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Ferromagnetism and spin waves in double exchange materials[⋆,⋆⋆]

P. Wurth[a] and E. Müller-Hartmann

Institut für Theoretische Physik, Universität zu Köln, Zülpicher Strasse 77, 50937 Köln, Germany

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Abstract. We study the influence of the on-site Hubbard repulsion U between the conduction electrons on the stability of the fully polarized ferromagnetic state in the ferromagnetic Kondo lattice model. Using single spin flip variational wave functions including local correlations in the vicinity of the flipped spin we investigate in detail how each of the two distinct mechanisms Hubbard repulsion and double exchange leads to ferromagnetism in this model, which is relevant for the Colossal Magnetoresistance (CMR) materials. In the ferromagnetic region of the phase diagram variational bounds on the spin wave energies are obtained. In particular the doping dependency of the deviations of the spin wave dispersion from a conventional Heisenberg form is analyzed. The astonishingly good agreement of our variational results in one dimension with results from numerical calculations on finite chains both for the stability region and the spin wave dispersion suggests that our results for the square lattice and the simple cubic lattice give an even better description of the actual properties of the model under consideration.

PACS. 75.30.Ds Spin waves – 71.10.Fd Lattice fermion models (Hubbard model, etc.) – 75.10.Lp Band and itinerant models

1 Introduction

The discovery of a huge magnetoresistance (Colossal Magnetoresistance CMR) in substances like $R_{1-x}X_xMnO_3$ with R = La, Pr or Nd and X = Sr, Ca, Ba or Pb [1–5] has motivated a large number both of theoretical and experimental works dealing with this materials. More than forty years ago Zener introduced the double exchange model in order to explain the interplay between magnetic order and conductivity in these manganite compounds with perovskite structure [6–8]. The d-shell of the Mn^{3+} in the undoped antiferromagnetic insulators contains three electrons in the tightly bound t_{2g} orbitals forming a core spin of magnitude $S = 3/2$ which due to strong Hund's rule couples ferromagnetically to one additional electron in one of the e_g orbitals. For doping concentrations $0.2 \lesssim x \lesssim 0.5$ the CMR materials are ferromagnetic metals because of additional holes in the e_g conduction bands. The ferromagnetic coupling between core spins and conduction electrons favors ferromagnetic ordering, because the hopping amplitudes of the conduction electrons reach the maximum possible values if the core spins are all aligned.

Some doubts have been raised whether the double exchange model alone can account for the large change of resistivity in the CMR materials [9]. The coupling of the electrons to lattice degrees of freedom may play an important role in understanding the physics of the CMR materials completely (see for example [10–13]). In this context the importance of the degeneracy of the e_g orbitals for the double exchange model and for the interaction of electrons and phonons has been discussed [14–16]. The physics of the double exchange model is however far from trivial. The Berry phase of the conduction electrons could lead to strong localization in the paramagnetic phase [17,18].

In this paper we will assume that the e_g-degeneracy is lifted due to small deviations from cubic symmetry and thus we will focus on a single band ferromagnetic Kondo lattice model. For reasons of simplicity we will, nevertheless, later use a simple cubic lattice. We will study effects of correlations between the conduction electrons taking into account the Hubbard interaction U for the conduction electrons. Thus we can study the interplay between two distinct mechanisms favoring ferromagnetism: double exchange and Hubbard repulsion.

In the case of the Hubbard model with infinite on-site repulsion U Nagaoka's theorem proves the existence of a fully polarized ferromagnetic ground state (Nagaoka state) in the case of one additional electron in the half filled band (and one additional hole for bipartite lattices) for a large number of lattices, especially for the square lattice and the simple cubic lattice [19,20]. Extensions of this theorem to finite electron densities in the thermodynamic limit have not yet been obtained. In the case of more than one additional electron in a half filled band, but still a vanishing electron density in the thermodynamic limit, ground states with lower total spin have been obtained

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⋆⋆ Dedicated to J. Zittartz on the occasion of his 60th birthday

[a] e-mail: pw@thp.uni-koeln.DE

[21–24]. Nevertheless for non bipartite lattices the regions of possible stability of the Nagaoka state at large Hubbard repulsion close to half filling turn out to be very robust with respect to single spin flips [25].

Here we will improve variational bounds for the possible stability of a ferromagnetic ground state for the simple cubic lattice in the thermodynamic limit using variational wave functions which we have employed successfully in the case of the Hubbard model on the square lattice in a previous publication [26].

We will then generalize these wave functions which include local correlations in the vicinity of the flipped spin as well as the ansatz *RES*3 given in [25] to the ferromagnetic Kondo lattice model with Hubbard repulsion. Although the ferromagnetic Kondo coupling is supposed to be more efficient in stabilizing a ferromagnetic ground state the additional degrees of freedom of the core spins complicate rigorous proofs of ferromagnetism. The ferromagnetic Kondo lattice is known to exhibit ferromagnetism for one electron for an arbitrary finite exchange coupling [27,28]. The ground state of a chain with open boundary conditions and infinite Hund's rule coupling was also shown to be a fully polarized ferromagnet for all electron concentrations $0 \neq n \neq 1$ [27]. For the square lattice and the simple cubic lattice however no rigorous results for finite electron concentrations have yet been given.

We will therefore analyze the region of possible stability for the Nagaoka state for the simple cubic lattice using our variational ansatz. Our results not only improve previous variational bounds quantitatively. We have also obtained a qualitative improvement of the results shown in [29,30] by showing the instability of the Nagaoka state for any finite Hund's rule coupling close to half filling. This result was obtained using a very simple scattering state ansatz to describe the antiferromagnetic correlations in this region.

In the ferromagnetic region of the phase diagram we will give upper bounds on the energies of spin wave excitations and on the bottom of the scattering continuum assuming a fully polarized ground state. The measured spin wave dispersion for $La_{0.7}Pb_{0.3}MnO_3$ throughout the whole Brillouin zone (BZ) is found in quite good agreement with the simple magnon dispersion of a Heisenberg model [31,32]. We will investigate closer the doping dependence of deviations from the Heisenberg model dispersion, which also follows from an expansion in $1/S$ in the Kondo lattice model at $J_H = \infty$ [33,34]. We will be able to reproduce exact numerical results for spin wave energies for finite chains with core spins of size $S = 1/2$ [35] very accurately, so we can be confident that our variational results for the large $S = 3/2$ spin in the simple cubic lattice are very reliable.

Finally we will use our variational results for the excitation energies at $T = 0$ to give a rough estimate of the Curie temperature both for the pure Hubbard model and for the ferromagnetic Kondo lattice model in the simple cubic case.

