A new spin-polaron technique to treat the triangular-lattice antiferromagnet

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By expressing the Holstein–Primakoff transformation in a symmetric form a new spin-polaron technique for treating the triangular-lattice antiferromagnet is developed. With the technique, we have treated an extended $t-J$ model, calculated the quasiparticle dispersion, and compared the dispersion with that obtained by other method.

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1. Introduction

It is found that the cobalt oxide $Na_xCoO_2 \cdot yH_2O$ ($x \sim 0.35$, $y \sim 1.3$) has a triangular lattice in the CoO_2 planes [1–4]. This materials is a fully frustrated system when only the nearest-neighbor (NN) correlation is taken into account. So it should be necessary to pay more attention on the triangular-lattice antiferromagnet (TAFM) system. With this motivation, we developed a modified spin-polaron technique to discuss the quasiparticle dispersion of the TAFM.

2. Holstein–Primakoff transformation

In order to develop a spin-polaron technique on the TAFM, we first express the Holstein–Primakoff (HP) transformation in a symmetric form on the square- and triangular-lattice, respectively.

2.1. Square lattice. A square-lattice AFM consists of two sublattices, one spin-up and other spin-down. We introduce a two-component vector

$$\beta_i = \frac{1}{\sqrt{2S}} \begin{pmatrix} \sqrt{2S - a_i^\dagger a_i} \\ a_i \end{pmatrix} \tag{1}$$

(with a_i being boson operators). Then, the HP transformation can be expressed in terms of the vector β_i as

$$S_i^z = S - a_i^\dagger a_i = S\beta_i^\dagger \sigma_z \beta_i = S\beta_i^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \beta_i, \tag{2}$$

$$S_i^x = \frac{1}{2}\left(a_i^\dagger \sqrt{2S - a_i^\dagger a_i} + \sqrt{2S - a_i^\dagger a_i}\, a_i \right) = S\beta_i^\dagger \sigma_x \beta_i, \tag{3}$$

$$S_i^y = \frac{i}{2}\left(a_i^\dagger \sqrt{2S - a_i^\dagger a_i} - \sqrt{2S - a_i^\dagger a_i}\, a_i \right) = S\beta_i^\dagger \sigma_y \beta_i, \tag{4}$$

or

$$\mathbf{s}_i = S\beta_i^\dagger \boldsymbol{\sigma} \beta_i, \tag{5}$$

where $\boldsymbol{\sigma}$ is Pauli matrix.

In the spin-wave theory (SWT), in order to introduce only one type boson, a canonical transformation is usually performed to change the Néel configuration $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$ into a ferromagnetic state with all spins up, *i.e.*, the z axis of spin-down sublattice must be upturned, forming the new local coordinate $o{-}x'y'z'$. Now we investigate how the vector β_i is rotated with the coordinaye rotation. Suppose the new coordinate is obtained by rotating the old one by 180° about its x axis, with z' pointing along the local Néel direction, the direction of x'-axis is invariable and y'-axis is pointing along — y. Accordingly, the spin components become as

$$\begin{pmatrix} S_j'^x \\ S_j'^y \\ S_j'^z \end{pmatrix} = \begin{pmatrix} S_j^x \\ -S_j^y \\ -S_j^z \end{pmatrix} = R \begin{pmatrix} S_j^x \\ S_j^y \\ S_j^z \end{pmatrix}, \tag{6}$$

where

$$R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{7}$$

is $SO(3)$ matrix. (S_j^x, S_j^y, S_j^z) are spin components in the old coordinate frame, and $(S_j'^x, S_j'^y, S_j'^z)$ in the new local coordinate frame.

With the coordinate rotation, β_j, become β_j'. We suppose that 1) they are related through a indeterminate matrix $u(R)$:

$$\beta_y' = u(R)\beta_j, \tag{8}$$

and 2) the HP transformation is unchanged in its form, *i.e.*,

$$\mathbf{s}_j' = S\beta_j'^\dagger \boldsymbol{\sigma} \beta_j'. \tag{9}$$

Then, we have immediately the relation

$$\begin{pmatrix} S_j'^x \\ S_j'^y \\ S_j'^z \end{pmatrix} = \begin{pmatrix} S\beta_j^\dagger u^\dagger(R)\sigma_x u(R)\beta_j \\ S\beta_j^\dagger u^\dagger(R)\sigma_y u(R)\beta_j \\ S\beta_j^\dagger u^\dagger(R)\sigma_z u(R)\beta_j \end{pmatrix}. \tag{10}$$

