Doping dependence of the spin gap in a two-leg ladder

L. Campos Venuti and A. Muramatsu
Institut für Theoretische Physik III, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Federal Republic of Germany
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A spin-fermion model relevant for the description of cuprates ladders is studied in a path integral formalism, where, after integrating out the fermions, an effective action for the spins in term of a Fermi-determinant results. The determinant can be evaluated in the long-wavelength, low-frequency limit to all orders in the coupling constant, leading to a non-linear σ model with doping dependent coupling constants. An explicit evaluation shows that the magnon gap diminishes upon doping, as opposed to previous mean-field treatments.

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I. INTRODUCTION

Doped quantum antiferromagnets constitute a major unresolved problem in condensed matter physics, which is at the center of current research since the discovery of high T_c superconductivity.[1] In particular, the case of a doped spin liquid—where no symmetry is spontaneously broken—is very challenging, since the starting point, the spin liquid state, cannot be described by a classical Néel state.

This problem is not only of theoretical relevance. Cu_2O_3 ladders are present in $Sr_{14-x}Ca_xCu_{24}O_{41}$, and many experiments support the presence of a spin gap and a finite correlation length,[2–7] two crucial ingredients signaling a spin liquid state. With isovalent Ca^{2+} substitution of Sr^{2+} holes are transferred from the CuO_3 chains to the ladders,[8] increasing the conductivity of the latter. The spin gap, as measured by Knight shift or NMR experiments[3–5] is seen to diminish. With increasing doping, superconductivity is ultimately stabilized under pressure,[9,10] a phenomenon that suffices to justify the interest for the subject.

The simplest model which is believed to grasp the physics of the problem is the *t-J* model on a two leg ladder. It is believed in general that this system evolves continuously from the isotropic case to the limit of strong rung interaction. In this limit some simplifying pictures are at hand: without doping the gap is the energy of promoting a singlet rung to a triplet ($\sim J_\perp$). Interaction among the rungs leads eventually to the usual magnon band. Upon doping the systems shows two different kinds of spin excitations.[11,12] One is still the singlet-triplet transition as before, and the other corresponds to the splitting of a hole pair into a couple of quasiparticles (formed by a spinon and an holon), each carrying charge $+|e|$ and spin 1/2. The number of possible excitations is proportional to $(1-\delta)$ (for the magnons) and δ (for the quasiparticles), respectively, where δ is the number of holes per copper site. For this reason, at a low doping concentration, the magnon gap will be the most important in influencing the form of the static susceptibility or dynamical structure factor.

Sigrist *et al.*[13] and more recently Lee *et al.*[14] attacked the problem ultimately with some sort of mean-field decoupling. Their results agreed in predicting an increase of the magnon gap (Δ_M, originated from the singlet-triplet transition), while Lee *et al.* were also able to calculate a decrease of the quasiparticle gap (Δ_{QP} originating from the splitting of a hole pair) for small doping concentrations.

In contrast to the mean-field results above, Ammon *et al.*[15] obtained a decrease of the magnon gap and an almost doping independent Δ_{QP} using a temperature density matrix renormalization group (TDMRG) calculation. The behavior of the magnon gap observed numerically is consistent with the one observed in several experiments, and hence it is natural to ascribe those experimental observations to Δ_M.

In this paper we concentrate on the behavior of the magnon gap upon doping. Due to the contradiction above it is imperative to go beyond mean field and include the role of fluctuations in a controlled manner. A mapping from an antiferromagnetic Heisenberg model to an effective field theory, the non linear σ model (NLσM), proved very efficient in describing the magnetic properties of two dimensional spin lattices,[16] chains,[17] and ladders.[18] This mapping was extended in Ref. 19 to the case of a doped two dimensional anitferromagnet using a procedure that we will closely follow.

II. MAPPING TO AN EFFECTIVE SPIN ACTION

Since no satisfactory analytical treatment of the *t-J* model away from half filling is possible at present, we focus on the so called spin-fermion model. This Hamiltonian can be derived in fourth order degenerate perturbation theory[20,21] from the *p-d*, three band, Emery model,[22] that gives a detailed description of the cuprate materials. There the role of perturbation is played by the hybridization term between the *p* orbital (oxygen) and the *d* orbital (copper). A further simplification of the model was proposed by Zhang and Rice,[23] that leads to the *t-J* model.

A typical copper-oxide two leg ladder, like those present in $Sr_{14-x}Ca_xCu_{24}O_{41}$ is depicted in Fig. 1. It is generally

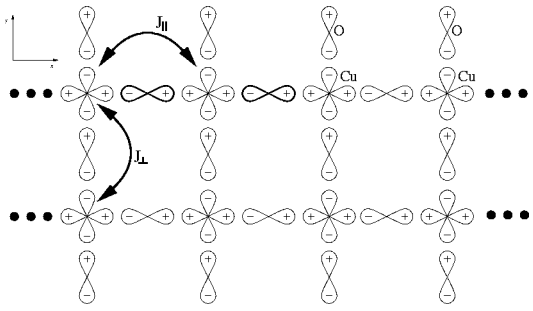

FIG. 1. Schematic picture of a two-leg ladder copper oxide.

accepted that the dopant holes reside on *p*-orbitals on the oxygens sites, whereas on the Cu^{2+} ions a localized hole resides, represented by spin 1/2 operator which interact via a nearest neighbor exchange.

