# Stability of the ground state of ordered dimers of the *t–J* model

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The stability region of the dimerized state of spin-Peierls ground state of the Hubbard model for a two-dimensional lattice has been determined. The spin excitation spectrum has a gap in this region.

Various versions other than the ferromagnetic and antiferromagnetic state of the Hubbard model for a two-dimensional lattice began to be studied with the work of Anderson.[1] The phases in which the spins at the adjacent sites are strongly correlated but the average spin at each site is zero[2] have been suggested. The dimerized or spin-Peierls phase was found to have the minimum energy. To describe such a strongly correlated state, we have developed a magnetic perturbation theory in which the correlation between the adjacent sites in a dimer is taken into account in zeroth-order perturbation theory. We begin with the Hamiltonian of the Hubbard exchange model for a simple 2D square lattice, which is specified on the space of a single-particle filling of sites and which is taken into account the tunneling between the neighboring sites $t$ and the two competing antiferromagnetic exchanges: the nearest exchange $J_1$ and the diagonal exchange $J_2$

$$H = -t \sum_{ij} (1 - n_{i-\sigma}) C^{+}_{i\sigma} C_{j\sigma} (1 - n_{j-\sigma}) + \mu \sum_{i} C^{+}_{i\sigma} C_{i\sigma} + \sum_{ij} J_{ij} \left(\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} n_i n_j\right). \quad (1)$$

Here $C_{i\sigma}$ is the operator which creates an electron at the site $i$, $\mathbf{S}_i$ is the spin, and $\mu$ is the chemical potential.

Let us divide the Hamiltonian into two parts. We assign the terms in (1), which operate at the links represented by heavy lines in Fig. 1, to the first unperturbed part. In the zeroth-order approximation the wave function is the product of the two-site

  

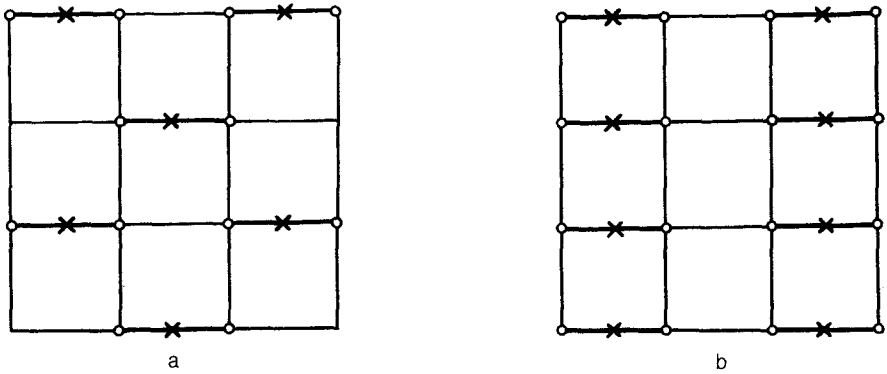


FIG. 1.

wave functions and the ground state of each pair of sites or the vacuum is the singlet $|\uparrow\downarrow - \downarrow\uparrow\rangle$. The total set of the states is given by the Bose creation operators $a_i^+$, $b_i^+$, and $c_i^+$, which operates on the space of the dimerized functions and which convert the vacuum into one of the triplet states, and by the Fermi creation operators $\alpha_{\uparrow i}^+$ and $\alpha_{\downarrow i}^+$, which creates a hole from the singlet vacuum

$$\langle \uparrow\uparrow | a^+ | \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\rangle = \langle \downarrow\downarrow | b^+ | \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\rangle$$
$$= \langle \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) | c^+ | \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\rangle = 1 \tag{2}$$
$$\langle \frac{1}{\sqrt{2}}(\uparrow 0 + 0\uparrow) | \alpha_\uparrow^+ | \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\rangle = \langle \frac{1}{\sqrt{2}}(\downarrow 0 + 0\downarrow) | \alpha_\downarrow^+ | \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\rangle = 1 .$$

For the terms in (1), which operate at the remaining couplings, we introduce a small parameter $\lambda$ ($\lambda J_1$, $\lambda J_2$, and $\lambda t$) and decompose over it according to perturbation theory. The results corresponding to Hamiltonian (1) are obtained for the value $\lambda = 1$. A direct verification shows that the spin operators can be expressed in terms of the Bose operators which we introduced[3]

$$M_z = a^+a - b^+b, \qquad M^+ = \sqrt{2}(a^+c - c^+b), \qquad M^- = \sqrt{2}(c^+a - b^+c)$$
$$L_z = -(c^+U + Uc), \qquad L^+ = \sqrt{2}(a^+U + Ub), \qquad L^- = \sqrt{2}(b^+U + Ua), \tag{3}$$

where $\mathbf{M}_i = \mathbf{S}_{2i} + \mathbf{S}_{2i-1}$ and $\mathbf{L}_i = \mathbf{S}_{2i} - \mathbf{S}_{2i-1}$ are the sum and the difference in the spins of the two neighbors, and $U = (1 - a^+a - b^+b - c^+c)^{1/2}$. After substituting (3) we see that the commutation relations $[M_iM_j] = i\epsilon_{ijk}M_k$, $[L_iL_j] = \epsilon_{ijk}M_k$, and $[M_iL_j] = i\epsilon_{ijk}L_k$ are valid. The matrix elements of the transition between the physical and nonphysical states vanish. Therefore, (3) is the analog of the Holstein-Primakoff transformation for systems with zero ground-state spin.

