

# Antiferromagnetism in two-dimensional $t$ - $J$ model: A pseudospin representation

Daisuke Yamamoto\* and Susumu Kurihara

*Department of Physics, Waseda University, Okubo, Shinjuku, Tokyo 169-8555, Japan<sup>†</sup>*

(Received 30 November 2006; revised manuscript received 13 February 2007; published 30 April 2007)

We discuss a pseudospin representation of the two-dimensional  $t$ - $J$  model. We introduce pseudospins associated with empty sites, deriving a representation of the  $t$ - $J$  model that consists of local spins and spinless fermions. We show, within a mean-field approximation, that our representation of  $t$ - $J$  model corresponds to the *isotropic* antiferromagnetic Heisenberg model in an effective magnetic field. The strength and the direction of the effective field are determined by the hole doping  $\delta$  and the orientation of pseudospins associated with empty sites, respectively. We find that the staggered magnetization in the standard representation corresponds to the component of magnetization perpendicular to the effective field in our pseudospin representation. Using a many-body Green's function method, we show that the staggered magnetization decreases with increasing hole doping  $\delta$  and disappears at  $\delta \approx 0.06$ – $0.12$  for  $t/J = 2.5$ – $5$ . Our results are in good agreement with experiments and numerical calculations in contradistinction to usual mean-field methods.

DOI: [10.1103/PhysRevB.75.134520](https://doi.org/10.1103/PhysRevB.75.134520)

PACS number(s): 74.72.-h, 71.27.+a, 71.10.Pm, 75.10.Jm

## I. INTRODUCTION

It is well known that most of the physical properties of the copper oxide materials are described by the two-dimensional  $t$ - $J$  model.<sup>1-3</sup> The action of this model is restricted to the single occupancy sector of Hilbert space,  $\sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} \leq 1$ . At half-filling, the  $t$ - $J$  model reduces to the antiferromagnetic Heisenberg model. In the doped case, on the other hand, due to the single occupancy constraint, electrons can move only onto empty sites. Thus, the constrained electron operators no longer obey the fermionic anticommutation relations.

The slave particle mean-field methods<sup>3-10</sup> were the first approaches to overcome this problem. In these methods, the constrained electron operators are expressed in terms of auxiliary fermions and bosons. However, as the local single occupancy constraints are replaced by a global average constraint, these mean-field methods lead to considerable errors: for example, the antiferromagnetic long-range order is overestimated.<sup>7-10</sup>

Another approach<sup>11-15</sup> is to express the constrained electron operators in terms of spinless fermions and spin-1/2 operators by introducing pseudospins associated with empty sites. Using this representation, the  $t$ - $J$  Hamiltonian can be described without any constraint in contrast with the slave particle methods. The “spin-up” and “spin-down” symmetries (time-reversal symmetry) of this representation are discussed by Wang and Rice<sup>13</sup> and by Loos.<sup>14</sup> In the present paper, we develop this idea and calculate the critical doping  $\delta_c$ , where the antiferromagnetic long-range order disappears.

Our representation of the  $t$ - $J$  model corresponds to the *isotropic* antiferromagnetic Heisenberg model in an effective magnetic field within a mean-field approximation. In order to calculate the staggered magnetization of the model, we employ the many-body Green's function method developed by Fröbrich and Kuntz.<sup>16</sup> Unlike the slave particle methods, we show that the critical doping  $\delta_c$  for the disappearance of antiferromagnetic long-range order is in good agreement with the numerical calculations.<sup>17-22</sup>

This paper is organized as follows. In Sec. II, we introduce a transformation mapping the original Hilbert space of

the constrained electrons to the tensor-product space of the spinless fermion and spin states. We also discuss the difference between our method and the preceding methods.<sup>13,14</sup> In Sec. III, using the many-body Green's function method, we calculate the staggered magnetization of the model obtained in Sec. II within a mean-field approximation. A summary is presented in Sec. IV.

## II. PSEUDOSPIN REPRESENTATION

We consider the  $t$ - $J$  Hamiltonian

$$H = -t \sum_{\langle i,j \rangle \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.}) - \mu \sum_{i\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} + J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j, \quad (1)$$

where  $c_{i\sigma}$  is the electron annihilation operator with spin  $\sigma$  at site  $i$ ,  $\mu$  is the chemical potential, and  $\mathbf{s}_i = \frac{1}{2} \sum_{\alpha\beta} c_{i\alpha}^{\dagger} \boldsymbol{\tau}_{\alpha\beta} c_{i\beta}$  is the spin operator with the Pauli matrices  $\boldsymbol{\tau}$ . The sum is taken over all nearest-neighbor bonds. The electron in this model is subjected to the constraint of no double occupancy, i.e.,

$$\sum_{\sigma} c_{i\sigma}^{\dagger} c_{i\sigma} \leq 1. \quad (2)$$

Consequently, the basis of possible states in the  $t$ - $J$  model consist of the states  $|i\sigma\rangle$  and  $|i0\rangle$ , which correspond to a site singly occupied by an electron with spin  $\sigma$  and to an empty site, respectively. The constrained electron operators  $c_{i\sigma}$  act on this basis as

$$c_{i\sigma} |i\sigma\rangle = |i0\rangle, \quad c_{i\sigma}^{\dagger} |i0\rangle = |i\sigma\rangle. \quad (3)$$