2 Model and ansatz

The starting point for our investigation is the following Hamiltonian

$$H = -\sum_{\langle \mathbf{x},\mathbf{y}\rangle} t_{\mathbf{x},\mathbf{y}} c^+_{\mathbf{y}\sigma} c_{\mathbf{x}\sigma} + U \sum_{\mathbf{x}} n_{\mathbf{x}\downarrow} n_{\mathbf{x}\uparrow} - J_H \sum_{\mathbf{x}} \mathbf{S}_{\mathbf{x}} \cdot \mathbf{s}_{\mathbf{x}} + \frac{J_H S}{2} \sum_{\mathbf{x}} n_{\mathbf{x}} . \quad (1)$$

The operators $c^+_{\mathbf{x}\sigma}$ ($c_{\mathbf{x}\sigma}$) create (annihilate) conduction electrons at site $\mathbf{x}$. The spin of the conduction electrons is given as $\mathbf{s}_{\mathbf{x}} = \frac{1}{2}\sum_{\sigma,\sigma'} c^+_{\mathbf{x}\sigma} \boldsymbol{\sigma}_{\sigma,\sigma'} c_{\mathbf{x}\sigma'}$ while the core spin at site $\mathbf{x}$ is denoted by $\mathbf{S}_{\mathbf{x}}$ ($\boldsymbol{\sigma}$ are the Pauli matrices). $n_{\mathbf{x}}$ is the electron density of the conduction electrons at site $\mathbf{x}$. The usual tight binding approximation (only hopping processes between nearest neighbor sites allowed in the kinetic energy) leads to the band structure

$$\epsilon_{\mathbf{k}} = -2t \sum_{\nu=1}^{d} \cos(k_\nu) \quad (2)$$

with minimum $\epsilon_B = -zt$ and maximum $\epsilon_T = zt$ for a d-dimensional hypercubic lattice with coordination number $z = 2d$. In addition to the on-site Coulomb repulsion U the electron spins interact with the core spins *via* a ferromagnetic Hund's rule coupling $J_H > 0$. The last term simply ensures that the Hund's rule energy is compensated for sites with maximal total spin of conduction electron and core spin. We will only consider electron densities $0 \leq n \leq 1$.

The fully polarized ferromagnetic state (Nagaoka state)

$$|\mathcal{N}\rangle \quad := |\mathcal{N}\rangle_c \otimes |LS, LS\rangle_{core} \quad (L \text{ is the number of sites})$$

with

$$|\mathcal{N}\rangle_c := \prod_{\substack{\mathbf{k}\in BZ \\ \epsilon_{\mathbf{k}} \leq \epsilon_F}} c^+_{\mathbf{k}\uparrow} |0\rangle_c . \quad (3)$$

is an eigenstate of the Hamiltonian with vanishing Hund's rule and Coulomb energy and with the kinetic energy per site given by

$$e_{\mathcal{N}} = \int_{\epsilon_B}^{\epsilon_F} d\epsilon \rho(\epsilon) \epsilon \quad (4)$$

where the one electron density of states ρ is defined by

$$\rho(\epsilon) := \langle \delta(\epsilon_{\mathbf{k}} - \epsilon_F) \rangle_{\mathbf{k}\in BZ}. \quad (5)$$

In a previous publication we investigated the stability of the Nagaoka state with respect to a single spin flip in the Hubbard model on the square lattice [26]. This corresponds to the limit of vanishing core spin of the Hamiltonian (1). The local ansatz for the scattering states and spin waves used in [26] can be easily generalized to the ferromagnetic Kondo lattice model by including additional

variational parameters for a reduced z-component of a core spin at one lattice site. The resulting scattering state is of the general form

$$|SLOC\rangle := \frac{1}{\sqrt{L}} \sum_{\mathbf{x}} e^{i\mathbf{q}\mathbf{x}} \sum_{\nu} \Big\{ \psi_c^{\nu} c_{\mathbf{x}\downarrow}^{+} A_{\mathbf{x}}^{\nu} + \psi_s^{\nu} S_{\mathbf{x}}^{-} B_{\mathbf{x}}^{\nu} \Big\} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle \tag{6}$$

with a finite number of variational parameters ψ_c^{ν} and ψ_s^{ν}. In view of the translational invariance of the Hamiltonian we choose the local operators B^{ν} and A^{ν} as

$$A_{\mathbf{x}}^{\nu} := T_{\mathbf{x}}^{-1} A_{\mathbf{0}}^{\nu} \, T_{\mathbf{x}} \quad \text{and} \quad B_{\mathbf{x}}^{\nu} := T_{\mathbf{x}}^{-1} B_{\mathbf{0}}^{\nu} \, T_{\mathbf{x}} \tag{7}$$

with the translation operator $T_{\mathbf{x}}$. They describe correlations in the vicinity of the flipped spin

$$A_{\mathbf{0}}^{\nu} \in \Big\{ 1, c_{\mathbf{y}_{1,1}\uparrow} c_{\mathbf{y}_{1,2}\uparrow}^{+}, c_{\mathbf{y}_{2,1}\uparrow} c_{\mathbf{y}_{2,2}\uparrow} c_{\mathbf{y}_{2,3}\uparrow}^{+} c_{\mathbf{y}_{2,4}\uparrow}^{+}, c_{\mathbf{y}_{3,1}\uparrow} c_{\mathbf{y}_{3,2}\uparrow} c_{\mathbf{y}_{3,3}\uparrow} c_{\mathbf{y}_{3,4}\uparrow}^{+} c_{\mathbf{y}_{3,5}\uparrow}^{+} c_{\mathbf{y}_{3,6}\uparrow}^{+} | \; |\mathbf{y}_{i,j}|_{\infty} < 5 \Big\}$$

and

$$B_{\mathbf{0}}^{\nu} \in \Big\{ c_{\mathbf{y}_{1,1}\uparrow}^{+}, c_{\mathbf{y}_{2,1}\uparrow} c_{\mathbf{y}_{2,2}\uparrow}^{+} c_{\mathbf{y}_{2,3}\uparrow}^{+}, c_{\mathbf{y}_{3,1}\uparrow} c_{\mathbf{y}_{3,2}\uparrow} c_{\mathbf{y}_{3,3}\uparrow}^{+} c_{\mathbf{y}_{3,4}\uparrow}^{+} c_{\mathbf{y}_{3,5}\uparrow}^{+} | \; |\mathbf{y}_{i,j}|_{\infty} < 5 \Big\}. \tag{8}$$

The operators $A_{\mathbf{0}}^{\nu}$ create between 0 and 3 localized particle hole pairs in the spin up Fermi sea, $B_{\mathbf{0}}^{\nu}$ create a particle in addition to up to 2 particle hole pairs. The Manhattan distance $|\mathbf{y}_{i,j}|_{\infty}$ of the particles and holes from the flipped spin will be assumed smaller than 5. It is always the best choice to create the spin-$\downarrow$ electron at the bottom of the band $\mathbf{q} = 0$ so that the ansatz can be simplified by choosing variational parameters reflecting the symmetry of the hypercubic lattice.

