from the partition function \( Z \), we will also be interested in dynamical observables, notably in the one-particle retarded Green’s function \( \ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega \) in global spin-quantization. This function follows from

\[
\ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega = \int \mathcal{D}[S] \ w(S) \ ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega.
\]

The one-particle Green’s function \( \ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega \), corresponding to a particular corespin configuration \( S \), is determined from the Green’s function in local spin-quantization by employing Eqs. (6) and (11)

\[
\ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega = U(S_i) a_{\beta \sigma}^{\dagger}(S_j) \ll a_{\alpha \sigma} \gg_\omega.
\]

To arrive at Eq. (16), we used the fact that in local quantization only the spin-up channel contributes to \( \ll c_{\alpha \sigma}^{\dagger} c_{\beta \sigma} \gg_\omega \), i.e. \( \sigma = \sigma' = \uparrow \). The spin-down channel has structures corresponding to the upper Kondo band in which we are not interested here. In global quantization, both spin directions contribute. The spin-integrated Green’s function reads

\[
\sum_{\sigma} \ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega = \int \mathcal{D}[S] \ w(S) \ ll a_{\beta \sigma}^{\dagger} \gg_\omega.
\]

The unbiased Monte-Carlo result for the spin-integrated one-particle Green’s function is therefore determined from

\[
\sum_{\sigma} \ll a_{\alpha \sigma}^{\dagger} a_{\beta \sigma} \gg_\omega = \int \mathcal{D}[S] \ w(S) \ll a_{\beta \sigma}^{\dagger} \gg_\omega.
\]

We note that the one-particle density of states (DOS) is independent of the choice of the spin-quantization, because it can be determined from diagonal Green’s functions in real space.

**III. UNIFORM HOPPING APPROACH**

The impact of the DE mechanism on the electronic kinetic energy can be mimicked by an average hopping amplitude \([\text{14}\]. In a previous paper \([\text{15}\]) we introduced what we called the “uniform hopping approach” (UHA). It gave strikingly good results for ground state properties. The idea behind UHA is to replace the terms \( u_{ij}^{\uparrow \uparrow} \) in the hopping amplitude, Eq. (1), which correspond to \( \cos(\theta_{ij}/2) \) as discussed before, by a uniform value \( u \). In Ref. \([\text{16}\)] the optimal UHA parameter \( u \) was determined by minimizing the ground state energy. Here we will extend this approach to finite temperatures by taking entropic effects into account.
In order to introduce the finite-temperature UHA, we proceed as follows: For a given corespin configuration characterized by the set of angles \{\theta_i, \phi_i\}, we define the average \( u(S) \) value

\[
uu(S) = \frac{1}{N_p} \sum_{(ij)} u_{ij}^\uparrow\uparrow(S) .
\]

Here \( N_p \) is the number of n.n. pairs \( \langle ij \rangle \). We now replace the individual factors \( u_{ij}^\uparrow\uparrow \) in Eq. (13) by \( u(S) \). Besides \( u_{ij}^\uparrow\uparrow \) the Hamiltonian depends on \( |u_{ij}^\sigma - u_{ij}^\sigma|^2 \) and on \( S_i \cdot S_j \), which correspond to \( \sin^2(\theta_{ij}/2) \) and \( \cos \theta_{ij} \), respectively. As a further approximation (see below), these terms are respectively replaced by \( 1 - u^2(S) \) and \( 2u^2(S) - 1 \).

The introduction of UHA leads to the partition function

\[
Z = \int D[S] \int_0^1 du \delta(u - u(S)) \tr e^{-\beta(H(u) - \mu N)} = \int_0^1 du \Gamma_{N_p}(u) e^{-\beta \Omega(u)} .
\]

The integrand can be interpreted as the (non-normalized)

\[
\hat{H}_{p}(u) = -u \sum_{<i,j>, \alpha,\beta} t_{\alpha\beta} c_i^\dagger c_j - (1 - u^2) \sum_{<\alpha,j>, \alpha',\beta} \frac{t_{\alpha\beta}}{2J_H} c_i^\dagger c_{\alpha\beta} + \sum_{i,j,\alpha,\beta} V_{\alpha\beta} n_{\alpha\beta} + J' N_p (2u^2 - 1) .
\]