### A. Pseudospin associated with empty site

One of the most popular techniques to handle the single occupancy constraint [Eq. (2)] is the slave particle method.<sup>3-10</sup> In the slave boson representation, the constrained electron operators are given by the mapping  $c_{i\sigma} \rightarrow b_i^{\dagger} f_{i\sigma}$ , where  $b_i$  is the bosonic operator annihilating the empty state and  $f_{i\sigma}$  is the fermionic operator annihilating the single occupied state. In this case, the nonholonomic con-

straint [Eq. (2)] is replaced by the holonomic constraint  $b_i^\dagger b_i + \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} = 1$ . For practical purposes, however, these local constraints for each site are almost inevitably replaced by an average global constraint, resulting in errors: one of the most serious drawbacks is that the antiferromagnetic long-range order is overestimated.<sup>7-10</sup>

In this paper, we develop another approach, rewriting the  $t$ - $J$  model in terms of spinless fermionic operators (charge degree of freedom) and local spin- $\frac{1}{2}$  operators.<sup>11-15</sup> In this approach, the Hilbert space is mapped onto a tensor product space,  $|\cdot\rangle_h \otimes |\cdot\rangle_s$  as

$$|i\sigma\rangle \rightarrow |i0\rangle_h |i\sigma\rangle_s, \quad |i0\rangle \rightarrow |i1\rangle_h |iS\rangle_s, \quad (4)$$

where

$$|iS\rangle_s \equiv C_1 |i\uparrow\rangle_s + C_2 |i\downarrow\rangle_s, \quad (5)$$

with  $|C_1|^2 + |C_2|^2 = 1$  the pseudospin state associated with an empty site. We introduce the fermionic ‘‘holon’’ operator  $h_i$  and the ‘‘spin’’ operator  $S_i$  acting as

$$\begin{aligned} h_i^\dagger |i0\rangle_h &= |i1\rangle_h, & h_i |i1\rangle_h &= |i0\rangle_h, \\ S_i^\dagger |i\downarrow\rangle_s &= |i\uparrow\rangle_s, & S_i |i\uparrow\rangle_s &= |i\downarrow\rangle_s. \end{aligned} \quad (6)$$

Owing to Eq. (4), the constrained electron operators are written as

$$\begin{aligned} c_{i\uparrow} &\rightarrow \tilde{c}_{i\uparrow} = h_i^\dagger (C_1 S_i^+ S_i^- + C_2 S_i^-), \\ c_{i\downarrow} &\rightarrow \tilde{c}_{i\downarrow} = h_i^\dagger (C_1 S_i^+ + C_2 S_i^- S_i^+). \end{aligned} \quad (7)$$

Clearly, the new operator  $\tilde{c}_{i\sigma}$  has the same action as the operator  $c_{i\sigma}$  on the basis vectors [Eq. (4)]. The four-dimensional space  $|\cdot\rangle_h \otimes |\cdot\rangle_s$  consists of the orthonormal vectors  $|i0\rangle_h |i\sigma\rangle_s$ ,  $|i1\rangle_h |iS\rangle_s$ , and  $|i1\rangle_h |i\bar{S}\rangle_s$  with  $|i\bar{S}\rangle_s \equiv C_1^* |i\downarrow\rangle_s - C_2^* |i\uparrow\rangle_s$ . However, all physical quantities, which can be written in terms of  $\tilde{c}_{i\sigma}$ , are determined only by the vectors  $|i0\rangle_h |i\sigma\rangle_s$  and  $|i1\rangle_h |iS\rangle_s$ . It is easy to prove that the operator  $\tilde{c}_{i\sigma}$  acts on the  $|i1\rangle_h |i\bar{S}\rangle_s$  state as

$$\tilde{c}_{i\sigma} |i1\rangle_h |i\bar{S}\rangle_s = 0, \quad \tilde{c}_{i\sigma}^\dagger |i1\rangle_h |i\bar{S}\rangle_s = 0. \quad (8)$$

Consequently,

$$\tilde{H} |i1\rangle_h |i\bar{S}\rangle_s = 0, \quad \tilde{H} |i1\rangle_h |i\bar{S}\rangle_s = 0, \quad (9)$$

where  $\tilde{H}$  is the pseudospin representation of the  $t$ - $J$  Hamiltonian  $H$ .  $t$ - $J$  Hamiltonian and all physical quantities can be written in terms of  $\tilde{c}_{i\sigma}$ . Therefore, no physical quantity is affected by the unphysical state  $|i1\rangle_h |i\bar{S}\rangle_s$ . In fact, no local constraint is needed [see Eq. (12)]. In this pseudospin representation, the ‘‘true’’ spin operator and the constrained electron number operator are expressed as

$$\mathbf{s}_i \rightarrow (1 - h_i^\dagger h_i) \mathbf{S}_i, \quad (10)$$

$$\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \rightarrow \sum_{\sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{i\sigma} = 1 - h_i^\dagger h_i. \quad (11)$$