Let us briefly look at some simple choices of operators $A_{\mathbf{0}}$ which have been investigated before in the case of the Hubbard model. The most simple ansatz of this form is the Gutzwiller projected single spin flip scattering state [36]. This ansatz corresponds to the choice of only two operators $A_{\mathbf{0}} = 1$ and $A_{\mathbf{0}} = c_{\mathbf{0}\uparrow} c_{\mathbf{0}\uparrow}^{+}$ and is sufficient to obtain a critical hole density $\delta_{cr} = 0.49$ at infinite Coulomb repulsion U. For all larger hole densities the Nagaoka state is unstable with respect to a single spin flip. In the following we will call this ansatz *GUTZ*.

The easiest way to improve *GUTZ* at infinite U is to allow the spin-$\uparrow$ electron to avoid the flipped spin rather than just to project out double occupancies [37–39]. If one confines the hopping of the spin-$\uparrow$ electron to nearest neighbor sites of the flipped spin this ansatz, which will be called *BE* in this paper, corresponds to the choice of additional operators $A_{\mathbf{0}} = c_{\mathbf{0}\uparrow} c_{\boldsymbol{\nu}\uparrow}^{+}$ where $\boldsymbol{\nu}$ is a nearest neighbor site of $\mathbf{0}$. These and all the other wave functions studied in [40,26] can easily be generalized to the case of finite core spins and ferromagnetic Hund's rule coupling. For each operator $A_{\mathbf{0}}$ without double occupancy the corresponding operator $B_{\mathbf{0}}$ is obtained by leaving out the first annihilation operator at site $\mathbf{0}$. In the extreme case of infinite J_H the total spin of conduction electron and core spin at each lattice site has to be $S+1/2$. In this case the operators $B_{\mathbf{0}}$ and $A_{\mathbf{0}}$ have to be combined properly to give $S^{tot,-}$. For the ansatz *GUTZ* for example the only variational wave function with finite energy in this limit is obtained by the combination $S_{\mathbf{0}}^{tot,-} c_{\mathbf{0}\uparrow}^{+} = \mathrm{S}_{\mathbf{0}}^{-} c_{\mathbf{0}\uparrow}^{+} + c_{\mathbf{0}\downarrow}^{+} c_{\mathbf{0}\uparrow} c_{\mathbf{0}\uparrow}^{+}$.

At finite Coulomb repulsion additional operators containing double occupancies become important. Close to half filling both in the Hubbard model and in the ferromagnetic Kondo lattice model ferromagnetism is unstable against a phase separation between a ferromagnetic phase containing all the holes and an antiferromagnetic half filled phase [41–44]. In order to describe the antiferromagnetic correlations close to half filling properly it is not sufficient to consider just the Gutzwiller projected ansatz *GUTZ* or any other of the states discussed above. In contrast to statements in [45] one can however show the instability of the Nagaoka state close to half filling with a very simple variational scattering state constructed from the two states

$$|0\rangle := \frac{1}{\sqrt{Lz}} \sum_{\mathbf{x}} e^{i\mathbf{q}\mathbf{x}} \sum_{\langle \boldsymbol{\nu}, \mathbf{0} \rangle} c_{\mathbf{x}\downarrow}^{+} c_{\mathbf{x}+\boldsymbol{\nu}\uparrow} c_{\mathbf{x}\uparrow}^{+} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle \tag{9}$$

$$|1\rangle := \frac{1}{\sqrt{(2S+1)L\delta}} \times \sum_{\mathbf{x}} e^{i\mathbf{q}\mathbf{x}} \Big(S_{\mathbf{x}}^{-} + c_{\mathbf{x}\downarrow}^{+} c_{\mathbf{x}\uparrow} \Big) c_{\mathbf{x}\uparrow}^{+} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle. \tag{10}$$

This corresponds to the choice of operators $A_{\mathbf{0}} = c_{\mathbf{0}\uparrow} c_{\mathbf{0}\uparrow}^{+}$, $B_{\mathbf{0}} = c_{\mathbf{0}\uparrow}^{+}$ and $A_{\mathbf{0}} = c_{\boldsymbol{\nu}\uparrow} c_{\mathbf{0}\uparrow}^{+}$. With this ansatz the antiferromagnetic exchange interaction is taken into account. We define the energy cost of a double occupancy as $U' := J_H S + U$ and the coupling $U'_{cr}(\delta)$ by the condition that the Nagaoka state is unstable at a given hole density δ for all $U' < U'_{cr}(\delta)$. By calculating the energy of the two states given in equations (9) and (10) and taking the limit $\delta \to 0$ one obtains a divergence of the critical coupling $U'_{cr}(\delta)$ for $\delta \to 0$ as

$$U'_{cr}(\delta) \sim \frac{8zt^2 \rho(\epsilon_T)}{(2S+1)\delta} \tag{11}$$

for the square lattice and

$$U'_{cr}(\delta) \propto \delta^{-2/3} \tag{12}$$

for the simple cubic lattice. In this way we easily understand and prove the instability of the Nagaoka state close to half filling for any finite J_H and for any finite U.

In order to obtain quantitatively improved results we applied the method described in [26] to the Hubbard model on the simple cubic lattice and to the ferromagnetic Kondo lattice with Hubbard repulsion between the conduction electrons for the simple cubic lattice and for the square lattice. We used a C++-program to create and to test a large number of local operators $A_{\mathbf{0}}$ and $B_{\mathbf{0}}$ in order to be able to include the most efficient operators in our final ansatz. For one dimensional chains the results obtained using our variational ansatz can be compared

with results from exact calculations for finite chains for $U = 0$ and $S = 1/2$ and $S = 3/2$. Even for $S = 1/2$ our variational bounds are in good agreement with the numerical results from [43,44] (for example at $\delta = 0.4$ the deviation is 19%). This gives rise to the expectation that our approach gives an even better approximation for the phase diagram for the simple cubic lattice and for larger spin since correlations get more localized the higher the dimension and since the *RPA* gets exact for $S = \infty$.

The generalization of the calculation for the ferromagnetic Kondo lattice model is straightforward. Particularly helpful is the fact that states containing a core spin with a reduced value of S^z are orthogonal to states containing a spin-$\downarrow$ electron. Therefore, we will not repeat the details of the calculation given in [26] here.