The uniform hopping approach presents an enormous simplification of the original problem. Firstly, the evaluation of the fermionic trace simplifies considerably: for non-interacting electrons \((V = 0)\) it can even be computed analytically. Secondly, the high dimensional configuration space of the corespins shrinks to a unit interval. Once the density of corespin states \( \Gamma_{N_p}(u) \) has been determined, the integration over the corespin states can be carried out.

The thermal probability density \( p(u | \beta) \) in Eq. (24) contains two competing factors. The density of corespin states \( \Gamma_{N_p}(u) \) peaks near \( u = 2/3 \) and decreases algebraically to zero as \( u \) approaches the bounds of the unit interval. A tendency towards ferromagnetic (antiferromagnetic) order is reflected by an exponential increase of the Boltzmann factor towards \( u = 1 \) \((u = 0)\). This factor becomes increasingly important with decreasing temperature. In the ferromagnetic case, the combined distribution peaks, depending on the value of \( \beta \), somewhere between \( 2/3 \) and 1 (see Fig. 1 for an illustration in 3D). With increasing \( \beta \) the peak shifts towards \( u = 1 \).

In summary, the configuration space of the corespins is reduced to the one-parametric space of the UHA parameter \( u \). This simplification is based on the assumption that, as far as the Boltzmann factor is concerned, the effect of the corespins on the electrons can be replaced by a mean effective hopping. Fluctuations of the corespins are allowed for by the density \( \Gamma_{N_p}(u) \) and by fluctuations of the UHA parameter, resulting in a finite lifetime of the quasiparticles even in the FM phase, and in a finite bandwidth even in the AFM phase. The density \( \Gamma_{N_p}(u) \) takes care of the correct inclusion of the corespin entropy, which will become crucial in the ensuing discussion.

**Validity of the additional approximation**

In order to assess the additional approximation introduced by the substitution of the terms \( \langle \sin^2(\theta/2) \rangle \approx 1 - \langle \cos \theta/2 \rangle^2 \approx 1 - u^2 \) and \( \langle \cos \theta \rangle \approx 2(\cos \theta/2)^2 - 1 \approx 2u^2 - 1 \), a Monte Carlo simulation with random spins on a \( 16^3 \) simple cubic (sc) lattice has been performed. For each spin configuration, the mean values of the functions \( \cos(\theta/2), \cos(\theta), \) and \( \sin^2(\theta/2) \) have been computed. The resulting scatter plot is depicted in Fig. 2. Astonishingly, the data follow a unique curve and moreover they are fairly well described by the approximation employed.

\[
p(u | \beta) = \Gamma_{N_p}(u) e^{-\beta \Omega(u)} .
\]
IV. UHA VS MONTE CARLO IN 1D

In this section we scrutinize the uniform hopping approach by a detailed comparison of its results with MC data obtained for the original Hamiltonian Eq. (11). Since the UHA affects only the treatment of the corespins, we will restrict our attention to a one-orbital model and neglect the degeneracy of the $e_g$ orbitals. In this case, the Hamiltonian (23) simplifies to

\[
\hat{H}_p(u) = -u \sum_{<ij>} c_i^\dagger c_j - \frac{1-u^2}{2J_H} \sum_i z_i n_i + V \sum_{<ij>} n_i n_j + J' N_p (2u^2 - 1),
\]

where $z_i$ denotes the number of nearest neighbors of site $i$.

For a one-dimensional chain with open boundary condition, $\Gamma_{N_p}(u)$ can be calculated exactly. For a two-site lattice we find $\Gamma_1(u) = 2u \chi_{B}(u)$, where $\chi_B(u)$ denotes the characteristic function of the set $B$. Since the relative angles of the $N_p = L-1$ nearest-neighbor pairs of a chain of length $L$ are independent, $\Gamma_{N_p}(u)$ reduces to a $(N_p-1)$-fold convolution of $\Gamma_1(u)$. Therefore, $\Gamma_{N_p}(u)$ is piecewise polynomial and can be evaluated numerically. It can be approximated by a Gaussian, which is not surprising because the central limit theorem applies. In combination with the Boltzmann factor, however, a Gaussian approximation is not good enough because the Boltzmann factor amplifies the tails of the distribution.