Consequently, the single occupancy constraint

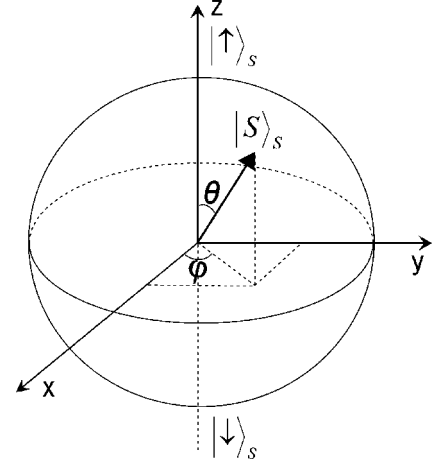


FIG. 1. Bloch sphere describing the orientation of pseudospins.

$$\sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} \leq 1 \rightarrow 1 - h_i^\dagger h_i \leq 1 \quad (12)$$

is automatically satisfied. Thus, no approximations for the constraint are necessary unlike the slave particle methods.<sup>3-10</sup>

## B. Pseudospin representation of $t$ - $J$ model

In our pseudospin representation, the  $t$ - $J$  model is found to be expressed as

$$\begin{aligned} \tilde{H} = & -t \sum_{\langle i,j \rangle} \{ h_i h_j^\dagger [ C_1^2 (S_i^+ S_i^- S_j^+ S_j^- + S_i^- S_i^+) \\ & + C_1 C_2^* (S_i^+ S_j^+ S_j^- + S_i^- S_i^+ S_j^+) \\ & + C_1^* C_2 (S_i^+ S_i^- S_j^- + S_i^- S_j^- S_i^+) \\ & + C_2^2 (S_i^- S_i^+ S_j^- S_j^+ + S_i^+ S_j^+) ] + \text{H.c.} \} \\ & - \mu \sum_i h_i^\dagger h_i + J \sum_{\langle i,j \rangle} h_i h_j^\dagger \mathbf{S}_i \cdot \mathbf{S}_j h_j h_j^\dagger, \end{aligned} \quad (13)$$

which can be rewritten in the following more convenient form with  $C_1 = \cos \frac{\theta}{2}$  and  $C_2 = e^{i\varphi} \sin \frac{\theta}{2}$  (Fig. 1):

$$\begin{aligned} \tilde{H} = & -t \sum_{\langle i,j \rangle} \left\{ h_i h_j^\dagger \left[ \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} + \mathbf{n} \cdot \left( \frac{1}{2} \mathbf{S}_i + \frac{1}{2} \mathbf{S}_j + i \mathbf{S}_i \times \mathbf{S}_j \right) \right] \right. \\ & \left. + \text{H.c.} \right\} - \mu \sum_i h_i^\dagger h_i + J \sum_{\langle i,j \rangle} h_i h_j^\dagger \mathbf{S}_i \cdot \mathbf{S}_j h_j h_j^\dagger, \end{aligned} \quad (14)$$

where  $\mathbf{n} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$  is a unit vector in the orientation of pseudospins. Loos<sup>14</sup> put a certain restriction on the orientation of the pseudospins so that the time-reversal symmetry of the  $t$ - $J$  model is preserved, assuming that the spin operators  $\mathbf{S}_i$  are transformed in the time-reversal operation similar to the true spin operators  $\mathbf{s}_i$ . In contrast, we put no restriction on the parameters  $\theta$  and  $\varphi$ . In Sec. III B, we show that our results are independent of the parameters  $\theta$  and  $\varphi$ .

The representation of the  $t$ - $J$  model introduced in Ref. 12 can be obtained by setting  $\theta=0$  in Eq. (14). The similar

expression is also introduced for the Hubbard model in Ref. 15. For simplicity, in this paper, we also choose the parameters as  $\theta=0$ ; i.e., the pseudospins are aligned along the  $z$  axis. Consequently, the pseudospin representation of the  $t$ - $J$  model is obtained as

$$\begin{aligned} \tilde{H} = & -t \sum_{\langle i,j \rangle} \left\{ h_i h_j^\dagger \left[ \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} + \frac{1}{2} S_i^z + \frac{1}{2} S_j^z + i(\mathbf{S}_i \times \mathbf{S}_j)_z \right] \right. \\ & \left. + \text{H.c.} \right\} - \mu \sum_i h_i^\dagger h_i + J \sum_{\langle i,j \rangle} h_i h_i^\dagger \mathbf{S}_i \cdot \mathbf{S}_j h_j h_j^\dagger. \end{aligned} \quad (15)$$

Only for true spins, the  $J$  term in Eq. (15) represents the ordinary magnetic energy. At half-filling, the  $t$ - $J$  Hamiltonian  $\tilde{H}$  [Eq. (15)] is reduced to the Heisenberg Hamiltonian.

### C. Mean-field approximation

Within the mean-field approximation, the  $t$ - $J$  Hamiltonian  $\tilde{H}$  [Eq. (15)] can be decoupled into a holon part  $\tilde{H}_h^{\text{MF}}$  and a spin part  $\tilde{H}_S^{\text{MF}}$  as

$$\tilde{H}_h^{\text{MF}} = \sum_{\langle i,j \rangle} (t_{\text{eff}} h_j^\dagger h_i + \text{H.c.}) - \mu \sum_i h_i^\dagger h_i, \quad (16)$$

$$\tilde{H}_S^{\text{MF}} = J_{\text{eff}} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - B_{\text{eff}}^z \sum_i S_i^z, \quad (17)$$

with  $t_{\text{eff}} = t \langle \mathbf{S}_i \cdot \mathbf{S}_j + \frac{1}{4} + \frac{1}{2} S_i^z + \frac{1}{2} S_j^z + i(\mathbf{S}_i \times \mathbf{S}_j)_z \rangle$ ,  $J_{\text{eff}} = J \{ (1 - \delta)^2 - \phi^2 \} + 2t\phi$ , and  $B_{\text{eff}}^z = -4t\phi$ , where  $\langle \dots \rangle$  is an average over the ensemble. The hole doping and the particle-hole order parameter are defined as  $\delta = \langle h_i^\dagger h_i \rangle$  and  $\phi = \langle h_i^\dagger h_{i+\hat{\gamma}} \rangle$  with  $\hat{\gamma} = \pm \hat{x}, \pm \hat{y}$ , respectively.