In [25] an ansatz *RES*3 was introduced which contains an infinite number of variational parameters. The generalization of this ansatz to the case of the ferromagnetic Kondo lattice model has the form

$$\begin{aligned}|RES4\rangle :=& \frac{1}{\sqrt{L}} \sum_{\mathbf{x},\mathbf{k}} \psi_{\mathbf{k}}^{c,1} e^{i(\mathbf{q}+\mathbf{k})\mathbf{x}} c_{\mathbf{x}\downarrow}^{+} c_{\mathbf{x}\uparrow} c_{\mathbf{k}\uparrow}^{+} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle \\ &+ \frac{1}{\sqrt{L}} \sum_{\mathbf{x},\mathbf{k}} \psi_{\mathbf{k}}^{c,2} e^{i(\mathbf{q}-\mathbf{k})\mathbf{x}} c_{\mathbf{x}\downarrow}^{+} c_{\mathbf{x}\uparrow}^{+} c_{\mathbf{k}\uparrow} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle \\ &+ \frac{1}{\sqrt{L}} \sum_{\mathbf{x},\mathbf{k}} \psi_{\mathbf{k}}^{s} e^{i(\mathbf{q}+\mathbf{k})\mathbf{x}} \left(S_{\mathbf{x}}^{-} + c_{\mathbf{x}\downarrow}^{+} c_{\mathbf{x}\uparrow} \right) c_{\mathbf{k}\uparrow}^{+} c_{\mathbf{k}_F\uparrow} |\mathcal{N}\rangle. \end{aligned} \tag{13}$$

The variational equation and the corresponding system of linear equations obtained by integration are given in Appendix. This ansatz describes correlations at an arbitrary distance of the spin flip. Local correlations in the vicinity of the spin-$\downarrow$ electron are however described not as well as in the ansatz *SLOC* because only one particle hole pair $c_{\mathbf{x}\uparrow} c_{\mathbf{k}\uparrow}^{+}$ or $c_{\mathbf{x}\uparrow}^{+} c_{\mathbf{k}\uparrow}$ is included. The scattering state studied in [29] is contained in the ansatz (13) by choosing $\psi_{\mathbf{k}}^{c,1} \equiv \psi_{\mathbf{k}}^{c,2} \equiv 1/\sqrt{L}$. We will call this ansatz *OKA* in the following.

In the same way as the scattering states the local spin wave ansatz studied in [26] can be generalized for the ferromagnetic Kondo lattice model giving

$$|SWLO\rangle = \frac{1}{\sqrt{L}} \sum_{\mathbf{x}} e^{i\mathbf{q}\mathbf{x}} \sum_{\nu} \left\{ \psi_c^{\nu} c_{\mathbf{x}\downarrow}^{+} C_{\mathbf{x}}^{\nu} + \psi_s^{\nu} S_{\mathbf{x}}^{-} A_{\mathbf{x}}^{\nu} \right\} |\mathcal{N}\rangle \tag{14}$$

with operators C obeying

$$C_{\mathbf{x}}^{\nu} := T_{\mathbf{x}}^{-1} C_{\mathbf{0}}^{\nu} \; T_{\mathbf{x}} \tag{15}$$

and

$$\begin{aligned} C_{\mathbf{0}}^{\nu} \in \Big\{ & c_{\mathbf{y}_{1,1}\uparrow}, c_{\mathbf{y}_{2,1}\uparrow} c_{\mathbf{y}_{2,2}\uparrow} c_{\mathbf{y}_{2,3}\uparrow}^{+}, \\ & c_{\mathbf{y}_{3,1}\uparrow} c_{\mathbf{y}_{3,2}\uparrow} c_{\mathbf{y}_{3,3}\uparrow} c_{\mathbf{y}_{3,4}\uparrow}^{+} c_{\mathbf{y}_{3,5}\uparrow}^{+} |\; |\mathbf{y}_{i,j}|_{\infty} < 5 \Big\}. \end{aligned} \tag{16}$$

This ansatz can be evaluated in exactly the same manner as the ansatz (6). We will denote by *SWGU* the ansatz containing all operators $C_{\mathbf{0}}$ of the form $c_{\mathbf{y}\uparrow}$ and $c_{\mathbf{y}\uparrow} c_{\mathbf{y}'\uparrow} c_{\mathbf{0}\uparrow}^{+}$ with $|\mathbf{y}|_{\infty} \leq 1, |\mathbf{y}'|_{\infty} \leq 1$ and the corresponding operators $A_{\mathbf{0}}$ which approximate the spin wave corresponding to *GUTZ*. The ansatz containing $C_{\mathbf{0}}$ operators of the type $c_{\mathbf{y}\uparrow}$ and $c_{\mathbf{y}\uparrow} c_{\mathbf{y}'\uparrow} c_{\nu\uparrow}^{+}$ with $|\mathbf{y}|_{\infty} \leq 1, |\mathbf{y}'|_{\infty} \leq 1$ for nearest neighbor sites $\boldsymbol{\nu}$ of $\mathbf{0}$ and the corresponding operators $A_{\mathbf{0}}$ we name SWBE. In the thermodynamic limit all the variational spin wave wave functions only contain terms with $S^{tot} = S - 1$ for $\mathbf{q} \neq \mathbf{0}$. Therefore the spin wave energies calculated this way are variational upper bounds for the spin wave excitations assuming a fully saturated ferromagnetic ground state.

3 Results

In Figure 1 we show regions of guaranteed instability for the Nagaoka state for the simple cubic lattice for the Hamiltonian from equation (1) with two sets of parameters. Figure 1a shows the situation in the case of the pure Hubbard model ($S = 0$), Figure 1b corresponds to the choice $S = 3/2$ and $J_H = 0.5zt$. In both cases we show the reduced coupling $U_{red} := \frac{U}{U+U_{BR}}$ with the critical coupling $U_{BR} = 16|e_{\mathcal{N}}^{0}| \approx 16.04t$ from [46] used as the reference energy. Only the areas above all lines are left for a Nagaoka ground state. We show the result from variational calculations using the four different single spin flip wave functions *OKA* (from [29]), *GUTZ*, *RES*4 and *SLOC*, which we discussed in the previous section (*cf.* Eqs. (13) and (6)). The ansatz *SLOC* used in this case contains 241 local operators in the case of the Hubbard model and 125 operators in the ferromagnetic Kondo lattice case.

In both figures it is obvious that the new wave functions *RES*4 and *SLOC* considerably improve the results obtained with the variational wave functions *GUTZ* and *OKA*. For the Hubbard model the critical hole density at $U = \infty$ is reduced from the best previous value of $\delta_{cr} = 0.237$ (obtained with the ansatz *RES*3 [25,47]) to $\delta_{cr} = 0.185$. The critical coupling $U_{cr} := \min_{\delta} U_{\mathrm{cr}}(\delta)$ is enhanced from $U_{cr} = 48.9t$ to $U_{cr} = 78.6t$. As expected the wave functions *RES*4 and *SLOC* correctly show the divergence of the coupling $U_{cr}(\delta)$ for vanishing hole density in contrast to the wave functions *OKA* and *GUTZ*.