The spin-fermion Hamiltonian is defined as follows:

$$H_{SF}=t\sum_{\langle j,j';i\rangle,i,\sigma}(-1)^{\alpha_{i,j}+\alpha_{i,j'}}c^{\dagger}_{j,\sigma}c_{j',\sigma}+J_K\sum_i \mathbf{R}_i\cdot\mathbf{S}_i + J_H\sum_{\langle i,i'\rangle}\mathbf{S}_i\cdot\mathbf{S}_{i'}. \quad (1)$$

The index i (j) runs over the Cu (O) sites, $c^{\dagger}_{j,\sigma}$ creates a hole in an oxygen p band and $\mathbf{S}_j$ are spin operators for the copper ions. The coefficients $\alpha_{i,j}$ take care of the sign of the p-d overlap and $\alpha_{i,j}=1$ if $j=i+\frac{1}{2}\hat{x}$ or $i+\frac{1}{2}\hat{y}$ and $\alpha_{i,j}=2$ if $j=i-\frac{1}{2}\hat{x}$ or $i-\frac{1}{2}\hat{y}$. Finally the operator $\mathbf{R}_i$ is defined as

$$\mathbf{R}_i=\sum_{\langle j,k;i\rangle,i,\alpha,\beta}(-1)^{\alpha_{i,j}+\alpha_{i,k}}c^{\dagger}_{j,\alpha}\boldsymbol{\sigma}_{\alpha,\beta}c_{k,\beta}. \quad (2)$$

Following Ref. 23 we can define the following operator centered on the copper site $P_{i,\sigma}=(1/2)\Sigma_{\langle j;i\rangle}(-1)^{\alpha_{i,j}}c_{j,\sigma}$ which represents nonorthogonal orbitals with a high weight on the i site. Their anticommutation relations are

$$\{P_{i,\sigma},P^{\dagger}_{i',\sigma'}\}=\delta_{\sigma,\sigma'}\left(\delta_{i,i'}-\frac{1}{4}\delta_{\langle i,i'\rangle}\right), \quad (3)$$

and we can rewrite the Hamiltonian in terms of these operators as follows:

$$H_{SF}=4t\sum_{\substack{l=1\ldots L\\ \lambda=1,2,\sigma}}P^{\dagger}_{l,\lambda,\sigma}P_{l,\lambda,\sigma} + 4J_K\sum_{\substack{l=1\ldots L\\ \lambda=1,2,\alpha,\beta}}P^{\dagger}_{l,\lambda,\alpha}\boldsymbol{\sigma}_{\alpha,\beta}P_{l,\lambda,\beta}\cdot\mathbf{S}_{l,\lambda} + J_{\perp}\sum_{l=1\ldots L}\mathbf{S}_{l,1}\cdot\mathbf{S}_{l,2}+J_{||}\sum_{\substack{l=1\ldots L\\ \lambda=1,2}}\mathbf{S}_{l,\lambda}\cdot\mathbf{S}_{l+1,\lambda}. \quad (4)$$

L is the number of the rungs along the ladder, and $\lambda=1,2$ distinguishes the two legs. For the sake of generality, an anisotropy in the Heisenberg term is allowed.

The different steps of our procedure are the following: first find orthogonal (Wannier states) for the holes, then go to a (coherent states) path integral formulation for spins and fermions and perform the Gaussian integration of the fermionic degrees of freedom. The remaining part of the calculation is devoted to the evaluation of the resulting Fermi determinant in the long-wavelength low-frequency limit. This expansion includes the coupling constant J_K to all order.

Wannier states are easily find via $P_{\mathbf{k},\sigma}=\sqrt{\epsilon(\mathbf{k})}f_{\mathbf{k},\sigma}$, where

$$\epsilon(\mathbf{k})=\left(1-\frac{\cos(k_x a)+\cos(k_y a)/2}{2}\right).$$

Here a is the lattice constant and we used a two-dimensional Fourier transform where k_y takes only values 0 and π/a distinguishing between symmetric (bonding) and antisymmetric (antibonding) states. The partition function can be expressed as a path integral,

$$Z=\int D[f^*]D[f]D[\hat{\Omega}]e^{-S_{SF}}, \quad (5)$$

where $S_{SF}=S_h+S_s$. The action S_s contains all terms with spins degree of freedoms only,[24]

$$S_s=\int_0^{\beta}d\tau\left[-iS\sum_{l,\lambda}\mathbf{A}(\hat{\Omega}_{l,\lambda})\cdot\frac{\partial\hat{\Omega}_{l,\lambda}}{\partial\tau}+H_{\mathrm{Heis}}[S\hat{\Omega}(\tau)]\right], \quad (6)$$

where $\hat{\Omega}$ is a unimodular field, S is the spin per site (1/2 in our case), and $\mathbf{A}$ is the vector potential for a (Dirac) monopole: $\epsilon^{abc}(\partial A_a/\partial\hat{\Omega}_b)=\hat{\Omega}_c$.

It is by now well accepted that the effective low energy field theory of the d-dimensional Heisenberg antiferromagnetic model is given by the $(d+1)$ NLσM.[17,25,26] In the case of a ladder one obtains the $(1+1)$ NLσM.[18,27] For this reason, here we will deal mainly with the part of the action which contains fermionic degrees of freedom S_h:

$$S_h=\sum_{kq\alpha\beta}f^*_{k,\alpha}[(i\omega_n+4t\epsilon(\mathbf{k})-\mu)\delta_{k,q}\delta_{\alpha,\beta} + g\sqrt{\epsilon(\mathbf{k})\epsilon(\mathbf{q})}\boldsymbol{\sigma}_{\alpha,\beta}\cdot\hat{\Omega}_{k-q}]f_{q,\beta}; \quad (7)$$

here $k=(k_x,k_y,\omega_n)$, where $\omega_n=\pi(2n+1)/\beta$ are the fermionic Matsubara frequency and $g=4J_KS$. It is natural to decompose the inverse propagator into $G^{-1}=G_0^{-1}-\Sigma$, where the free part is

$$G_0^{-1}=(i\omega_n+4t\epsilon(\mathbf{k})-\mu)\delta_{k,q}\delta_{\alpha,\beta} \quad (8)$$

and the fluctuating external potential is

$$\Sigma=-g\sqrt{\epsilon(\mathbf{k})\epsilon(\mathbf{q})}\boldsymbol{\sigma}_{\alpha,\beta}\cdot\hat{\Omega}_{k-q}. \quad (9)$$