The spin part  $\tilde{H}_S^{\text{MF}}$  [Eq. (17)] corresponds to the Hamiltonian describing the *isotropic* antiferromagnet in a uniform magnetic field with the effective exchange constant  $J_{\text{eff}}$  and the effective magnetic field  $B_{\text{eff}}^z$  along the  $z$  axis. We note that the direction of the effective field depends on the choice of the orientation of the pseudospin.

### III. DOPING DEPENDENCE OF STAGGERED MAGNETIZATION

In this section, we consider the doping dependence of the staggered magnetization of the mean-field Hamiltonian [Eqs. (16) and (17)]. In Sec. III A, we calculate the components of magnetization for the Heisenberg antiferromagnet,

$$\bar{H} = \sum_{\langle i,j \rangle} (\bar{J} \mathbf{S}_i \cdot \mathbf{S}_j + D^x S_i^x S_j^x) - B^z \sum_i S_i^z, \quad (18)$$

where  $\bar{J}$  is the exchange constant,  $D^x$  is the anisotropy parameter, and  $B^z$  is the magnetic field along the  $z$  axis. The Heisenberg model [Eq. (18)] corresponds to the spin part of the mean-field Hamiltonian [Eq. (17)] with

$$\bar{J} \rightarrow J_{\text{eff}}, \quad D^x \rightarrow 0, \quad B^z \rightarrow B_{\text{eff}}^z. \quad (19)$$

Using this correspondence, we calculate the staggered magnetization of the mean-field Hamiltonian [Eqs. (16) and (17)] in Sec. III B.

### A. Antiferromagnet in a magnetic field

The magnetic properties of two-dimensional antiferromagnets have been the focus of many preceding theoretical studies.<sup>16,23-28</sup> In particular, the properties of a two-dimensional anisotropic antiferromagnet in a transverse field were recently studied with rotating frame method<sup>28</sup> and in the nonrotating frame,<sup>16</sup> of which differences were discussed by Fröblich and Kuntz.<sup>16</sup> In this section, we calculate the components of magnetization of the Heisenberg model [Eq. (18)] directly in the nonrotating frame as in Ref. 16. The retarded Green's functions are defined as

$$\begin{aligned} G_{ij}^{\alpha-}(t-t') &= -i\theta(t-t') \langle [S_i^\alpha(t), S_j^-(t')] \rangle \\ &= \langle \langle S_i^\alpha; S_j^- \rangle \rangle, \quad \alpha = +, -, z, \end{aligned} \quad (20)$$

where  $\theta(t)$  is the step function. The Fourier transform of Green's functions are denoted by  $\langle \langle S_i^\alpha; S_j^- \rangle \rangle_\omega$  in the energy space. The equations of motion for Green's functions given in Eq. (20) are expressed as

$$\omega G_{ij}^{\alpha-}(\omega) = \begin{pmatrix} 2\langle S_i^z \rangle \delta_{ij} \\ 0 \\ -\langle S_i^x \rangle \delta_{ij} \end{pmatrix} + \langle \langle [S_i^\alpha, \bar{H}]; S_j^- \rangle \rangle_\omega. \quad (21)$$

In order to close the system of equations, we adopt the Tyablikov (random-phase approximation) decoupling<sup>29</sup> of higher-order Green's functions,

$$\langle \langle S_i^\alpha S_k^\beta; S_j^- \rangle \rangle_\omega \approx \langle S_i^\alpha \rangle G_{kj}^{\beta-} + \langle S_k^\beta \rangle G_{ij}^{\alpha-}. \quad (22)$$

Fourier transformations to momentum space are given by

$$G_{\mu\nu}^{\alpha-}(\mathbf{q}) = \frac{2}{N} \sum_{i\mu j\nu} G_{i\mu j\nu}^{\alpha-} e^{-i\mathbf{q} \cdot (\mathbf{R}_{i\mu} - \mathbf{R}_{j\nu})}, \quad (23)$$

where subscripts  $\mu$  and  $\nu$  denote sublattice indices ( $A$  or  $B$ ). Each sublattice consists of  $N/2$  lattice sites. Furthermore, to simplify the calculations, we assume that the magnetic components can be defined as  $\langle S_{i_A}^x \rangle = -\langle S_{i_B}^x \rangle \equiv m^x$  and  $\langle S_{i_A}^z \rangle = \langle S_{i_B}^z \rangle \equiv m^z$  due to the symmetry of the present case. We now rewrite Eq. (21) in a matrix form,

$$(\omega \mathbf{1} - \mathbf{\Gamma}) \mathbf{G} = \mathbf{\Lambda}. \quad (24)$$