Figure 1a tells us that in the pure Hubbard model the Nagaoka state is a possible ground state only for large Coulomb repulsion and small hole density. This situation is very different in the case of the ferromagnetic Kondo lattice. Our variational calculations confirm the scenario suggested by the rigorous results concerning ferromagnetism [27,28] in the thermodynamic limit for the simple cubic lattice: We do not find any instability with respect to single spin flip at infinite Hund's rule coupling and for arbitrary small values of J_H we find a region of possible stability for low particle density ($\delta \to 1$) [48].

Figure 1b shows the effect of switching on Hund's rule coupling to core spins of size $S = 3/2$. There is a stability region for low electron density even at vanishing Coulomb repulsion ($U_{red} = 0$). The stability region close to half filling is substantially enlarged and includes regions

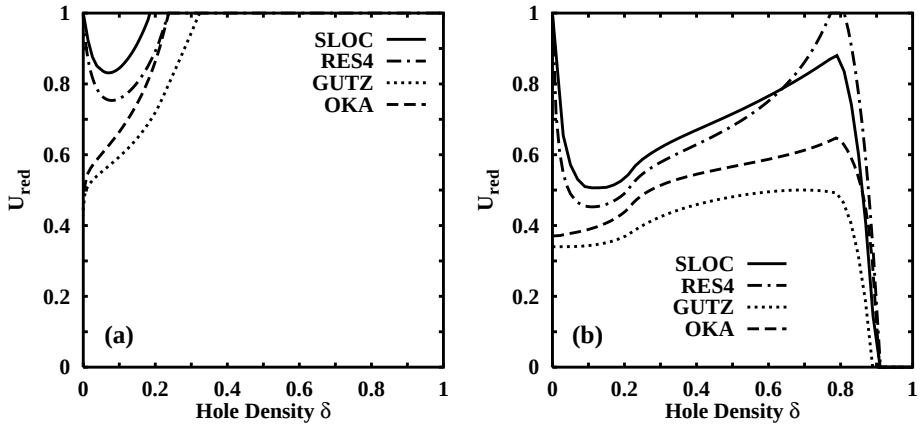

Fig. 1. Instability of the Nagaoka state for (a) the Hubbard model and (b) the ferromagnetic Kondo lattice with $J_H = 0.5zt$ and $S = 3/2$ for the simple cubic lattice.

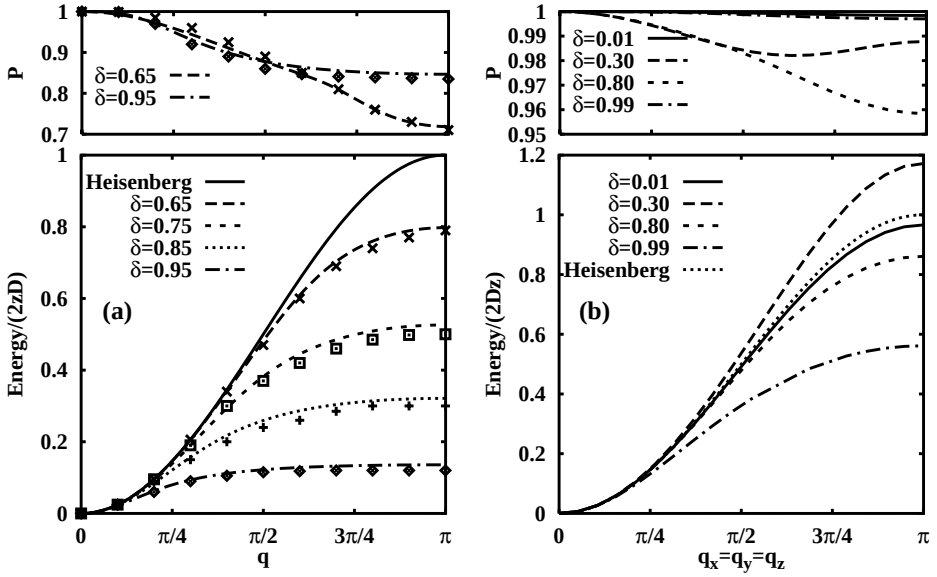

Fig. 2. Spin wave dispersion for the $J_H = \infty$ Kondo lattice model for (a) chains with $S = 1/2$ and (b) the simple cubic lattice with $S = 3/2$. The symbols in (a) show the exact results from [35].

with higher hole densities and lower Hubbard repulsion. Our new wave functions *RES*4 and *SLOC* give again the strongest restrictions for the region of possible stability of the Nagaoka state. The ansatz *RES*4 gives better results at small particle density while the ansatz *SLOC* including further local correlations is more efficient in the region of small and intermediate hole density. If the Hund's rule coupling is further increased the two separated regions of possible stability of the Nagaoka state shown in Figure 1b merge to give one growing stability region. At large but finite J_H only a window of very small hole density close to half filling shows instability of the Nagaoka state with respect to a single spin flip [48].

In the following we will focus on the excitation spectrum in the region of possible stability of the Nagaoka state. A simple Random-Phase-Approximation (*RPA*) for the spin wave energies at $J_H = \infty$ gives a dispersion which has exactly the same form as the magnon dispersion in a Heisenberg ferromagnet [33,34]. Figure 2 shows the deviation of the actual spin wave dispersion approximated by our variational ansatz from this form in the one-dimensional case with $S = 1/2$ (a) and for the simple cubic lattice with $S = 3/2$ (b). Both figures show the spin wave dispersion normalized such that the stiffness D defined by $\omega(\mathbf{q}) \sim Dq^2$ for $q \to 0$ coincides for all curves. For the chains we compare our results with those obtained by exact diagonalization for finite chains [35]. The figures also include the spectral weight

$$P := \frac{|\langle \mathcal{N}|\mathrm{S}^{tot,+}_{\mathbf{q}}|\psi(\mathbf{q})\rangle|^2}{\langle \mathcal{N}|\mathrm{S}^{tot,+}_{\mathbf{q}}\mathrm{S}^{tot,-}_{\mathbf{q}}|\mathcal{N}\rangle} \tag{17}$$

which is proportional to the weight of a spin wave peak in a measurement of the susceptibility in a neutron scattering experiment. Figure 2a shows that our variational ansatz gives a good description of the spin wave excitation even in the extreme quantum case of one dimension and low spin where quantum fluctuations are expected to be most pronounced. The results shown in Figure 2b