Since, according to Eq. (7) the action S_{SF} is bilinear in the fermionic variables, we can integrate them out. This leads to $S_{SF}=S_s-\mathrm{tr}\ln G^{-1}$. Defining the matrix

$$A=\sqrt{\epsilon(\mathbf{k})}\delta_{k,q}\delta_{\alpha,\beta} \quad (10)$$

and a rescaled propagator $\hat{G}^{-1}$ through

$$\hat{G}^{-1}=A^{\dagger-1}G^{-1}A^{-1}, \quad (11)$$

we can write

$$\mathrm{tr}\ln(G^{-1})=\mathrm{tr}\ln(AA^{\dagger})+\mathrm{tr}\ln(\hat{G}^{-1}), \quad (12)$$

the first term gives just a constant and we can ignore it. Again we decompose the rescaled inverse propagator as $\hat{G}^{-1}=\hat{G}_0^{-1}-\hat{\Sigma}$ which brings us to

$$\hat{G}_0^{-1} = \left(\frac{i\omega_n + 4t\epsilon(\mathbf{k}) - \mu}{\epsilon(\mathbf{k})} \right) \delta_{kq}\delta_{\alpha\beta} \equiv g_0^{-1}(k_x, k_y, \omega_n)\,\delta_{k,q}\delta_{\alpha,\beta}, \tag{13}$$

$$\hat{\Sigma} = -g\Omega_{\mathbf{k}-\mathbf{q},\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}. \tag{14}$$

The remaining part of the calculation is devoted to the evaluation of $S_{h\ \mathrm{eff}} = -\mathrm{tr}\ln(\hat{G}^{-1})$ in the continuum limit.

Parametrizations

As we already mentioned, in the undoped regime where no holes are present, it has proven very effective a mapping from a antiferromagnetic Heisenberg spin ladder to a 1+1 NLσM. This mapping rely on the idea that although long range order (here antiferromagnetic) is prohibited in one dimension, the most important contribution to the action are given by paths in which antiferromagnetic order survives at short distance. Accordingly the dynamical unimodular field is decomposed in a Néel modulated field **n** plus a ferromagnetic fluctuating contribution. A gradient expansion in the dynamical field brings then to the 1+1 NLσM. The gradient expansion is justified when the correlation length of the spin is much larger than the lattice constant a. However the prediction of the NLσM, i.e., a finite correlation length and a triplet of massive modes above the ground state[17,28–30] remain valid until $\xi \approx 2.5a$, as numerical calculations on the isotropic Heisenberg ladder have shown.[31]

The basic assumption of this work is then that such a parametrization is still meaningful as long as the spin liquid state is not destroyed by doping, as seems to be the case in experiments, where a finite spin gap is also seen in the doped case.[2–7] Then, as, e.g., in Ref. 24, we parametrize the spin field in the following way:

$$\Omega_{i,\lambda}(\tau) = (-1)^{i+\lambda}\mathbf{n}_{i,\lambda}\sqrt{1-\left|\frac{a\mathbf{l}_{i,\lambda}}{S}\right|^2} + \frac{a\mathbf{l}_{i,\lambda}}{S}. \tag{15}$$

$\mathbf{n}_{i,\lambda}$ and $\mathbf{l}_{i,\lambda}$ are two slowly varying, orthogonal, vector fields describing locally antiferromagnetic and ferromagnetic configurations, respectively. $\mathbf{n}_{i,\lambda}$ is normalized such that $|\mathbf{n}_{i,\lambda}|^2 = 1$. The lattice constant a in front of $\mathbf{l}_{i,\lambda}$ in Eq. (15) makes explicit the fact that $\mathbf{l}_{i,\lambda}$ is proportional to a generator of rotations of $\mathbf{n}_{i,\lambda}$, namely, to a first-order derivative of $\mathbf{n}_{i,\lambda}$.

In the particular geometry of a ladder, this decomposition give rise to two local order parameters $\mathbf{n}_{i,1}$ and $\mathbf{n}_{i,2}$. However, we assume that spins across the chain are rather strongly correlated such that they will sum up to give rise to an antiferromagnetic configuration, or subtract and give a ferromagnetic fluctuation. A further parametrization is then

$$\mathbf{n}_{i,\lambda} = \mathbf{N}_i\sqrt{1-a^2|\mathbf{M}_i|^2} + (-1)^{\lambda}a\mathbf{M}_i, \tag{16}$$

with $\mathbf{N}_i\cdot\mathbf{M}_i = 0$ and $|\mathbf{N}_i|^2 = 1$. This parametrization, with two ferromagnetic fluctuating fields **l** and **M**, is the most correct one since it preserves the correct number of degrees of freedom. In the case of a two leg ladder, one sees, *a posteriori*, that the field **M** decouples completely and does not play any role, both in the undoped and in the doped case.

The next step is the gradient expansion, or equivalently, in Fourier space, an expansion in powers of k. In 1+1 dimensions the field **N** will have no scaling dimension, whereas the fields **l** and **M** have a scaling dimension -1. Accordingly, in the subsequent expansion we will need to keep terms with up to two derivative and any power of the field **N**. Terms containing **l** and **M** are marginal whenever two fields or one field and one derivative are present. Higher order terms are irrelevant and will be discarded. This correspond to expand all our quantities up to $O(a^2)$.

The self energy then has the expansion

$$\hat{\Sigma} = \Sigma_{00} + \Sigma_{01} + \Sigma_{02} + \Sigma_1 + \Sigma_2 + O(a^3), \tag{17}$$

where the various quantity are

$$\Sigma_{00} = -g\,\delta_{k_y-q_y,\pi}\mathbf{N}_{k_x-q_x+\pi,\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{18}$$

$$\Sigma_{01} = -ag\,\delta_{k_y-q_y,0}\mathbf{M}_{k_x-q_x+\pi,\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{19}$$

$$\Sigma_{02} = \frac{a^2 g}{2}\,\delta_{k_y-q_y,\pi}(\mathbf{N}|\mathbf{M}|^2)_{k_x-q_x+\pi,\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{20}$$

$$\Sigma_1 = -\frac{ag}{S}\mathbf{l}_{\mathbf{k}-\mathbf{q},\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{21}$$

$$\Sigma_2 = \frac{a^2 g}{2S^2}(\mathbf{N}|\mathbf{l}|^2)_{\mathbf{k}-\mathbf{q}+\mathbf{Q},\omega-\nu}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{22}$$

where $\mathbf{Q} = (\pi/a, \pi/a)$ is the antiferromagnetic modulation vector suitable for a ladder geometry. We also regroup the zeroth order term in $F^{-1} \equiv \hat{G}_0^{-1} - \Sigma_{00}$.