From this equation the indeterminate matrix $u(R)$ can be easily solved, and the results is

$$u(R) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{11}$$

Because the new coordinate is fixed on the spin-down sublattice and the old one on the spin-up sublattice, the vector β_i has the form of Eq.(1) on spin-up sublattice, and the form

$$\beta'_j = u(R)\beta_j = \frac{1}{\sqrt{2S}} \begin{pmatrix} a_j \\ \sqrt{2S - a_j^\dagger a_j} \end{pmatrix} \tag{12}$$

on spin-down sublattice. If the prime is omitted and the spin-up and spin-down sublattices are distinguished by indices, we have

$$\beta_i = \begin{cases} \frac{1}{\sqrt{2S}} \begin{pmatrix} \sqrt{2S - a_i^\dagger a_i} \\ a_i \end{pmatrix} & (i \in \text{spin-up sublattice}), \\ \frac{1}{\sqrt{2S}} \begin{pmatrix} a_i \\ \sqrt{2S - a_i^\dagger a_i} \end{pmatrix} & (i \in \text{spin-down sublattice}). \end{cases} \tag{13}$$

The HP transformation can be merged into an unison form on both the sublattices:

$$\mathbf{s}_\alpha = S\beta_\alpha^\dagger \boldsymbol{\sigma} \beta'_\alpha, \tag{14}$$

with $\alpha = i, j$ corresponding to spin-up and spin-down sublattices, respectively. It is easily verified that on both sublattices the two-component vector satisfies the normal condition

$$\beta_i^\dagger \beta_i = 1. \tag{15}$$

2.2. Triangular lattice. Now we express the HP transformation on the TAFM. Unlike the square-lattice AFM, the TAFM has three sublattices (called A, B and C) with three 120°-Néel states, and their local coordinates can't be simply divided into spin-up and spin-down sublattices, but into three.

Following Miyake [5,6], we define the local (spatially varying) coordinates $o{-}x'y'z'$, with y' pointing along the old z direction and z' pointing along the local 120°-Néel direction. When x' is rotated by $0, 120$ and $240°$C about $y'(z)$ axis respectively, three new local coordinates are formed, which are fixed on the sublattices A, B and C, respectively. In the three new coordinates a spin operator has three forms:

$$(S_i'^x, S_i'^y, S_i'^z) = \begin{cases} (S_i^y, S_i^z, S_i^x) & (i \in A) \\ \left(-\frac{\sqrt{3}}{2} S_i^x - \frac{1}{2} S_i^y, S_i^z, -\frac{1}{2} S_i^x + \frac{\sqrt{3}}{2} S_i^y\right) & (i \in B) \\ \left(\frac{\sqrt{3}}{2} S_i^x - \frac{1}{2} S_i^y, S_i^z, -\frac{1}{2} S_i^x - \frac{\sqrt{3}}{2} S_i^y\right) & (i \in C). \end{cases} \tag{16}$$

We merge the three form into one

$$\begin{pmatrix} S_i'^x \\ S_i'^y \\ S_i'^z \end{pmatrix} = R_\alpha^{-1} \begin{pmatrix} S_i^x \\ S_i^y \\ S_i^z \end{pmatrix} \quad (\alpha = A, B, C). \tag{17}$$

Then the matrix R_α^{-1} can be easily resolved from the Eqs. (6), and the inverse matrices are

$$R_A = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad R_B = \begin{pmatrix} -\frac{\sqrt{3}}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \end{pmatrix},$$

$$R_C = \begin{pmatrix} \frac{\sqrt{3}}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 & -\frac{\sqrt{3}}{2} \\ 0 & 1 & 0 \end{pmatrix}. \tag{18}$$

Similarly to Section 2.1 we introduce here a two-component vector

$$\beta_i(0) = \frac{1}{\sqrt{2S}} \begin{pmatrix} \sqrt{2S - a_i^\dagger a_i} \\ a_i \end{pmatrix} \tag{19}$$

in the old coordinate frame, and the HP transformation is still expressed in terms of $\beta_i(0)$ as

$$\mathbf{s}_i = S\beta_i^\dagger(0) \boldsymbol{\sigma} \beta_i(0). \tag{20}$$

When the coordinate is rotated, spin operator changes from $\mathbf{s}_i$ to $\mathbf{s}'_i$, and the introduced matrix from $\beta_i(0)$ to $\beta_i(\alpha)$ (where $\alpha = A, B, C$ correspond to the three new coordinates, respectively). We suppose the HP transformations on the new coordinates are expressed in a unison form

$$\mathbf{s}_i = S\beta_i^\dagger(\alpha) \boldsymbol{\sigma} \beta_i(\alpha), \tag{21}$$

and we suppose also that

$$\beta_i(\alpha) = u(R_\alpha)\beta_i(0). \tag{22}$$

From the Eqs. (21) and (22), we can express $\mathbf{s}'_i$ in terms of $\beta_i(0)$

$$\mathbf{s}'_{i\alpha} = S\beta_i^\dagger(0) u^\dagger(R_\alpha) \boldsymbol{\sigma} u(R_\alpha) \beta_i(0) \quad (\alpha \in A, B, C). \tag{23}$$