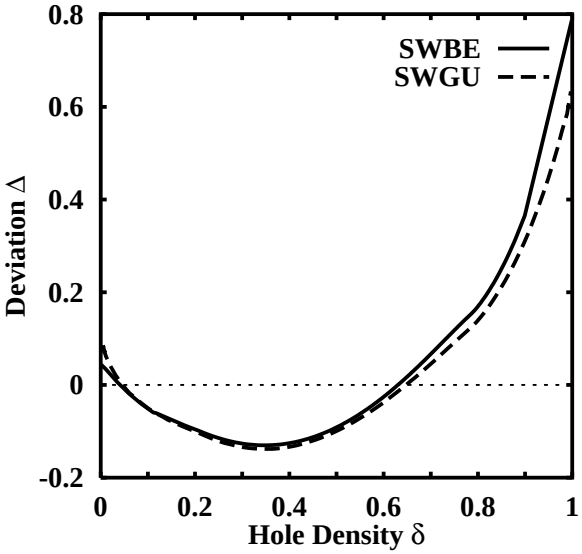

Fig. 3. Doping dependence of the deviation from a Heisenberg form for $J_H = \infty$, $S = 3/2$ and the simple cubic lattice.

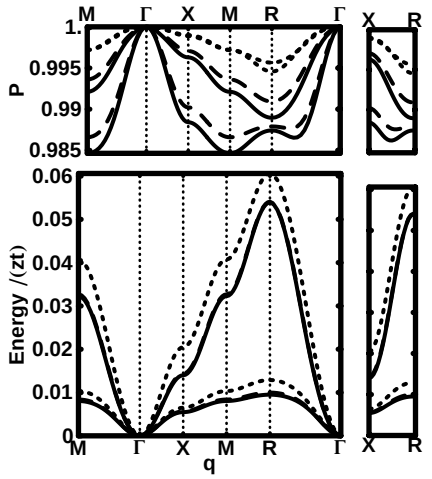

Fig. 4. Spin wave dispersion and spectral weight for the simple cubic lattice with $S = 3/2$, $J_H = zt$, $U = 10zt$ and $\delta = 0.3$ (upper lines) and $\delta = 0.95$ (lower lines). *SWBE*: full line, *SWGU*: long dashed line, *RPA*: dotted line.

should therefore be even closer to the actual excitations in the ferromagnetic Kondo lattice model. It is obvious that the deviation of the spin wave dispersion from a simple Heisenberg form is large for low electron concentration (δ close to 1) in the thermodynamic limit for the simple cubic lattice.

In order to demonstrate the doping dependence of this deviation Figure 3 shows the quantity

$$\Delta := \frac{2zD}{\omega(\mathbf{Q})} - 1 \tag{18}$$

for the simple cubic lattice with $J_H = \infty$ ($Q_i = \pi$ for i=1, ..., d). Δ is exactly zero for a Heisenberg dispersion. The deviation is large for large hole density, but there is also a finite deviation at smaller hole density. The corresponding analysis for one-dimensional systems is again in good agreement with results from numerical calculations for finite chains [49].

Figure 4 shows the spin wave dispersion at $\delta = 0.3$ and $\delta = 0.95$ obtained by the wave functions *SWBE*, *SWGU* and *RPA* for values of $J_H = zt$ and $U = 10zt$ which are reasonable for the CMR materials. The reduction relative to the *RPA* value of the spin wave energy due to correlation effects is stronger for the small particle density. For $\delta = 0.95$ the additional correlations in the ansatz *SWBE* compared to the ansatz *SWGU* also become more important. The correlation effect is however not negligible even for the low hole density $\delta = 0.3$. The largest deviation of the energy of the ansatz *SWBE* from the *RPA* value in this case is approximately 35%. Since the deviations of the spin wave dispersion from a Heisenberg dispersion are relatively small, it is not surprising, that the measured spin wave dispersion for $La_{0.7}Pb_{0.3}MnO_3$ shown in [31,32] appeared close to the spin wave dispersion for a Heisenberg model.

Finally we want to give a rough estimate for the Curie temperature extrapolated from our variational bounds for the spin excitations at zero temperature. For the ferromagnetic Kondo lattice with $J_H = \infty$ we use the approximation

$$k_B T_{Curie} = J(2.90S'(S'+1) - 0.36) \tag{19}$$

for the critical temperature for a Heisenberg model with spin S' [50]. We choose a value of $S' = S + n\frac{1}{2}$ for the effective spin and a coupling constant J which reproduces the spin wave stiffness D of the variational wave function. The resulting critical temperatures for the *RPA* spin wave and the spin wave *SWLO* are shown in Figure 5a. Even the *RPA* spin wave gives reasonable values for the critical temperature. Using the ansatz *SWLO* we get $T_{Curie} = 0.122t \approx 280$ K for $\delta = 0.3$ for a realistic hopping amplitude $t = 0.2$ eV. The critical temperature of $La_{2/3}Ca_{1/3}MnO_3$ for example is $T_{Curie} = 250$ K [51].

In the case of the Hubbard model the spin wave excitations are not well separated from the bottom of the scattering continuum. Here we assume the magnons to be independent bosons. Since the low lying excitations close to $\mathbf{q} = \mathbf{0}$ are most important we approximate the spin wave dispersion by $\omega(\mathbf{q}) = Dq^2$. For hole densities close to the critical hole density the scattering continuum becomes also important. Thus we show in Figure 5b an estimate for the critical temperature which also takes into account the bottom of the scattering continuum $\epsilon_{\rm scat}$ by choosing

$$\omega(\mathbf{q}) = \begin{cases} Dq^2 & \text{if} \quad Dq^2 < \epsilon_{scat} \\ \epsilon_{scat} & \text{else.} \end{cases} \tag{20}$$

In the case of the Hubbard model the effect of additional correlations is again more pronounced. The reduction of the critical temperature in comparison to an estimate using the *RPA* spin wave is much stronger than in the $S = 3/2$, $J_H = \infty$ case [48].