In Eq. (24), the  $6 \times 6$  matrix  $\mathbf{\Gamma}$  is given by

$$\mathbf{\Gamma} = \begin{pmatrix} -a & 0 & -b & c_{\mathbf{q}} & d_{\mathbf{q}} & -e_{\mathbf{q}} \\ 0 & a & b & -d_{\mathbf{q}} & -c_{\mathbf{q}} & e_{\mathbf{q}} \\ -\frac{1}{2}b & \frac{1}{2}b & 0 & -\frac{1}{2}e_{\mathbf{q}} & \frac{1}{2}e_{\mathbf{q}} & 0 \\ c_{\mathbf{q}} & d_{\mathbf{q}} & e_{\mathbf{q}} & -a & 0 & b \\ -d_{\mathbf{q}} & -c_{\mathbf{q}} & -e_{\mathbf{q}} & 0 & a & -b \\ \frac{1}{2}e_{\mathbf{q}} & -\frac{1}{2}e_{\mathbf{q}} & 0 & \frac{1}{2}b & -\frac{1}{2}b & 0 \end{pmatrix}, \quad (25)$$

with  $a = zJm^z - B^z$ ,  $b = z(J + D^x)m^x$ ,  $c_{\mathbf{q}} = z(J + \frac{1}{2}D^x)\gamma_{\mathbf{q}}m^z$ ,  $d_{\mathbf{q}} = \frac{1}{2}zD^x\gamma_{\mathbf{q}}m^z$ , and  $e_{\mathbf{q}} = zJ\gamma_{\mathbf{q}}m^x$ , where  $z=4$  is the number of nearest neighbors and  $\gamma_{\mathbf{q}} = \frac{1}{2}(\cos q_x + \cos q_y)$  is the Fourier factor for a square lattice: we set the lattice constant to be unity. The  $6 \times 2$  matrix  $\mathbf{G}$  is defined as

$$\mathbf{G} = \begin{pmatrix} \mathbf{G}_{AA} & \mathbf{G}_{AB} \\ \mathbf{G}_{BA} & \mathbf{G}_{BB} \end{pmatrix}, \quad (26)$$

with

$$\mathbf{G}_{\mu\nu} = \begin{pmatrix} G_{\mu\nu}^{+-} \\ G_{\mu\nu}^{--} \\ G_{\mu\nu}^{z-} \end{pmatrix}, \quad \mu, \nu = A, B, \quad (27)$$

while the  $6 \times 2$  matrix  $\mathbf{\Lambda}$  is given by

$$\mathbf{\Lambda} = \begin{pmatrix} \Lambda_{AA} & \Lambda_{AB} \\ \Lambda_{BA} & \Lambda_{BB} \end{pmatrix}, \quad (28)$$

with

$$\Lambda_{\mu\nu} = \begin{pmatrix} 2\langle S_{i\mu}^z \rangle \delta_{\mu\nu} \\ 0 \\ -\langle S_{i\mu}^x \rangle \delta_{\mu\nu} \end{pmatrix}, \quad \mu, \nu = A, B. \quad (29)$$

By solving Eq. (24), we obtain Green's functions. One finds that each Green's function  $G_{\mu\nu}^{\alpha\alpha'}$  has six poles,

$$\begin{aligned} \omega &= 0, \quad 0, \quad \pm\omega_1, \quad \pm\omega_2, \\ \omega_1 &= \sqrt{(a+c)^2 + b^2 - d^2 - e^2}, \\ \omega_2 &= \sqrt{(a-c)^2 + b^2 - d^2 - e^2}. \end{aligned} \quad (30)$$

Dealing with the pole  $\omega=0$  is known to be difficult, in that the anticommutator Green's function is required.<sup>30</sup> However, we can avoid this difficulty by introducing the new expression

$$\begin{aligned} G_{AA}^{+-} - G_{AA}^{--} &= \frac{1}{2\omega_1} \left[ \frac{m^x(b+e) - m^z(a+c+d) + m^z\omega_1}{\omega - \omega_1} \right. \\ &\quad \left. - \frac{m^x(b+e) - m^z(a+c+d) - m^z\omega_1}{\omega + \omega_1} \right] \\ &\quad + \frac{1}{2\omega_2} \left[ \frac{m^x(b-e) - m^z(a-c-d) + m^z\omega_2}{\omega - \omega_2} \right. \\ &\quad \left. - \frac{m^x(b-e) - m^z(a-c-d) - m^z\omega_2}{\omega + \omega_2} \right]. \end{aligned} \quad (31)$$

Since the pole  $\omega=0$  is absent in this expression, we can use the standard spectral theorem.<sup>30</sup> Applying this theorem to Eq. (31) and using the relation for spin  $S=1/2$ ,

$$\langle S_i^z \rangle = 1/2 - \langle S_i^- S_i^+ \rangle, \quad (32)$$

we derive

$$\begin{aligned} \frac{1}{2} &= \frac{1}{N} \sum_{\mathbf{q}} \left[ \frac{m^x(b+e) - m^z(a+c+d)}{2\omega_1} \coth \frac{\beta\omega_1}{2} \right. \\ &\quad \left. + \frac{m^x(b-e) - m^z(a-c-d)}{2\omega_2} \coth \frac{\beta\omega_2}{2} \right]. \end{aligned} \quad (33)$$