The evaluation of the various contribution in the continuum limit, proceeds very similarly as in Ref. 19, and we refer to that paper for a more detailed explanation. The quantity to be evaluated is

$$S_{h\mathrm{eff}} = -\mathrm{tr}\ln(F^{-1}) - \mathrm{tr}\ln[\mathbb{1} - F(\Sigma_{01} + \Sigma_{02} + \Sigma_1 + \Sigma_2)]. \tag{23}$$

We then need to find the inverse of F^{-1} up to $O(a)$. It turns out that

$$F = \overline{F}D^{-1} - a\overline{F}D^{-1}RD^{-1} + O(a^2), \tag{24}$$

where the various matrices are

$$\overline{F} = \overline{g_0^{-1}}(\mathbf{k},\omega)\,\delta_{kq}\delta_{\alpha\beta} - g\,\delta_{k_y-q_y,\pi}\mathbf{N}_{k_x-q_x+\pi}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{25}$$

$$D = D(\mathbf{k},\omega)\,\delta_{kq}\delta_{\alpha\beta}, \tag{26}$$

$$R = -g\,\delta_{k_y-q_y,\pi} \times \sum_{r=x,\tau}(k_r - q_r + \delta_{r,x}\pi/a)\,\partial_r g_0^{-1}(\mathbf{k},\omega)\mathbf{N}_{k-q+Q}\cdot\boldsymbol{\sigma}_{\alpha\beta}, \tag{27}$$

and we used the shorthand notation

$$\bar{g}_0^{-1}(\mathbf{k},\omega_n)=g_0^{-1}(\mathbf{k}+\mathbf{Q},\omega_n), \tag{28}$$

$$D(\mathbf{k},\omega_n)=g_0^{-1}(\mathbf{k},\omega_n)\bar{g}_0^{-1}(\mathbf{k},\omega_n)-g^2. \tag{29}$$

We first consider the term

$$\mathrm{tr}\ln(F^{-1})=\mathrm{tr}\ln(\hat{G}_0^{-1})+\mathrm{tr}\ln(\mathbb{1}-\hat{G}_0\Sigma_{00}). \tag{30}$$

The second term of this equation is reduced to the calculation of

$$\sum_{m=1}^{\infty}\frac{1}{n}\mathrm{tr}(\hat{G}_0\Sigma_{00})^m, \tag{31}$$

where each term has the following expansion:

$$\begin{aligned}\mathrm{tr}(\hat{G}_0\Sigma_{00})^m=(g)^m\sum_{k,q_2\cdots q_m} & g_0(k)\bar{g}_0(k+q_2)g_0(k+q_3)\\ &\times\bar{g}_0(k+q_4)\cdots g_0(k+q_{m-1})\bar{g}_0(k+q_m)\\ &\times\mathbf{N}_{-q_2}^{a_1}\mathbf{N}_{q_1-q_2}^{a_2}\cdots\mathbf{N}_{q_m}^{a_2}\,\mathrm{tr}(\sigma_1^a\sigma_2^a\cdots\sigma_m^a),\end{aligned} \tag{32}$$

with m an even integer. The trace over the Pauli matrices can be carried out using a trace reduction formula.[32] The gradient expansion in Eq. (32) is then obtained by performing an expansion of the product of propagators $g_0(k)\cdots\bar{g}_0(k+q_m)$ in powers of the variables $q_2,q_3,\ldots q_m$ that appear as argument of the vector field $\mathbf{N}$. The result obtained is[19]

$$\mathrm{tr}\ln(\mathbb{1}-\hat{G}_0\Sigma_{00})=\int dx\,d\tau\left[\frac{\bar{\chi}_{xx}}{2}\left|\partial_x\mathbf{N}\right|^2+\frac{\bar{\chi}_{\tau\tau}}{2}\left|\partial_\tau\mathbf{N}\right|^2\right], \tag{33}$$

with the definition

$$\bar{\chi}_{\alpha\beta}=\frac{\partial^2}{\partial q_\alpha\partial q_\beta}\sum_k\ \ln[1-g^2g_0(k)g_0(k+q+Q)]\delta_{q_y0}|_{q=0}. \tag{34}$$

We can now pass to the evaluation of the second term in Eq. (23). This does not present particular problems, since after expanding all the quantities, it reduces to the evaluation of a finite number of traces. The result is

$$\begin{aligned}&\mathrm{tr}\ln[\mathbb{1}-F(\Sigma_{01}+\Sigma_{02}+\Sigma_1+\Sigma_2)]\\ &\quad=i\frac{g^3}{S}\int dx\,d\tau\hat{\chi}_\tau(\mathbf{N}\times\partial_\tau\mathbf{N})\cdot(\mathbf{l}_1+\mathbf{l}_2)\\ &\quad-\frac{g^2}{8S^2}\int dx\,d\tau\tilde{\chi}(\mathbf{l}_1+\mathbf{l}_2)^2.\end{aligned} \tag{35}$$

Here we omitted to write a Gaussian term $\propto\mathbf{M}^2$, completely decoupled, which can be integrated out without further consequences. The quantities $\hat{\chi}_\tau$ and $\tilde{\chi}$ are given by

$$\hat{\chi}_\tau=-i\sum_k\ D^{-1}(k)\partial_{\omega_n}g_0^{-1}(k)D^{-1}(k+Q), \tag{36}$$

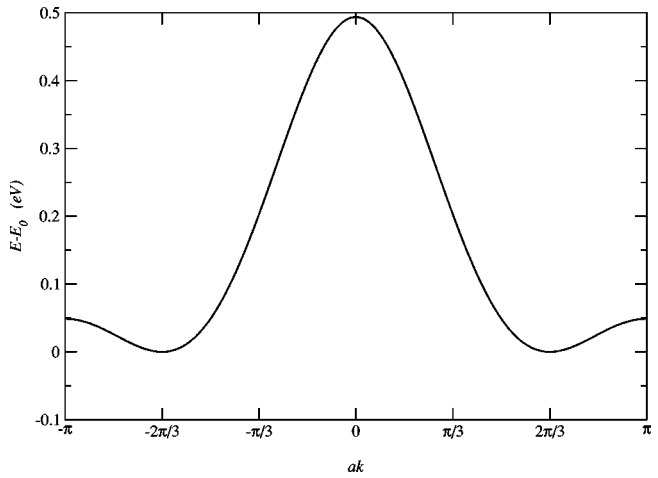

FIG. 2. Effective lowest-band holes emerging from our theory. The parameters are $t=0.24$ and $J_K=1$ eV. The minimum falls exactly at $(ak)=2\pi/3$.