A. Energy distribution

In this subsection we will compare UHA with MC results for the DE model with $V = J' = 0$, $J_H = \infty$ for a one dimensional system with one $e_g$ orbital per site. The Hamiltonian of Eq. (24) reduces to a one-particle tight-binding Hamiltonian

\[
\hat{H}_p(u) = -u \sum_{<i,j>} c_i^\dagger c_j,
\]

with only kinetic energy. The hopping integral $u$ is the only remnant of the interaction with the $t_{2g}$ corespins. The grand potential reads

\[
-\beta \Omega(u) = \sum_k \log(1 + e^{-\beta(\epsilon_k - \mu)})
\]

\[
= \int dE \rho_L(E) \log(1 + e^{-\beta(E-\mu)}).
\]

where the one-particle eigenvalues $\epsilon_k = -2u \cos k$ depend on $u$ and $\rho_L(E)$ denotes the tight-binding DOS of the $L$-site lattice. $\Omega(u)$ can now be computed easily, and along with exact results for $\Gamma_{N_p}(u)$ we have access to the partition function and thermal quantities such as the kinetic energy. In Fig. 3, the results for the kinetic energy are compared with those of unbiased MC simulations. One finds an impressively agreement between the two results. The energies are reproduced within the error bars for all values of $\beta$. At higher temperatures this agreement is not obvious at all, because the corespins are strongly fluctuating. The impact of the fluctuations seems to be well described by the UHA.

For a canonical ensemble at sufficiently low temperatures (canonical low-T approximation) one can derive an analytical result for UHA. To do so, the function $\Omega(u)$ is replaced by the ground state energy of the tight-binding Hamiltonian which we write as

\[
\Omega(u) = u E_k,
\]

with a factor $E_k$ (total energy of a tight-binding system with unit hopping amplitude) independent of $u$. The
The canonical partition function then reads

\[ Z = \int \mathcal{D}[S] \ e^{-\beta u E_k}. \]

Since \( u \) can be expressed as the average \( u = \frac{1}{N_p} \sum \cos(\vartheta_{ij}/2) \), the exponential function can be written as a product of factors containing only n.n. spins. In the case of a 1D chain with open boundary conditions or for a Bethe lattice, the relative angles of neighboring spins can thus be integrated independently. Consequently, the partition function factorizes and (up to some unimportant constant factors) can be transformed to

\[ Z = \left( \int_0^1 du \ \Gamma_1(u) \ e^{-u\zeta} \right)^{N_p} = \left( 2 - e^{-\zeta(1 + \zeta)} \frac{1}{\zeta^2} \right)^{N_p}, \]

with \( \zeta = \beta E_k/N_p \). By differentiation with respect to \( \beta \), we obtain the kinetic energy

\[ E_{\text{kin}} = E_k \frac{\zeta^2 + 2\zeta + 2 - 2e^\zeta}{\zeta(\zeta + 1 - e^\zeta)}. \]

This result is shown as a dashed line in Fig. 3. The comparison with MC results shows increasingly close agreement for \( \beta \gtrsim 10 \).

The above considerations show that UHA on average correctly describes the kinetic processes. In order to give a more critical assessment of UHA, we study the fluctuations of the kinetic energy. It should be kept in mind that the motivation of UHA is to describe the mean energy correctly. It is thus not a priori obvious whether UHA also properly reflects its fluctuations. In UHA the fluctuations of the kinetic energy are exclusively due to fluctuations of the uniform hopping parameter \( u \), that in turn is related to the relative n.n. angles of corespins. In the full model, however, the relative n.n. angles fluctuate locally.