In Eq. (33), the sum runs over the first Brillouin zone. Moreover, using the fact that the commutator Green's function has to be regular at the origin,<sup>16</sup> i.e.,

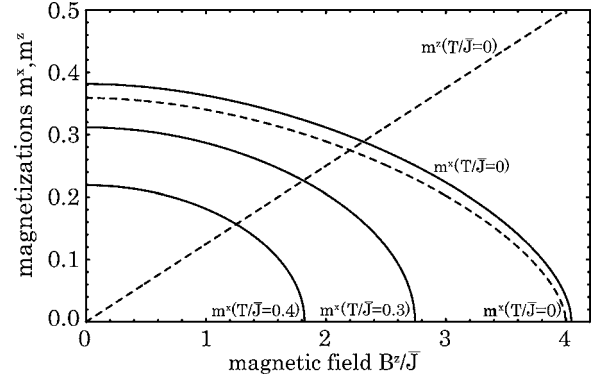


FIG. 2. Components of magnetization  $m^x$  and  $m^z$  as a function of  $B^z$  at different temperatures  $T$  for  $D^x/\bar{J}=0.01$  (solid lines) and  $D^x/\bar{J}=0$  (dotted lines).

$$\lim_{\omega \rightarrow 0} \omega G_{ij}^{\alpha\alpha'} = 0, \quad (34)$$

we obtain

$$m^z = \frac{B^z}{z(2\bar{J} + D^x)} \quad (\text{for } m^x \neq 0). \quad (35)$$

From Eqs. (33) and (35), all components of the magnetization,  $m^x$  and  $m^z$ , are determined. As seen in the results in Fig. 2, the magnetization  $m^x$  perpendicular to the magnetic field decreases with increasing the field strength, and disappears around field strength  $B^z/\bar{J} \approx 4$  at  $T=0$  for  $D^x/\bar{J}=0$ .

## B. Doping dependence of staggered magnetization

In this section, we consider the staggered magnetization of the  $t$ - $J$  Hamiltonian [Eq. (1)]. We take  $x$  axis, which is aligned perpendicular to the orientation of pseudospins, to be in a direction parallel to the easy axis of the staggered magnetization (i.e.,  $|\langle s_i^x \rangle| \neq 0$  and  $|\langle s_i^z \rangle| = |\langle s_i^y \rangle| = 0$ ). From transformation (10), the staggered magnetization  $|\langle s_i^x \rangle|$  in the original representation is transformed into the pseudospin representation as

$$|\langle s_i^x \rangle| \rightarrow |\langle (1 - h_i^\dagger h_i) S_i^x \rangle| = |\langle S_i^x \rangle| - |\langle h_i^\dagger h_i S_i^x \rangle| = |\langle S_i^x \rangle| \equiv M. \quad (36)$$

Equation (36) shows that the staggered magnetization in the pseudospin representation can be regarded as the component of magnetization perpendicular to the effective magnetic field (to the orientation of pseudospins). When deriving relation (36), we use the fact  $\langle h_i^\dagger h_i S_i^x \rangle = 0$ , choosing the orientation of pseudospins along the  $z$  axis. Thus, the other components of magnetization cannot fulfill the similar relation to Eq. (36). For example, one can easily show that  $|\langle s_i^z \rangle| \neq |\langle S_i^z \rangle|$ .

Instead of starting from the Heisenberg model [Eq. (18)], we now examine the spin part of the mean-field Hamiltonian

[Eq. (17)]. After some algebra similar to the one given in Sec. III A, we obtain

$$\frac{1}{2} = \frac{1}{N} \sum_{\mathbf{q}} \left[ \frac{M(\tilde{b} + \tilde{e}) - \tilde{M}(\tilde{a} + \tilde{c} + \tilde{d})}{2\tilde{\omega}_1} \coth \frac{\beta\tilde{\omega}_1}{2} + \frac{M(\tilde{b} - \tilde{e}) - \tilde{M}(\tilde{a} - \tilde{c} - \tilde{d})}{2\tilde{\omega}_2} \coth \frac{\beta\tilde{\omega}_2}{2} \right], \quad (37)$$

$$\tilde{M} = \frac{B_{\text{eff}}}{2zJ_{\text{eff}}} \quad (\text{for } M \neq 0), \quad (38)$$

$$\tilde{\omega}_1 = \sqrt{(\tilde{a} + \tilde{c})^2 + \tilde{b}^2 - \tilde{d}^2 - \tilde{e}^2}, \quad (39)$$

$$\tilde{\omega}_2 = \sqrt{(\tilde{a} - \tilde{c})^2 + \tilde{b}^2 - \tilde{d}^2 - \tilde{e}^2}, \quad (40)$$

with  $\tilde{M} = |\langle S_i^z \rangle|$ ,  $\tilde{a} = zJ_{\text{eff}}\tilde{M} - B_{\text{eff}}^z$ ,  $\tilde{b} = zJ_{\text{eff}}M$ ,  $\tilde{c}_{\mathbf{q}} = zJ_{\text{eff}}\gamma_{\mathbf{q}}\tilde{M}$ ,  $\tilde{d}_{\mathbf{q}} = 0$ , and  $\tilde{e}_{\mathbf{q}} = zJ_{\text{eff}}\gamma_{\mathbf{q}}M$ . In addition to Eqs. (37) and (38), the equations for the holon Green's functions are needed to obtain a closed system of equations. The holon Green's function are defined as

$$g_{ij}(t-t') = -i\theta(t-t')\langle\{h_i(t), h_j^\dagger(t')\}\rangle = \langle\langle h_i; h_j^\dagger \rangle\rangle. \quad (41)$$