$$\tilde{\chi}=\sum_k\ \{D^{-1}(k)[g_0^{-1}(k+Q)-g_0^{-1}(k)]\}^2. \tag{37}$$

They are generalized susceptibilities of the holes in presence of long-wavelength spin fields. In particular the zeros of $D(k)$ determine the dispersion of such holes. Through the dependence of the chemical potential we extract the doping concentration. The bands originating in such a way correspond to free holes moving in a staggered magnetic field. Such a staggered field would break translation invariance by one site and we would obtain four bands in the reduced Brillouin zone. Instead, in our procedure we never explicitly broke translation invariance, so that we obtain genuinely two bands in the Brillouin zone. The lowest of these two bands is symmetric in character (bonding). In Fig. 2 we show this for values of the constants relevant for the copper-oxide ladder i.e., a bandwidth of ≈ 0.5 eV (Ref. 33) and $J_K\approx 1$.[34–36] This band is in good agreement with accurate calculations on the one hole spectrum of the t-J model. In particular, in the isotropic t-J model, for $t/J\approx 2$ (which is a value relevant for the cuprates ladders) the same qualitative feature are observed: a global maximum at $(ka)=0$, global minima at $(ka)\approx\pm 2\pi/3$, and local maxima at $(ka)=\pm\pi$.[37,38]

Now that we calculated the long wavelength contribution coming from the holes, we still have to consider the continuum limit (in the low energy sector) of the pure spin action S_s given by Eq. (6). The result is

$$\begin{aligned}S_{\mathrm{seff}}=&-i\int dx\,d\tau(\mathbf{N}\times\partial_\tau\mathbf{N})\cdot(\mathbf{l}_1+\mathbf{l}_2)\\ &+a\left(J_\parallel+\frac{J_\perp}{2}\right)\int dx\,d\tau(\mathbf{l}_1+\mathbf{l}_2)^2\\ &+aJ_\parallel\int dx\,d\tau(\mathbf{l}_1-\mathbf{l}_2)^2+aS^2J_\parallel\int dx\,d\tau|\partial_x\mathbf{N}|^2.\end{aligned} \tag{38}$$

The very last step is the Gaussian integration of the $\mathbf{l}_\perp$ field, leaving us with the effective long-wavelength action for the antiferromagnetic order parameter, a (1+1) NLσM:

$$S_{\rm eff}=S_{h\rm eff}+S_{s\rm eff}=\frac{1}{2f}\int dx d\tau\left[v\left|\partial_x\mathbf{N}\right|^2+\frac{1}{v}\left|\partial_\tau\mathbf{N}\right|^2\right], \tag{39}$$

where the NLσM parameters are given by

$$f=\frac{1}{2}\left[\left(S^2J_\parallel-\frac{\overline{\chi}_{xx}}{2}\right)\left(\frac{\left(1+\frac{g^3}{S}\hat{\chi}_\tau\right)^2}{\left[4J_{||}+2J_\perp+\frac{g^2}{S^2}\tilde{\chi}\right]}-\frac{\overline{\chi}_{\tau\tau}}{2}\right)\right]^{-1/2}, \tag{40}$$

$$v=a\left[\frac{\left(S^2J_\parallel-\frac{\overline{\chi}_{xx}}{2}\right)}{\left(\frac{\left(1+\frac{g^3}{S}\hat{\chi}_\tau\right)^2}{\left[4J_{||}+2J_\perp+\frac{g^2}{S^2}\tilde{\chi}\right]}-\frac{\overline{\chi}_{\tau\tau}}{2}\right)}\right]^{1/2}. \tag{41}$$

Hence the spin-fermion model with mobile holes interacting with an antiferromagnetic background is mapped into an effective NLσM whose coupling constant depend on doping through the generalized susceptibilities in Eqs. (34), (36), and (37).

Now we can immediately transpose to our model of a doped spin liquid, some known result for the NLσM, e.g., mainly the presence of a gap which separates the singlet ground state from a triplet of magnetic excitations. This gap should persist as long as the continuum approximation is valid.

The fact that the NLσM in (1+1) dimension has a gap above the ground state can be established in a variety of ways. Using the two loop beta function[39] one obtains

$$\Delta=v\Lambda e^{-2\pi/f}\left(\frac{2\pi}{f}+1\right), \tag{42}$$

where Λ is a cutoff of the order of the inverse lattice constant. Now we have an explicit analytic form for the doping dependence of the spin gap in the spin-liquid state of a two leg ladder.

To study the behavior of the gap with doping we have to distinguish two regimes where the lowest effective band has minimum either at zero or at $2/3\pi$. For $J_K>2t$ the minima fall in $\pm 2/3\pi$. Here all the generalized susceptibilities in Eqs. (34), (36), and (37) contribute to lower f and since, from Eq. (42), Δ is an increasing function of f, they make the gap smaller for any value of the constants (see Fig. 3). This is comforting, since, as we mentioned, for J_K very large the physics of the spin-fermion model should be similar to that of the t-J model,[23] and for that one, TDMRG simulations show that the gap decreases at least in a strong anisotropic case ($J_\perp=10J_\parallel$). When $J_K<2t$ the band minimum falls in zero and there is one susceptibility, $\tilde{\chi}$, which instead makes f grow. In this regime there is then a (small) region of parameters where the gap grows with doping (see Fig. 4).