By sampling the contributions to the kinetic energy in a MC simulation including local fluctuations, we obtain histograms for the full model. They can be compared with the statistical distribution of the kinetic energy corresponding to the UHA density \( \Gamma_{N_p}(u) e^{-\beta H(u)} \). The result of this comparison is depicted in Fig. 4. We find perfect agreement between MC and UHA results, revealing a non-trivial justification of UHA.

### B. Spectral function and Coulomb Correlations

We will now comment on the influence of the n.n. Hubbard interaction on the spectral density and compare MC with UHA results. A thorough discussion of correlation effects in conjunction with the Kondo model will be given elsewhere. We have studied a 12 site chain with open boundaries at half filling of the effective spinless model, i.e. quarter filling of the original Kondo model. In this case the implementation of the ESF model reduces the dimension of the Lanczos basis from \( \binom{L}{N} \) = 134 596 to \( \binom{L}{N} \) = 924. Additionally UHA replaces the sampling of spin configurations with a simple scan in the UHA parameter \( u \) (several 100 000 spin configurations in MC versus approx. 20 \( u \)-values in the relevant \( u \)-range [0.8, 1.0] in UHA).

Without Hubbard interaction, the system is ferromagnetic due to the DE mechanism. The spectral density, calculated by MC and depicted in Fig. 12 of Ref. 18, is that of a tight-binding model. The peaks are slightly broadened due to spin fluctuations. In UHA, through the variation of the uniform hopping amplitude \( u \), we ob-
tain a superposition of tight-binding bands that combine to a broadened tight-binding band. For the parameters $L = 20$, $J_H = 6$ and $J' = 0.02$ and at $\beta = 50$, the average uniform hopping amplitude $\langle u \rangle$ is found to be $\langle u \rangle \approx 0.953$. This yields a band width $W$ of $W \approx 3.8$ which agrees with what we have found in MC simulations.

We now include the n.n. Hubbard term with $V = 2$ in the ESF model Eq. (24), or alternatively in the UHA Hamiltonian in Eq. (23). The Monte Carlo data are obtained by resorting to a Lanczos exact diagonalization scheme for each corespin configuration. The fermionic trace is then evaluated by summing over enough lowest eigenstates, such that convergence is ensured. Details will be given elsewhere.\(^4\)

In UHA, a $t-V$ model has to be diagonalized. The Lanczos diagonalization for this model is not really faster than the diagonalization of the original model, but the configuration space is drastically reduced, as only the parameter $u$ has to be sampled within the unit interval $u \in [0, 1]$.

Figure 5 shows the spectral density derived by both approaches. The electronic correlation has important impact on the spectral density. A gap appears in the middle of the original Brillouin zone at $k = \pi/2$, indicating the doubling of the unit cell due to charge ordering. In addition, the spectra exhibit more structure than just a simple quasi particle peak.

This result is neither new nor surprising. The point we want to make here is that UHA works well also for correlated electrons, indicating that it can reliably be employed to study more sophisticated and more realistic models for the manganites, e.g. by including correlation effects, phononic degrees of freedom, and more orbital degrees of freedom.

V. FM PHASE TRANSITION IN 3D

We now apply UHA to a sc crystal and determine the Curie temperature for the bare one-orbital DE model. The crucial difference between the 1D and the 3D geometry is that in the latter the relative angles of n.n. corespin-pairs are in general correlated. Therefore the correct density $\Gamma_{N_p}(u)$ is no longer a convolution of the density $\Gamma_1(u)$ of a single spin-pair.

A. Determination of $\Gamma_{N_p}(u)$

In order to determine $\Gamma_{N_p}(u)$ for a 3D geometry, we have to resort to numerical approaches. We have employed the Wang-Landau algorithm\(^5\) with single spin flip updates, which was invented for the determination of the density of states of classical models. Figure 6 shows the resulting density $\Gamma_{N_p}(u)$ as a function of $u$ for a sc lattice with linear dimensions $L_x = 4, 6, 10$ and 12. As in the one-dimensional case, $\ln(\Gamma_{N_p}(u))$ diverges as $u \to 0$ and $u \to 1$. In fact, one can show that

$$\ln(\Gamma_{N_p}(u)) \to (L - 1) \ln(1 - u)$$

in any spatial dimension. This divergence has important impact on the low-temperature thermodynamic behavior. The entropy diverges logarithmically and the specific heat has a finite value for $T \to 0$. The scale in Fig. 6 might appear exaggerated, but it is actually the tiny tail close to $u = 1$ which will become important for low temperatures.