The indeterminate matrix $u(R_\alpha)$ can be determined by substituting the Eqs. (20) and (23) into (17), and the results is

$$u(R_\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \tag{24}$$

with $\alpha = 0, 2\pi/3, -2\pi/3$ on sublattices A, B and C, respectively. Eventually, Eq. (21) is just the HP transformation in the three local coordinates of TAFM.

3. Modified spin-polaron technique

After expressing the HP transformation in terms of the introduced matrix, we now develop a modified spin-polaron technique. The spin-polaron picture was proposed early by Schmitt–Rink, Varma and Ruckenstein [7] to deal with the $t-J$ model on square lattice [8–11]. In this picture the electron-annihilation operators are expressed as pure hole operators or composite operators, for example,

$$C_{i\downarrow} = h_i^\dagger s_i^\dagger \tag{25}$$

with $s_i^\dagger$ being the hard-core Bose operators. A similar spin-polaron picture was proposed by Liu and Manousakis [8] by introducing two types of holes and two types of spinons on spin-up and spin-down sublattices, respectively.

Since the electronic operators $C_{i\sigma}(C_{i\sigma}^\dagger)$ appear always in pairs in physical quantities (for example, the kinetic operator $\sum_{\langle ij\rangle,\sigma} C_{i\sigma}^\dagger C_{j\sigma}$, current operator $\sum_{\langle ij\rangle,\sigma} \mathbf{R}_i C_{i\sigma}^\dagger C_{j\sigma}$, the Hamiltonian H, and for the $t-J$ model, the single-occupancy constraint $\sum_\sigma C_{i\sigma}^\dagger C_{i\sigma} \le 1$), we should deal directly with the pair operator $\sum_\sigma C_{j\sigma}^\dagger C_{j\sigma} = C_{i\uparrow}^\dagger C_{j\uparrow} + C_{i\downarrow}^\dagger C_{j\downarrow}$, rather than the single electronic operators $C_{i\sigma}(C_{i\sigma}^\dagger)$.

Because the electron hopping operators $C_{i\uparrow}^\dagger C_{j\uparrow}$ and $C_{i\downarrow}^\dagger C_{j\downarrow}$ correspond to the same hole hoppings from the site i to j, the term $C_{i\uparrow}^\dagger C_{j\uparrow} + C_{i\downarrow}^\dagger C_{j\downarrow}$ should be proportional to the hole hopping operators $h_i h_j^\dagger$, or

$$C_{i\uparrow}^\dagger C_{j\uparrow} + C_{i\downarrow}^\dagger C_{j\downarrow} = \kappa_{ij} h_i h_j^\dagger. \tag{26}$$

The factor κ_{ij} should be related to boson operators $a_{i(j)}$ and $a_{i(j)}^\dagger$, and one may expand it in terms of a series of these boson operators,

$$\kappa_{ij} = A_0 + A_1(a_i^\dagger + a_j) + A_2(a_i^\dagger a_j + a_j^\dagger a_i) + \dots, \tag{27}$$

where $A_0, A_1, \dots$ are indeterminate coefficients. Determination of them is determination of the modified spin-polaron technique.

On the one hand, in terms of the electron operators and the Pauli matrices, the spin operators can be expressed as $\mathbf{S}_i = \frac{1}{2}\sigma_{\alpha\alpha'} C_{i\alpha}^\dagger \sigma_{\alpha\alpha'} C_{i\alpha'}$, and the corresponding z-component reads

$$S_i^z = \frac{1}{2}\sum_{\alpha\alpha'} C_{i\alpha}^\dagger \sigma_{\alpha\alpha'}^z C_{i\alpha'} = S(C_{i\uparrow}^\dagger C_{i\uparrow} - C_{i\downarrow}^\dagger C_{i\downarrow}). \tag{28}$$

On the other hand, the component s_z can be expressed as

$$S_i^z = \beta_i^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \beta_i.$$