From the holon part of the mean-field Hamiltonian [Eq. (16)], we obtain the following expression of the holon Green's function:

$$g_{\mathbf{q}}(\omega) = \frac{1}{\omega - (\varepsilon_{\mathbf{q}} - \mu)}, \quad (42)$$

with  $\varepsilon_{\mathbf{q}} = zt_{\text{eff}}\gamma_{\mathbf{q}}$ .<sup>31</sup> Using the spectral theorem,<sup>30</sup> we also find

$$\delta = \frac{1}{2N} \sum_{\mathbf{q}} \left[ 1 - \tanh \frac{\beta(\varepsilon_{\mathbf{q}} - \mu)}{2} \right], \quad (43)$$

$$\phi = \frac{1}{2N} \sum_{\mathbf{q}} \gamma_{\mathbf{q}} \left[ 1 - \tanh \frac{\beta(\varepsilon_{\mathbf{q}} - \mu)}{2} \right]. \quad (44)$$

The set of self-consistency equations [Eqs. (37), (38), (43), and (44)] is numerically solved. In Fig. 3(b), we show the staggered magnetization and the particle-hole order parameter at  $T=0$  as functions of doping  $\delta$ . The staggered magnetization decreases with increasing  $\delta$ , and disappears at the critical doping  $\delta_c$ , which is calculated to be  $\delta_c \approx 0.12$  for  $t/J=2.5$ . Our results derived without the constraint are in good accord with the numerical results,<sup>17-22</sup> e.g.,  $\delta_c \approx 0.13$  for  $t/J=2.5$  in Ref. 17. However, according to the numerical calculations, the staggered magnetization decreases more quickly with increasing  $\delta$  than our results. By going beyond the Tyablikov decoupling [Eq. (22)], which we have adopted in the present work, our results will be closer to the numerical calculations. In usual mean-field theories, on the other hand, since the single occupancy constraint [Eq. (2)] is treated only on the average, the antiferromagnetic order is generally overestimated,<sup>7-10</sup> e.g.,  $\delta_c > 0.15$  for  $t/J=4.0$  in

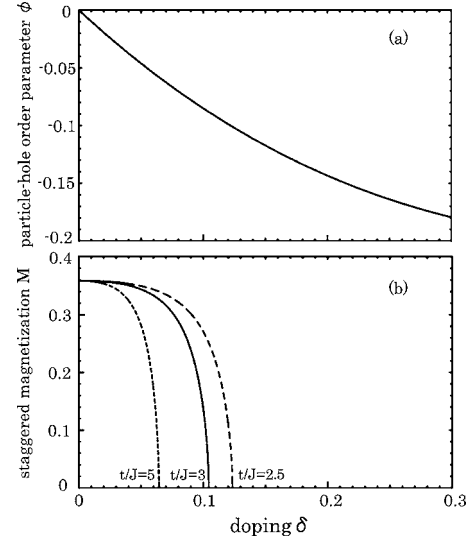


FIG. 3. (a) Particle-hole order parameter  $\phi$  as a function of doping  $\delta$  at  $T=0$  (independent of  $t/J$ ). (b) Staggered magnetization  $M$  as a function of doping  $\delta$  at  $T=0$  for  $t/J=2.5$ ,  $t/J=3$ , and  $t/J=5$ .

Ref. 9. For a more quantitative comparison with experiments, one must add other terms (e.g., next-nearest-neighbor hopping) to the Hamiltonian.

In this paper, we choose the pseudospin state as  $|i\uparrow\rangle_S$ . If the pseudospin state is chosen as  $(|i\uparrow\rangle_S + |i\downarrow\rangle_S)/2$ , the direction of the effective magnetic field is aligned along the  $x$  axis, and the staggered magnetization is mapped to the component of magnetization  $|\langle S_i^z \rangle|$  (perpendicular to the effective field).

#### IV. SUMMARY

In this paper, we have developed the pseudospin representation for the  $t$ - $J$  model. By introducing pseudospins associated with empty sites, we rewrote the  $t$ - $J$  model in terms of local spin and spinless fermionic operators. Using this representation, the  $t$ - $J$  Hamiltonian can be described without any constraint. The enlarged Hilbert space (the tensor product space) consists of three physical states and an unphysical state. According to Eq. (8), no physical quantity is affected by the unphysical state. Within a mean-field level, the influence of the unphysical state cannot be entirely excluded. However, since this influence is negligible in the low-doping limit, we believe that our method is a good approximation at least in the low-doping region. The spin part of the obtained mean-field model was regarded as the antiferromagnetic Heisenberg Hamiltonian in a uniform magnetic field with the correspondence  $B^z/\bar{J} \rightarrow B_{\text{eff}}^z/J_{\text{eff}} \equiv -4t\phi/\{J[(1-\delta)^2 - \phi^2] + 2t\phi\}$ . The strength and the direction of the effective field are determined by the doping  $\delta$  and the orientation of pseudospins, respectively. Our method yields a reasonable value of the critical doping  $\delta_c$ , at which the antiferromagnetic long-range order disappears, in good agreement with the numerical calculations.<sup>17-22</sup>



## ACKNOWLEDGMENTS

The authors would like to thank K. Kamide, N. Yokoshi, H. Shibata, and K. Iigaya for valuable comments and discussions. This work is supported by The 21st Century COE

Program (Holistic Research and Education Center for Physics of Self-organization Systems) at Waseda University from the Ministry of Education, Culture, Sports, Science and Technology of Japan.