The computational effort of finite-temperature UHA is now essentially reduced to the Wang-Landau determination of $\Gamma_{N_p}(u)$, while the integration over $u$ to calculate various physical results takes only a small amount of computer time. Therefore, results can be obtained for much larger lattices than with the conventional MC approach and, indeed, for a whole range of temperatures at once.

B. FM to PM transition at $J_H = \infty, J' = 0$

We now study the 3D DE model in the UHA. Based on the tests of the previous section, we expect the UHA results to be reliable also in this case. We restrict the present discussion to the case $J_H = \infty, J' = 0$. For these parameters, only the FM and PM phases exist.\(^6\)

The trend from PM to FM can already be seen in Fig. 4, where we show the expectation value $\langle u \rangle$ of the uniform hopping parameter and its standard deviation as a function of the inverse temperature $\beta$ at $\mu = 0$. Already
for a relatively small system, $p(u \mid \beta)$ is sharply peaked. Starting from $u = 2/3$ at high temperatures, the expectation value $\langle u \rangle$ tends towards unity, i.e. FM corespins, as $\beta \to \infty$. From Eq. (28) we find the asymptotic formula

$$u^* = 1 + \frac{1}{\beta \epsilon_k}$$

(29)

for the position $u^*$ of the maximum of $p(u \mid \beta)$, where $\epsilon_k$ denotes the kinetic energy per lattice site of the tight-binding model with unit hopping parameter. It turns out that for $\beta \gtrsim 10$, the curves for $u^*$ and $\langle u \rangle$ coincide. Well above this temperature, near $\beta \approx 5.5$, the variance of $p(u \mid \beta)$ shows a peak (see inset of Fig. 5), indicating important fluctuations near this temperature. For the determination of the Curie temperature of the DE model, we study the specific heat $C_v$ as a function of temperature for various system sizes. The peaks of the specific heat at quarter filling ($n = 0.5$) are plotted in Fig. 6. They show signs of divergence as the lattice size increases. This indicates the presence of a second order phase transition from FM to PM. We identify the position $T^* \approx 0.17$ of the peak as the phase transition temperature $T_C$ at $n = 0.5$. This value is somewhat higher than that determined with the Hybrid MC algorithm [19] ($T_C \approx 0.14$) for a 16$^3$ lattice but is better than the variational estimate [2] $T_C \approx 0.19$.

In order to facilitate the calculation, particularly for electron fillings different from $n = 0.5$ ($\mu = 0$), we consider a canonical ensemble and replace the Boltzmann factor by $e^{-\beta F}$. If the temperature is small on the electronic energy scale, we can replace the electronic free energy $F$ by the ground state energy $F \approx uE_k$. As introduced above, $E_k$ denotes the kinetic energy at $T = 0$ of the tight-binding model with unit hopping amplitude (now in 3D) for a given electron filling. This approximation is justified because $T_C \lesssim 0.17$ is indeed small enough. The partition function now reads

$$Z = \int_0^1 du \Gamma_{N_p}(u) e^{-\beta E_k u}.$$  

(30)

The impact of this “canonical low-T approximation” is illustrated in the inset of Fig. 5. We find that the position of the peak is not affected at all. The only difference to the full grand canonical result is the longer tail at higher temperatures of the full result, which is due to additional fluctuations of the electrons.

The specific heat approaches a constant value $C_v = 1$ as $T \to 0$. This can be inferred from Eq. (29), since, for low temperatures, the internal energy per lattice site is given by $\epsilon_k u^*$ whose derivative with respect to temperature exactly yields unity. This explains the plateau of $C_v$ for $T \lesssim 0.1$.