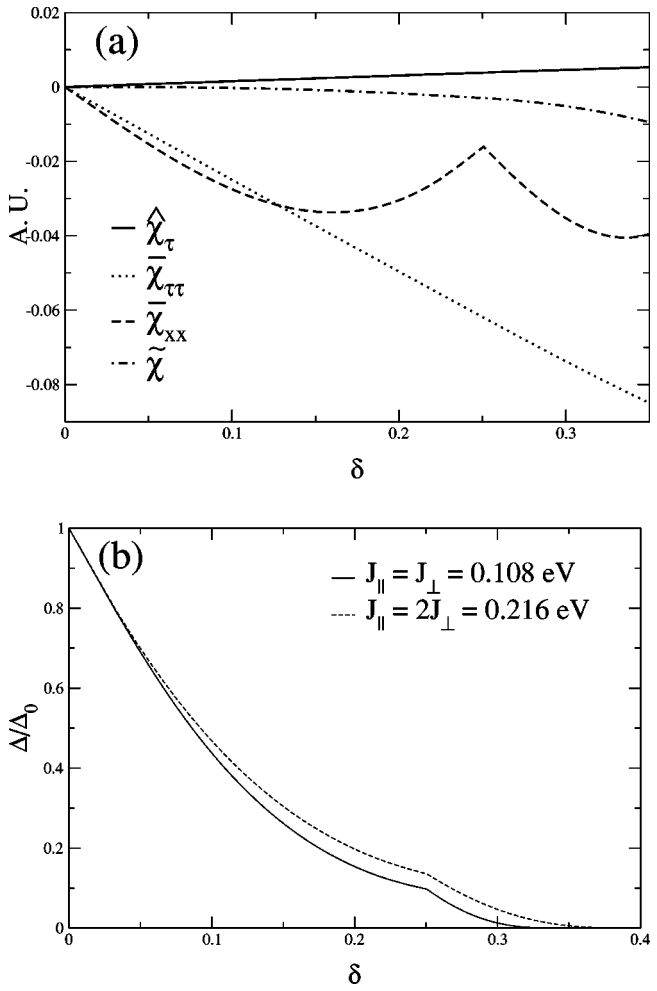

FIG. 3. $J_K>2t$. (a) Generalized susceptibilities of Eqs. (34), (36), and (37) for $J_K=2, t=0.76$ eV. For $J_K>2t$ all the susceptibilities contribute to lower f hence the gap decreases for small doping for any value of the constants. (b) Normalized gap from Eq. (42). Here we fixed $J_\perp=0.108$ eV. The solid line refers to isotropic couplings $J_{||}/J_\perp=1$. For comparison, an isotropic case with $J_{||}/J_\perp=2$ is also shown (dashed curve). It can be seen that anisotropy does not greatly influence the gap-vs-doping curve.

Before passing to a comparison with experiments, we want to comment on a possible simplifying understanding. A simple picture to explain the observed diminishing of the spin gap with doping in $Sr_{14-x}Ca_xCu_{24}O_{41}$, is that (at least for low doping concentration where speaking of a spin liquid is still feasible) the effect of the holes is that of renormalizing the anisotropy parameter $\lambda=J_\perp/J_\parallel$ for the spin part toward larger values. In many studies on the 2 leg ladder Heisenberg antiferromagnet,[40–42] the spin gap is seen to increase with λ. In fact, the same occurs in the NLσM without doping in the range $\lambda\approx 1-2$.

According to Eqs. (40) and (41) effective coupling constants $\tilde{J}_\parallel$, and $\tilde{J}_\perp$ can be defined for the doped system such that the form of the NLσM parameters is that for a pure spin system[18] i.e.,

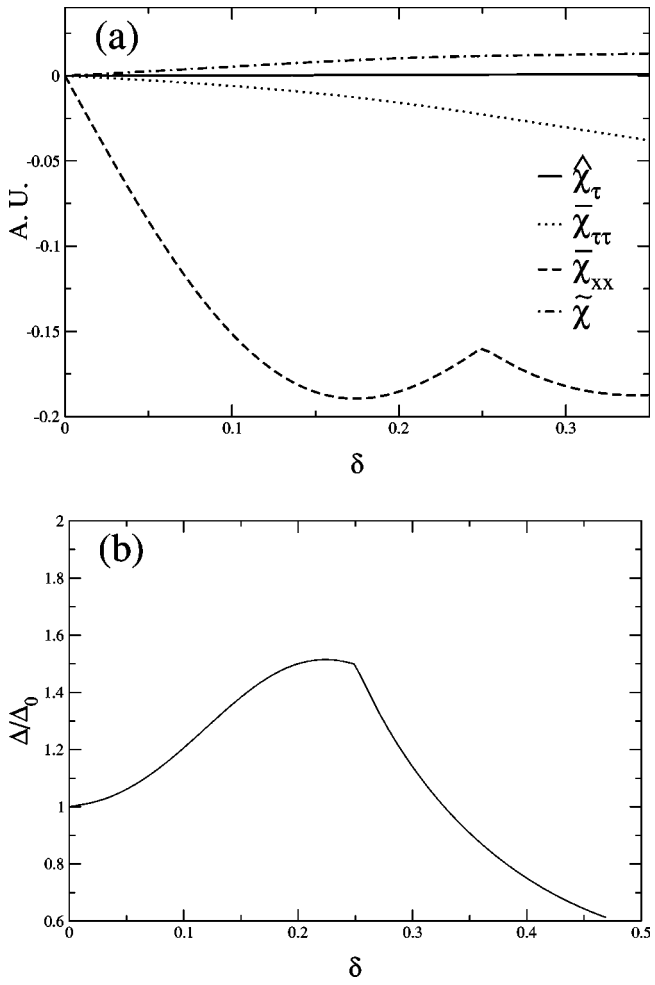

FIG. 4. $J_K<2t$. (a) Generalized susceptibilities of Eqs. (34), (36), and (37) for $J_K=3t=1.8$ eV. For $J_K<2t$, one susceptibility $\tilde{\chi}$ grows with doping and contributes to increase f and hence the gap. For $(J_K,t)\gg(J_\parallel,J_\perp)$ we can have an increasing gap for small doping. (b) Normalized gap of Eq. (42). Fixing the exchange constants to $J_\parallel=J_\perp=0.108$ eV is enough to have an increasing gap for small doping.

$$f=\frac{1}{S}\sqrt{1+\frac{\tilde{J}_\perp}{2\tilde{J}_\parallel}}, \tag{43}$$

$$v=2aS\tilde{J}_\parallel\sqrt{1+\frac{\tilde{J}_\perp}{2\tilde{J}_\parallel}}. \tag{44}$$

A small doping expansion in the regime $J_K>2t$ leads to

$$\tilde{J}_{||}=J_{||}+\frac{3}{4}\frac{(J_K^2-4t^2)}{J_K}\delta+O(\delta^2), \tag{45}$$

$$\tilde{J}_\perp=J_\perp-\left(\frac{3}{2}\frac{(J_K^2-4t^2)}{J_K}+2(4J_{||}+2J_\perp)+\frac{(4J_{||}+2J_\perp)^2}{8J_K}\right)\times\delta+O(\delta^2), \tag{46}$$

so indeed $\tilde{J}_\parallel$ and $\tilde{J}_\perp$ are seen respectively to increase, decrease, such that λ decreases. However, such an interpretation breaks down beyond $\delta\approx0.04$ whereas f,v are still well defined positive constants. This means that beyond such doping, this simplified picture cannot be naïvely applied and holes have a more effective way of lowering the gap.