\*Electronic address: yamamoto@kh.phys.waseda.ac.jp

†URL: <http://www.kh.phys.waseda.ac.jp/>

- <sup>1</sup>P. W. Anderson, *Science* **235**, 1196 (1987).
- <sup>2</sup>F. C. Zhang and T. M. Rice, *Phys. Rev. B* **37**, 3759 (1988).
- <sup>3</sup>P. A. Lee, N. Nagaosa, and X.-G. Wen, *Rev. Mod. Phys.* **78**, 17 (2006), and references therein.
- <sup>4</sup>G. Kotliar and J. Liu, *Phys. Rev. B* **38**, 5142 (1988).
- <sup>5</sup>T. Tanamoto, H. Kohno, and H. Fukuyama, *J. Phys. Soc. Jpn.* **62**, 717 (1993).
- <sup>6</sup>X.-G. Wen and P. A. Lee, *Phys. Rev. Lett.* **76**, 503 (1996).
- <sup>7</sup>M. Inui, S. Doniach, P. J. Hirschfeld, and A. E. Ruckenstein, *Phys. Rev. B* **37**, 2320 (1988).
- <sup>8</sup>C. L. Kane, P. A. Lee, T. K. Ng, B. Chakraborty, and N. Read, *Phys. Rev. B* **41**, 2653 (1990).
- <sup>9</sup>H. Matsukawa and H. Fukuyama, *J. Phys. Soc. Jpn.* **61**, 1882 (1992).
- <sup>10</sup>M. Inaba, H. Matsukawa, M. Saitoh, and H. Fukuyama, *Physica C* **257**, 299 (1996).
- <sup>11</sup>G. Khaliullin and P. Horsch, *Phys. Rev. B* **47**, 463 (1993).
- <sup>12</sup>J. L. Richard and V. Yu. Yushankhai, *Phys. Rev. B* **47**, 1103 (1993).
- <sup>13</sup>Y. R. Wang and M. J. Rice, *Phys. Rev. B* **49**, 4360 (1994).
- <sup>14</sup>J. Loos, *Phys. Rev. B* **53**, 12556 (1996).
- <sup>15</sup>S. Östlund and M. Granath, *Phys. Rev. Lett.* **96**, 066404 (2006).
- <sup>16</sup>P. Fröbrich and P. J. Kuntz, *Phys. Rep.* **432**, 223 (2006), and references therein.
- <sup>17</sup>M. Calandra and S. Sorella, *Phys. Rev. B* **61**, R11894 (2000).
- <sup>18</sup>T. K. Lee and Shiping Feng, *Phys. Rev. B* **38**, 11809 (1988).
- <sup>19</sup>T. Giamarchi and C. Lhuillier, *Phys. Rev. B* **43**, 12943 (1991).
- <sup>20</sup>A. Himeda and M. Ogata, *Phys. Rev. B* **60**, R9935 (1999).
- <sup>21</sup>M. Ogata and A. Himeda, *J. Phys. Soc. Jpn.* **72**, 374 (2003).
- <sup>22</sup>D. A. Ivanov, *Phys. Rev. B* **70**, 104503 (2004).
- <sup>23</sup>T. Tamaribuchi and M. Ishikawa, *Phys. Rev. B* **43**, 1283 (1991).
- <sup>24</sup>M. E. Zhitomirsky and T. Nikuni, *Phys. Rev. B* **57**, 5013 (1998).
- <sup>25</sup>A. Cuccoli, T. Roscilde, V. Tognetti, R. Vaia, and P. Verrucchi, *Phys. Rev. B* **67**, 104414 (2003).
- <sup>26</sup>M. E. Zhitomirsky and A. L. Chernyshev, *Phys. Rev. Lett.* **82**, 4536 (1999).
- <sup>27</sup>D. Petitgrand, S. V. Maleyev, Ph. Bourges, and A. S. Ivanov, *Phys. Rev. B* **59**, 1079 (1999).
- <sup>28</sup>P. J. Jensen, K. H. Bennemann, D. K. Morr, and H. Dreysse, *Phys. Rev. B* **73**, 144405 (2006).
- <sup>29</sup>S. V. Tyablikov, *Ukr. Mat. Zh.* **11**, 289 (1959).
- <sup>30</sup>S. V. Tyablikov, *Methods in the Quantum Theory of Magnetism* (Plenum, New York, 1967).
- <sup>31</sup>One derives the relation  $G_{AB}^{+-} = G_{BA}^{+-}$  from Eq. (24). The expression  $\langle (\mathbf{S}_i \times \mathbf{S}_{i+\eta})_z \rangle = 0$  is obtained from this symmetry relation.