So we have the relation

$$(C_{i\uparrow}^\dagger C_{i\uparrow} - C_{i\downarrow}^\dagger C_{i\downarrow}) = \beta_i^\dagger \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \beta_i.$$

If the negative sing is changed for positive, one immediately has

$$(C_{i\uparrow}^\dagger C_{i\uparrow} + C_{i\downarrow}^\dagger C_{i\downarrow}) = \beta_i^\dagger \begin{pmatrix} 1 & 0 \\ 0 & +1 \end{pmatrix} \beta_i. \tag{29}$$

This is exactly true as it is identity. Enlightened by this relation, we may extend it from the same site to different site:

$$(C_{i\uparrow}^\dagger C_{i\uparrow} + C_{i\downarrow}^\dagger C_{i\downarrow}) \propto \beta_i^\dagger \begin{pmatrix} 1 & 0 \\ 0 & +1 \end{pmatrix} \beta_i = \beta_i^\dagger \beta_j. \tag{30}$$

This extension implies that the factor κ_{ij} have been selected as

$$\begin{aligned} \kappa_{ij} &= \beta_i^\dagger \beta_j \\ &= \frac{1}{\sqrt{2S}}\left[(a_i^\dagger + a_j) - \frac{1}{4S}(a_i^\dagger a_i a_j + a^\dagger a_j^\dagger a_j) + \dots\right], \end{aligned} \tag{31}$$

and the coefficients as $A_0 = 0$, $A_1 = \frac{1}{\sqrt{2S}}$, $A_2 = 0$, $A_3 = \dots$. Finally, Eqs. (26) and (31) make up the modified spin-polaron transformation.

It should be stressed that there may be other selections of A's. For example, one may suppose $\kappa_{ij} = f(\beta_i, \beta_i^\dagger, \beta_j, \beta_j^\dagger)$ as long as the operators κ_{ij} satisfy the necessary requirements such as conjugation for the permutation of i and j, and unitarity when $i = j$. Different selection may correspond to different magnon-holon coupling strength.

Now we rewrite the modified spin-polaron transformation in a compact form

$$\sum_\sigma C_{i\sigma}^\dagger C_{j\sigma} = h_i \beta_i^\dagger(\alpha) h_j^\dagger \beta_j(\beta), \tag{32}$$

where the index $\alpha(\beta)$ is for distinguishing different sublattices, with the site $i(j)$ belonging to the sublattice $\alpha(\beta)$.

Because $\beta_i(\alpha)$ satisfies the normal condition

$$\beta_i^\dagger(\alpha)\beta_i(\alpha) = 1, \tag{33}$$

on the same site, with the modified spin-polaron technique the no-double occupancy constraint is automatically built in:

$$\sum_\sigma C_{i\sigma}^\dagger C_{i\sigma} = h_i \beta_i^\dagger(\alpha) h_i^\dagger \beta_i(\alpha) = h_i h_i^\dagger \le 1. \tag{34}$$

4. Application of the spin-polaron technique to the TAFM

Now we use the modified spin-polaron technique to treat the TAFM. Here we use the extended $t-J$ model to describe its physics. Then, when the long-range correlations are teken into account, the Hamiltonian reads

$$H = H_{tt'} + H_J,$$

$$H_{tt'} = -t \sum_{\langle ij\rangle_1 \sigma} C^\dagger_{i\sigma} C_{j\sigma} - t' \sum_{\langle ij\rangle_2 \sigma} C^\dagger_{i\sigma} C_{j\sigma} - \mu \sum_i C^\dagger_{i\sigma} C_{j\sigma}, \quad (35)$$

$$H_J = J \sum_{\langle ij\rangle_1} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (36)$$

where the summations $\langle i, j\rangle_1$ and $\langle i, j\rangle_2$ run over the NN and next-nearest neighbor (NNN) pairs respectively and the operators $C^\dagger_{i\sigma}$ are subjected to the single-occupancy constraint.