III. COMPARISON WITH EXPERIMENTS

We come now to the comparison with experiments. Our theory depends on four parameters $t,J_K,J_\parallel,J_\perp$ which we now want to fix to physical values. Angle-resolved photoemission spectroscopy experiment on $Sr_{14}Cu_{24}O_{41}$ were performed by Takahashi *et al.*,[33] who found a band matching the periodicity of the ladder with a bandwidth of $\sim$0.5–0.4 eV. Adjusting our lowest band to have such a bandwidth we obtain a relation between t and J_K. On the other hand, experiments on the CuO_2 cell materials and band theory calculation[34–36] agreed in assuming a value of J_K of the order of $J_K\approx1-2$ eV. This in turn gives us a value of $t\approx0.24-0.76$ eV, which is also consistent with the same calculation.

The debate around an anisotropy of the spin exchange constants in $Sr_{14-x}Ca_xCu_{24}O_{41}$ is not completely settled yet.[6,7] Recent Raman data[2] gave $J_\perp/J_{||}\approx0.8$. We adjusted the value of the momentum cutoff Λ by fixing the theoretical gap with the experimental one for the undoped compound $Sr_{14}Cu_{24}O_{41}$. Finally, to compare with the measured values of the gap for different doping concentration x in $Sr_{14-x}A_xCu_{24}O_{41}$ (where A can be either divalent Ca^{2+},Ba^{2+} or trivalent Y^{3+},La^{3+}), we still need a relation between the A substitution x and the number of holes per copper site present in the ladder δ. This is another unsettled issue of the telephone number compound. In particular Osafune *et al.*,[8] studying the optical conductivity spectrum, inferred that with increasing Ca substitution x holes are transferred from the chain to the ladder. On the other hand Nücker *et al.*[43] argued that in the series compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ the number of holes in the ladder is almost insensitive to Ca substitution x (although a small increase is observed). Here we will assume that $Sr_{14-x}A_xCu_{24}O_{41}$ is an example of doped spin liquid and will use the data from Ref. 8. The result of our theory can be seen in Fig. 5. There we used isotropic exchange constant, but the theoretical curve did not change in a visible way if we used a value $J_\perp/J_{||}\approx0.8$ and in general is not very sensitive to the anisotropy of the ladder as can also be seen in Fig. 3(b). We see from the figure that the spin gap becomes zero for $\delta\approx0.37$; beyond this value the coupling constants f and v would become imaginary, signaling that our effective model cease to make sense. This means that for such doping ratios our parametrization (15) is no longer valid, in the sense that it does not incorporate the most important spin configurations. However, our theory could cease to make sense much before. If one takes the point of view of the t-J model (as we said, the spin-fermion model should map to it for large J_K) the holes introduced in the system couple rigidly to the spins forming singlet with the P_i states. In the worst case this would limit the correlation length of the spin

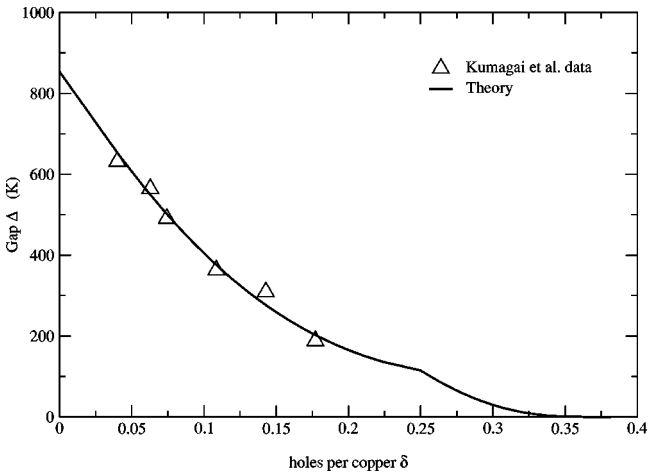

FIG. 5. Result of our theory and comparison with experiments. The values of the constants used in Eq. (42) are $t=0.76, J_K=2$ eV, and $J_\parallel/J_\perp=1$. The momentum cutoff Λ was fixed by fixing the the value of the gap with the one measured in $Sr_{14}Cu_{24}O_{41}$. For the anisotropic case $J_\perp/J_\parallel=0.8$, the curve does not change appreciably.

to the mean hole-hole distance $1/\delta$. In our case this happens at a doping ratio of $\delta\approx 0.15$.

A word of caution should be mentioned with respect to comparison with experimental results. A still unresolved controversy is present between NMR (Refs. 3–5) and neutron scattering[6,7] experiments, where the latter see essentially no doping dependence of the spin gap. Without being able to resolve this issue, we would like to stress, however, that beyond the uncertainties in experiments, the doping behavior obtained for the spin-gap agrees with the numerical results in TDMRG and is opposite to the one obtained in mean-field treatments, making clear the relevance of fluctuations.

IV. CONCLUSION

In this paper we studied the behavior of the spin gap of a two leg Heisenberg antiferromagnetic ladder as microscopically many holes are introduced in the system. Such a situation can be physically realized in the series compound $Sr_{14-x}A_xCu_{24}O_{41}$ with $A=$Ca, Y, La, and numerous result are now available from experiments. On the theoretical side, however, there is a contradiction between previous analytical treatments on the one hand, and TDMRG simulations or NMR experiments on the other hand. Whereas in the first case, a magnon gap increasing with doping is predicted, a decrease is observed in accurate numerical simulation and experiments.

Starting from the spin-fermion model we were able to solve the contradiction using a controlled analytical treatment that properly takes into account fluctuations in the continuum limit. Integrating out the fermions we were left with a Fermi determinant which we can evaluate exactly in that limit. The result is a nonlinear σ model with doping dependent parameters. The spontaneously generated mass gap of this theory is seen to decrease as holes are introduced. Once physical value for the parameters are given, we obtained very good agreement with NMR experiments performed on $Sr_{14-x}A_xCu_{24}O_{41}$.