Signatures of the FM to PM phase transition should show up especially in the magnetic susceptibility $\chi$. For its calculation, the density $\Gamma_{N_p}(u)$ is not sufficient because a value of $u$ of the average hopping does not determine the magnetization $m$. Given the conditional probability $p(m \mid u)$ the moments of the magnetization are

$$\langle |m|^n \rangle \equiv \frac{1}{Z} \int_0^1 du \Gamma_{N_p}(u) e^{-\beta \Omega(u)} M^{(n)}(u)$$

with

$$M^{(n)}(u) = \int_0^1 dm |m|^n p(m \mid u).$$

Estimates of the conditional moments $M^{(n)}(u)$ have been obtained in a second run of the Wang-Landau algorithm. A random walk in the space of all corespin configurations...
is performed whose acceptance is controlled by $1/\Gamma_N(u)$. An estimator of the susceptibility $\chi$ is then given by

$$\chi = \beta L \left( \langle m^2 \rangle - \langle |m| \rangle^2 \right).$$

Figure 8 shows the susceptibility as a function of the temperature for various lattice sizes. We observe clear signs of a divergence near $T \approx 0.18$ which corroborates the transition temperature obtained from the specific heat.

The filling dependence of $T_C$ is easily determined from Eq. (30). Since the filling dependence only enters via $E_k$, which shows up in combination with $\beta$, we have the simple relation

$$\beta E_k = \text{const}$$

for the transition temperature. Thus the Curie temperature $T_C$ is proportional to the kinetic energy $E_k$ of the tight-binding model which, in turn, is a function of the electron filling. The proportionality of $T_C$ to the bandwidth has already been found based on different approximations. In order to compare our calculations with experimental results, we fix the single free parameter in the DE model, i.e., the hopping amplitude. We choose $t = 0.2$ eV, a value reasonable for the material.

The dashed line of Fig. 9 shows the Curie temperature obtained from the DE model in UHA. We find astonishingly good agreement to the experimentally observed phase diagram of La$_{1-x}$Sr$_x$MnO$_3$ in the ferromagnetic regime. Our result is in sharp contrast to the claim made by Millis et al. that the DE model cannot even explain the right order of magnitude of $T_C$ for the manganites. The reasoning of Ref. 19 starts from similar ideas as the UHA but is based on additional uncontrolled approximations. Our results for the DE model are in accord with other estimates.

The experimentally observed phase diagram shows additional phases for small concentrations: ferromagnetic insulating (FI), paramagnetic insulating (PI) and a spin-canting insulating (SCI) state. These states are not accounted for in our present approach. For a correct description, a finite value of $J'$ is important, as well as generalizations of UHA, which will be discussed elsewhere.

VI. CONCLUSIONS

In this paper we have presented the uniform hopping approach (UHA) for the FM Kondo model at finite temperature. We have used our method to calculate the ferromagnetic to paramagnetic phase transition temperature of the one-orbital DE model for large 3D systems. We find that the DE model yields a Curie temperature that is comparable to the experimental data.

The finite temperature UHA in the frame of the ESF model reduces the numerical effort of a simulation by several orders of magnitude, while retaining all crucial physical features. In the example given in Sec. IV B, the reduction factor is at least $10^6$. The key idea is to map the physics of the high dimensional configuration space of the $t_{2g}$ corespins onto an effective one-parametric model. The density of states entering our approach can be determined by the Wang-Landau algorithm. A full thermodynamic evaluation of the UHA model takes into account entropy and fluctuations of the corespins. Tests for 1D systems reveal that UHA results are in close agreement with unbiased MC data for static and dynamic observables.

This reduction in numerical effort will allow us to include phononic and/or orbital degrees of freedom in future numerical simulations in order to study more realistic models for the manganites.
Acknowledgments

This work has been supported by the Austrian Science Fund (FWF), project no. P15834-PHY. We are indebted to W. Nolting for stimulating discussions and to V. Martín-Mayor for drawing our attention to Refs. [16].

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