The spin-spin correlation part H_J of the Hamiltonian can be treated with the HP transformation. In k space the free part of the spinon energy is

$$H_J = \sum_k \omega_k \alpha^\dagger_k \alpha_k, \quad (37)$$

where α_k are spinon operators. The spin-wave dispersion is

$$\omega_k = \frac{1}{2} JSz \sqrt{\left[(1 + 2\gamma^{(1)}_k)(1 - \gamma^{(1)}_k)\right]} \quad (38)$$

where $\gamma^{(1)}_k = \frac{1}{z} \sum_{\boldsymbol{\delta}^{(1)}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}^{(1)}}$ is the summations over the NN sites. And the vectors $+\boldsymbol{\delta}^{(1)}$ covers the six NN neighbors $\mathbf{e}_x$, $-\mathbf{e}_x$, $-\frac{1}{2}\mathbf{e}_x + \frac{\sqrt{3}}{2}\mathbf{e}_y$, $\frac{1}{2}\mathbf{e}_x - \frac{\sqrt{3}}{2}\mathbf{e}_y$, $-\frac{1}{2}\mathbf{e}_x - \frac{\sqrt{3}}{2}\mathbf{e}_y$ and $\frac{1}{2}\mathbf{e}_x + \frac{\sqrt{3}}{2}\mathbf{e}_y$, $\mathbf{e}_x$ being one of the basis vectors, and $\mathbf{e}_y$ normal to $\mathbf{e}_x$. Eq. (38) is exactly the same as that obtained by Leung and Runge [6].

With the transformation Eq. (32) the Hamiltonian H_{tt} can be expressed by boson and hopping operators. If we preserve the second order of bosons, it reads

$$H_{tt'} = H_t + H_{t'},$$

$$\begin{aligned} H_t \approx{}& \frac{1}{2} t \sum_{\langle ij\rangle_1} h_i h^\dagger_j - \sqrt{\frac{3}{4S}}\, t \\ &\times \left[\sum_{\langle ij\rangle_1, j\in B} h_i h^\dagger_j (a^\dagger_i - a_j) - \sum_{\langle ij\rangle_1, j\in C} h_i h^\dagger_j (a^\dagger_i - a_j)\right] \\ &- \frac{1}{8S} t \sum_{\langle ij\rangle_1} h_i h^\dagger_j \left(a^\dagger_i a_i + a^\dagger_j a_j - 2a^\dagger_i a_j\right) \\ &-\mu \sum_i h_i h^\dagger_i + \text{H.c,} \end{aligned} \quad (39)$$

$$H'_t \approx -t' \sum_{\langle ij\rangle_2} h_i h^\dagger_j \left[1 - \frac{1}{4S}\left(a^\dagger_i a_i + a^\dagger_j a_j - 2a^\dagger_i a_j\right)\right] + \text{H.c.} \quad (40)$$

In k space with Bogliubov transformation, we have

$$H_{tt} = \sum_k \epsilon_k h^\dagger_k h_k + H', \quad (41)$$

where h_k are holon operators. The first term describes the holon hopping, and holon dispersion is

$$\epsilon_k = -\frac{1}{2}\left[t\gamma^{(1)}_k - 2t'\gamma^{(2)}_k\right], \quad (42)$$

where $\gamma^{(2)}_k = \frac{1}{z} \sum_{\boldsymbol{\delta}^{(2)}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}^{(2)}}$ is the summations over the (NNN) sites. In Eq. (41) the second term H' desctibes the interaction between the holons and spinons

$$H' = \sum_{kp} \left(V^\dagger_{kp} h_k h^\dagger_p \alpha^\dagger_{k-p} + V_{kp} h_p h^\dagger_k \alpha_{k-p}\right), \quad (43)$$

where V_{kp} is the coherence factors. Here we will not discuss it in detail, but pay attention mainly to the holon dispersion.

Eq. (42) gives out the holon dispersion when both NN and NNN hoppings included. If the NNN hopping is ignored, the spectrum reduces to

$$\epsilon_k = -\frac{1}{2} t\gamma^{(1)}_k. \quad (44)$$

It is periodical function. Its amplitude is one half of Trumper's [12] and only one sixth of Azzouz's [13]. This means that the present dispersion is the least. Why? We know that the TAFM is fully frustrated, and the ground state is very disordered. The disorder certainly flattens the dispersion. So the property of spin frustration is more fully maintained within the present theory.

Quasiparticle dispersion can be probed in detail from the experiments of the angle-resolved photoelectron spectroscopy (ARPES) [14,15]. Through the ARPES study on the cobalt oxide $Na_{0.6}CoO_2$ some authors have measured the dispersion on the triangular lattice, and found that the hopping integral t is reduced by nearly ten times due to the strong correlation [15]. This conclusion provides an experimental support for the present theoretical result.

In summary, after introducing a two-components matrix we express the HP transformation in a symmetric form. Based on that, we developed a new modified spin-polaron technique. With the technique we have calculated the quasiparticle dispersion of an extended $t-J$ model. The result is more accurate than those obtained with other methods. The new technique is very suitable to treat the fully frustrated systems, especially TAFMs.

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