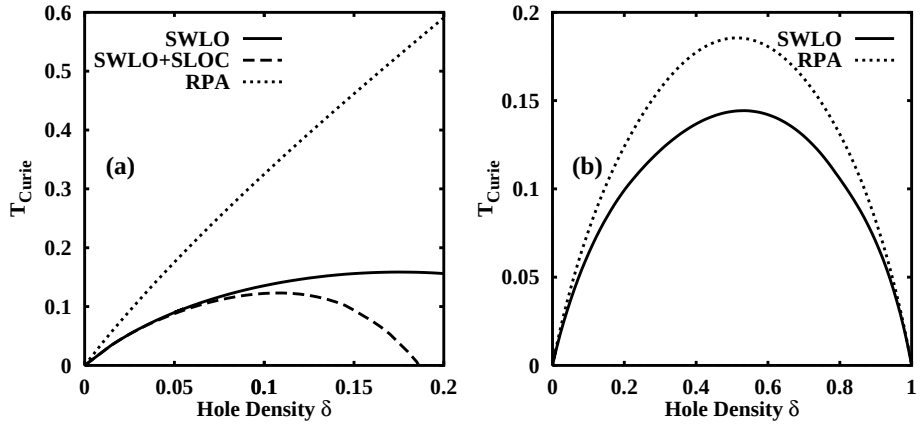

Fig. 5. Critical temperature for (a) the ferromagnetic Kondo lattice model with $J_H = \infty$ and $S = 3/2$ and (b) the Hubbard model at $U = \infty$ for the simple cubic lattice.

4 Summary and discussion

We investigated the stability of the fully polarized ferromagnetic state with respect to a single spin flip for the ferromagnetic Kondo lattice model including Hubbard repulsion for the conduction electrons. We used variational wave functions describing scattering states to obtain exact bounds for the region of possible stability of this Nagaoka state in the thermodynamic limit for the simple cubic lattice. As a special case the pure Hubbard model with $S = 0$ was re-investigated. We improved previous variational results for various values of core spin, Hund's rule coupling J_H and Hubbard repulsion U. For example the critical hole density for the pure Hubbard model was reduced from $\delta_{cr} = 0.237$ [25,47] to $\delta_{cr} = 0.185$ and the critical coupling was increased from $U_{cr} = 48.9t$ to $U_{cr} = 78.6t$. In addition to the quantitative improvements which require a large number of variational parameters we showed the instability of the Nagaoka state for any finite coupling J_H and U close to the half filled lattice including the exchange energy in the variational ansatz for a scattering state.

In the one dimensional ferromagnetic Kondo lattice model without Hubbard repulsion both for core spins of magnitude $S = 3/2$ and $S = 1/2$ our variational ansatz gives boundaries for the ferromagnetic regime in the thermodynamic limit which are very close to numerical results for finite chains [43,44]. Thus we expect that our results for the simple cubic lattice and $S = 3/2$ give a good description of the actual stability region in this case, where quantum fluctuations are expected to be more local. One advantage of the variational approach is the fact that it is possible to include a large Coulomb repulsion in the ferromagnetic Kondo lattice model without further approximations such as classical core spins or infinite J_H. In this sense the present work complements extensive numerical calculations for finite chains with $U = 0$ [43,44].

In regions of a possible ferromagnetic ground state we have calculated variational approximations for the spin wave energies assuming fully polarized ferromagnetism in the ground state. Especially we have calculated the doping dependence of the deviation of the spin wave dispersion from the one obtained for a Heisenberg ferromagnet. We found that the deviation is large for large hole densities but relatively small in the vicinity of the hole density $\delta = 0.3$ for which the spin wave dispersion has been measured throughout the Brillouin zone [31,32]. We obtained good agreement between our variational results and calculations for finite chains and a core spin of $S = 1/2$. This result for the extreme quantum case once more suggests that our method gives an even better approximation for the actual spin wave dispersion of the Kondo lattice for the higher spin $S = 3/2$ and the simple cubic lattice relevant for the CMR materials.

We estimated the Curie temperature using our variational bounds for the excitation energies at $T = 0$ and obtained values that are reasonable for the CMR materials in agreement with calculations using various other methods [52,44,53].

Appendix: Variational equation ansatz RES4

Using the definitions

$$\begin{aligned} \psi^{c,1}_{\mathbf{k}} &:= 0 \text{ if } \epsilon_{\mathbf{k}} < \epsilon_F, \\ \psi^{s}_{\mathbf{k}} &:= 0 \text{ if } \epsilon_{\mathbf{k}} < \epsilon_F, \\ \psi^{c,2}_{\mathbf{k}} &:= 0 \text{ if } \epsilon_{\mathbf{k}} > \epsilon_F \end{aligned} \tag{21}$$

and

$$\begin{aligned} I_{c1} &:= \frac{1}{(2\pi)^d}\int d^dk \psi^{c,1}_{\mathbf{k}}, \quad I_{c1\epsilon} := \frac{1}{(2\pi)^d}\int d^dk \epsilon_{\mathbf{k}}\psi^{c,1}_{\mathbf{k}}, \\ I_{c2} &:= \frac{1}{(2\pi)^d}\int d^dk \psi^{c,2}_{\mathbf{k}}, \quad I_{c2\epsilon} := \frac{1}{(2\pi)^d}\int d^dk \epsilon_{\mathbf{k}}\psi^{c,2}_{\mathbf{k}}, \\ I_{s} &:= \frac{1}{(2\pi)^d}\int d^dk \psi^{s}_{\mathbf{k}}\ , \quad I_{s\epsilon 1} := \frac{1}{(2\pi)^d}\int d^dk \epsilon_{\mathbf{k}}\psi^{s}_{\mathbf{k}} \end{aligned} \tag{22}$$

variation for $\mathbf{q}=0$ leads to the equations

$$\begin{aligned}0 &= \psi^{c,1}_{\mathbf{k}}\left[n\omega-|e_{\mathcal{N}}|-JSn-\epsilon_{\mathbf{k}}\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]\\ &+\psi^{s}_{\mathbf{k}}\left[n\omega-|e_{\mathcal{N}}|-\epsilon_{\mathbf{k}}\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]+I_s(\omega-\epsilon_B)\\ &-I_{c2\epsilon}\left(1+\frac{\epsilon_{\mathbf{k}}}{zt}\right)+I_{c2}(\epsilon_{\mathbf{k}}-\epsilon_B)+I_{c1}\left(\omega-\epsilon_B-JS\right),\end{aligned} \tag{23}$$

$$\begin{aligned}0 &= \psi^{c,2}_{\mathbf{k}}\left[\delta\omega-|e_{\mathcal{N}}|-JS\delta-U\delta+\epsilon_{\mathbf{k}}\left(\delta+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]\\ &+I_{c2}(\omega-\epsilon_B-JS-U)\\ &+I_{c1\epsilon}\left(1-\frac{\epsilon_{\mathbf{k}}}{zt}\right)-I_{c1}(\epsilon_{\mathbf{k}}+\epsilon_B)\\ &+I_{s\epsilon 1}\left(1-\frac{\epsilon_{\mathbf{k}}}{zt}\right)-I_s(\epsilon_{\mathbf{k}}+\epsilon_B),\end{aligned} \tag{24}$$

$$\begin{aligned}0 &= \psi^{s}_{\mathbf{k}}\left[(2S+n)\omega-|e_{\mathcal{N}}|-\epsilon_{\mathbf{k}}\left(2S+n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]\\ &+\psi^{c,1}_{\mathbf{k}}\left[n\omega-|e_{\mathcal{N}}|-\epsilon_{\mathbf{k}}\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]+I_s(\omega-\epsilon_B)\\ &-I_{c2\epsilon}\left(1+\frac{\epsilon_{\mathbf{k}}}{zt}\right)+I_{c2}(\epsilon_{\mathbf{k}}-\epsilon_B)+I_{c1}(\omega-\epsilon_B).\end{aligned} \tag{25}$$

By integration over $\mathbf{k}$ we obtain a system of linear equations in the variables I.