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[1] J. G. Bednorz and K. A. Müller, Z. Phys. B: Condens. Matter **64**, 188 (1986).
[2] A. Gozar, G. Blumberg, B. S. Dennis, B. S. Shastry, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **87**, 197202 (2001).
[3] K. I. Kumagai, S. Tsuji, M. Kato, and Y. Koike, Phys. Rev. Lett. **78**, 1992 (1997).
[4] K. Magishi, S. Matsumoto, Y. Kitaoka, K. Asayama, M. Uehara, T. Nagata, and J. Akimitsu, Phys. Rev. B **57**, 11 533 (1988).
[5] P. Carretta, P. Ghigna, and A. Lasciafari, Phys. Rev. B **57**, 11 545 (1998).
[6] R. S. Eccleston, M. Uehara, J. Akimitsu, H. Eisaki, N. Motoyama, and S. I. Uchida, Phys. Rev. Lett. **81**, 1702 (1998).
[7] S. Katano, T. Nagata, J. Akimitsu, M. Nishi, and K. Kakurai, Phys. Rev. Lett. **82**, 636 (1999).
[8] T. Osafune, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **78**, 1980 (1997).
[9] H. Mayaffre, P. Auban-Senzier, M. Nardone, D. Jérome, D. Poilblanc, C. Bourbonnais, U. Ammerahl, G. Dhalenne, and A. Revcolevschi, Science **279**, 345 (1998).
[10] Y. Piskunov, D. Jérome, P. Auban-Senzier, P. Wzietek, U. Ammerahl, G. Dhalenne, and A. Revcolevschi, Eur. Phys. J. B **13**, 417 (2000).
[11] H. Tsunetsugu, M. Troyer, and T. M. Rice, Phys. Rev. B **49**, 16 078 (1994).
[12] M. Troyer, H. Tsunetsugu, and T. M. Rice, Phys. Rev. B **53**, 251 (1996).
[13] M. Sigrist, T. M. Rice, and F. C. Zhang, Phys. Rev. B **49**, 12 058 (1994).
[14] Y. L. Lee, Y. W. Lee, and C.-Y. Mou, Phys. Rev. B **60**, 13 418 (1999).
[15] B. Ammon, M. Troyer, T. M. Rice, and N. Shibata, Phys. Rev. Lett. **82**, 3855 (1999).
[16] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. **60**, 1057 (1988).
[17] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[18] S. Dell'Aringa, E. Ercolessi, G. Morandi, P. Pieri, and M. Roncaglia, Phys. Rev. Lett. **78**, 2457 (1997).
[19] A. Muramatsu and R. Zeyher, Nucl. Phys. B **346**, 387 (1990).
[20] J. Zaanen and A. M. Oleś, Phys. Rev. B **37**, 9423 (1988).
[21] A. Muramatsu, R. Zeyher, and D. Schmeltzer, Europhys. Lett. **7**, 473 (1988).
[22] V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987).

[23] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[24] T. Dombre and N. Read, Phys. Rev. B **38**, 7181 (1988).
[25] I. Affleck, in *Strings and Critical Phenomena*, edited by E. Brézin and J. Zinn-Justin, Les Houches Session XLIX, 1988 (Elsevier, Amsterdam, 1989).
[26] A. Auerbach, *Interacting Electrons and Quantum Magnetism* (Springer-Verlag, Berlin, 1994).
[27] G. Sierra, cond-mat/9606183. Published in *Lecture Notes in Physics*, Vol. 478, edited by G. Sierra and M. A Martin-Delgado (Springer-Verlag, Berlin, 1997).
[28] A. M. Polyakov, Phys. Lett. B **59**, 79 (1975).
[29] A. M. Polyakov and P. B. Weigman, Phys. Lett. B **131**, 121 (1983).
[30] R. Shankar and N. Read, Nucl. Phys. B **336**, 457 (1990).
[31] S. White, R. Noack, and D. Scalapino, Phys. Rev. Lett. **73**, 886 (1994).
[32] M. Veltman, Nucl. Phys. B **319**, 253 (1989).
[33] T. Takahashi, T. Yokoya, A. Ashihara, O. Akaki, H. Fujisawa, A. Chainani, M. Uehara, T. Nagata, J. Akimitsu, and H. Tsunetsugu, Phys. Rev. B **56**, 7870 (1997).
[34] N. Nücker, J. Fink, J. C. Fuggle, P. J. Durham, and W. M. Temmerman, Phys. Rev. B **37**, 5158 (1988).
[35] R. R. P. Singh, P. A. Fleury, K. B. Lyons, and P. E. Sulewski, Phys. Rev. Lett. **62**, 2736 (1989).
[36] M. S. Hybersten, M. Schlüter, and N. E. Christensen, Phys. Rev. B **39**, 9028 (1989).
[37] J. Oitmaa, C. J. Hamer, and Z. Weihong, Phys. Rev. B **60**, 16 364 (1999).
[38] M. Brunner, S. Capponi, F. F. Assaad, and A. Muramatsu, Phys. Rev. B **63**, 180511(R) (2001).
[39] E. Brezin and J. Zinn-Justin, Phys. Rev. B **14**, 3110 (1976).
[40] S. Gopalan, T. M. Rice, and M. Sigrist, Phys. Rev. B **49**, 8901 (1994).
[41] M. Reigrotzki, H. Tsunetsugu, and T. M. Rice, J. Phys.: Condens. Matter **6**, 9235 (1994).
[42] M. Greven, R. J. Birgeneau, and U. J. Wiese, Phys. Rev. Lett. **77**, 1865 (1996).
[43] N. Nücker, M. Merz, C. A. Kuntscher, S. Gerhold, S. Schuppler, R. Neudert, M. S. Golden, J. Fink, D. Schild, S. Stadler, V. Chakarian, J. Freeland, Y. U. Idzerda, K. Conder, M. Uehara, T. Nagata, J. Goto, J. Akimitsu, N. Motoyama, H. Eisaki, S. Uchida, U. Ammerahl, and A. Revcolevschi, Phys. Rev. B **62**, 14 384 (2000).