First of all the variable $I_{s\epsilon}$ can be eliminated by subtracting equation (24) from (23) to obtain

$$(\omega-\epsilon_{\mathbf{k}})\psi^{s}_{\mathbf{k}}=-\frac{J}{2}\left(n\psi^{c,1}_{\mathbf{k}}+I_{c1}\right) \tag{26}$$

and expressing $I_{s\epsilon}$ by I_s and I_{c1}:

$$I_{s\epsilon 1}=\omega I_s+\frac{J}{2}I_{c1}. \tag{27}$$

We solve equation (23) for $\psi^{c,1}$ and equation (24) for $\psi^{c,2}$ and obtain two linear equations by integration and two linear equations by multiplication by $\epsilon_{\mathbf{k}}$ followed by integration. The fifth equation is calculated by direct integration of equation (23) leading to

$$\mathbf{M}\cdot(I_{c1},I_s,I_{c2},I_{c2\epsilon},I_{c1\epsilon})^T=\mathbf{0} \tag{28}$$

with

$$\begin{aligned}\mathbf{M}_{1,1} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_1(\epsilon,\omega)}\Bigg\{(\omega-\epsilon_B-JS)(\omega-\epsilon)\\ &-\frac{J}{2}\left[n\omega-|e_{\mathcal{N}}|-\epsilon\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]\Bigg\},\\ \mathbf{M}_{1,2} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_1(\epsilon,\omega)}(\omega-\epsilon),\\ \mathbf{M}_{1,3} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_1(\epsilon,\omega)}(\epsilon-\epsilon_B)(\omega-\epsilon),\\ \mathbf{M}_{1,4} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_1(\epsilon,\omega)}(\epsilon-\omega)\left(1+\frac{\epsilon}{zt}\right),\\ \mathbf{M}_{1,5} &= 0,\end{aligned} \tag{29}$$

$$\begin{aligned}\mathbf{M}_{2,1} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_1(\epsilon,\omega)}\Bigg\{(\omega-\epsilon_B-JS)(\omega-\epsilon)\\ &-\frac{J}{2}\left[n\omega-|e_{\mathcal{N}}|-\epsilon\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right)\right]\Bigg\},\\ \mathbf{M}_{2,2} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_1(\epsilon,\omega)}(\omega-\epsilon),\\ \mathbf{M}_{2,3} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_1(\epsilon,\omega)}(\epsilon-\epsilon_B)(\omega-\epsilon),\\ \mathbf{M}_{2,4} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_1(\epsilon,\omega)}(\epsilon-\omega)\left(1+\frac{\epsilon}{zt}\right),\\ \mathbf{M}_{2,5} &= 0,\end{aligned} \tag{30}$$

$$\begin{aligned}\mathbf{M}_{3,1} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_2(\epsilon,\omega)}\left[\frac{J}{2}\left(1-\frac{\epsilon}{zt}\right)-(\epsilon+\epsilon_B)\right],\\ \mathbf{M}_{3,2} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_2(\epsilon,\omega)}\left(1-\frac{\epsilon}{zt}\right),\\ \mathbf{M}_{3,3} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_2(\epsilon,\omega)}(\omega-\epsilon_B-JS-U),\\ \mathbf{M}_{3,4} &= 0,\\ \mathbf{M}_{3,5} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{1}{N_2(\epsilon,\omega)}\left(1-\frac{\epsilon}{zt}\right),\end{aligned} \tag{31}$$

$$\begin{aligned}\mathbf{M}_{4,1} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_2(\epsilon,\omega)}\left[\frac{J}{2}\left(1-\frac{\epsilon}{zt}\right)-(\epsilon+\epsilon_B)\right],\\ \mathbf{M}_{4,2} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_2(\epsilon,\omega)}\left(1-\frac{\epsilon}{zt}\right),\\ \mathbf{M}_{4,3} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_2(\epsilon,\omega)}(\omega-\epsilon_B-JS-U),\\ \mathbf{M}_{4,4} &= 0,\\ \mathbf{M}_{4,5} &= \int_{\epsilon_F}^{\epsilon_T}d\epsilon\rho(\epsilon)\frac{\epsilon}{N_2(\epsilon,\omega)}\left(1-\frac{\epsilon}{zt}\right)\end{aligned} \tag{32}$$

$$\begin{aligned}\mathbf{M}_{5,1} &= \omega-|e_{\mathcal{N}}|-JS-\delta\epsilon_B-\frac{J}{2}\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right),\\ \mathbf{M}_{5,2} &= \left(\delta-\frac{|e_{\mathcal{N}}|}{zt}\right),\\ \mathbf{M}_{5,3} &= |e_{\mathcal{N}}|-\delta\epsilon_B,\\ \mathbf{M}_{5,4} &= -\delta-\frac{|e_{\mathcal{N}}|}{zt},\\ \mathbf{M}_{5,5} &= -n-\frac{|e_{\mathcal{N}}|}{zt}\end{aligned} \tag{33}$$

where

$$f_1(\epsilon,\omega):=n\omega-|e_{\mathcal{N}}|-\epsilon\left(n+\frac{|e_{\mathcal{N}}|}{zt}\right),$$

$$f_2(\epsilon,\omega):=\delta\omega-|e_{\mathcal{N}}|+\epsilon\left(\delta+\frac{|e_{\mathcal{N}}|}{zt}\right),$$

$N_1(\epsilon,\omega):=(JSn-f_1(\epsilon,\omega))(\omega-\epsilon)+\frac{Jn}{2}f_1(\epsilon,\omega)$ and

$N_2(\epsilon,\omega):=\delta(JS+U)-f_2(\epsilon,\omega).$

All quantities can be evaluated by just one-dimensional integrations. The density of states ρ is calculated using a polynomial fit taking into account the van Hove singularities. At the lowest variational energy ω the matrix $\mathbf{M}$ is singular. Thus ω corresponds to the root of $\det(\mathbf{M})$ and is calculated numerically.

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