The lattice-site Hamiltonian, which is expressed in terms of the Bose and Fermi

operators in the quadratic approximation in the operators at the lattice doubled along the $x$ axis, and which is denoted by crosses in Fig. 1, is

$$H = H_c + H_{ab} + H_\alpha$$

$$H_c = \sum_{ij} [J_1 c_i^+ c_i - \lambda \frac{J_{ij}}{4}(c_i^+ c_j + c_j^+ c_i + c_i c_j + c_i^+ c_j^+)] \tag{4}$$

$$H_{ab} = \sum_{ij} [J_1(a_i^+ a_i + b_i^+ b_i)$$

$$- \lambda \frac{J_{ij}}{4}(a_i^+ b_i + b_i a_j^+ + b_i^+ a_j + a_i b_j^+ + a_i^+ a_j^+ + a_i a_j + b_i^+ b_j^+ + b_i b_j)]$$

$$H_\alpha = - \frac{\lambda t}{4} \sum_{ij} [\alpha_{i\uparrow}^+ \alpha_{j\uparrow}(U_i U_j + c_j^+ c_i + 2a_j^+ a_i)$$

$$+ \alpha_{i\downarrow}^+ \alpha_{j\downarrow}(U_i U_j + c_j^+ c_i + 2b_j^+ b_i)].$$

The term $H_\alpha$ was obtained by projecting the first term in (1) onto the space of dimerized functions which we introduced. We are concerned with the Bose excitation spectrum. To calculate it, we transform to a $k$ representation and retain in the Fermi part only the terms diagonal in $K$. The integral over $k$ gives the total density of the holes $N = N_\uparrow + N_\downarrow$.

It should be noted that the presence of holes in (4), in contrast with Ref. 4, does not reduce solely to a redefinition of the antiferromagnetic exchange in the Bose part of the Hamiltonian. The Bose Hamiltonian depends on the method of dividing the ground state into dimers. The domains of stability are, however, nearly the same. We will consider two cases (Fig. 1a and 1b) and compare the results.

Case $a$ (Fig. 1a)

$$H = \sum_\rho [J_1 + \lambda\{3R - (R + \frac{J_1}{2})\cos 2k_x - (R \pm J_1 \mp 2J_2)\cos k_x \cos k_y\}] x_{k\rho}^+ x_{k\rho}$$

$$- \frac{\lambda}{2}\{\frac{J_1}{2}\cos 2k_x + (J_1 - 2J_2)\cos k_x \cos k_y\}(x_{k\rho}^+ x_{-k\rho}^+ + x_{k\rho} x_{-k\rho}). \tag{5a}$$

Here $R = Nt/2$, and $\rho = 1,2,3$. The Hamiltonian contains three modes (two of which are degenerate). The superscript is used for $x_{k1} = c_k$ and $x_{k2} = a_k + b_k$ and the subscript is used for $x_{k3} = a_k - b_k$. The energy of the spin Bose excitation $E_k$ is

$$E_k^2 = [J_1 + \lambda\{3R - R\cos 2k_x - 2R\cos k_x \cos k_y\}]$$

$$\times [J_1 + \lambda\{3R - (R + J_1)\cos 2k_x - 2(R \pm J_1 \mp 2J_2)\cos k_x \cos k_y\}]. \tag{6a}$$

With $\lambda = 1$ we find the physical Hamiltonian (1). The domain of stability of the states ($E^2 > 0$ for all $k_x$ and $k_y$) for $\lambda = 1$ is determined by the inequalities

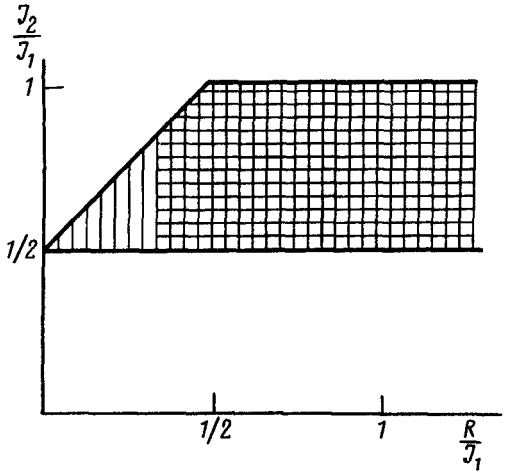


FIG. 2.

$$\frac{1}{2}J_1 \leqslant J_2 \leqslant J_1, \qquad J_2 \leqslant \frac{1}{2}J_1 + R \ .$$

The domain corresponding to these instabilities is represented in Fig. 2 by the vertical hatching.

Case $b$ (Fig. 1b)

$$H = \sum_{\rho} [J_1 + \lambda \{3R - (R \pm \frac{J_1}{2})\cos 2k_x - (2R \pm J_1 \mp J_2)\cos k_y \pm J_2 \cos k_y \cos 2k_x \}] x^+_{k\rho} x_{k\rho} - \frac{\lambda}{2}[\frac{J_1}{2}\cos 2k_x + (J_1 - J_2)\cos k_y - J_2 \cos k_y \cos 2k_x] \times (x^+_{k\rho}\, x^+_{-k\rho} + x_{k\rho}\, x_{-k\rho}) \ . \tag{5b}$$

The Hamiltonian also contains three modes, two of which $x_{k1} = c_k$ and $x_{k2} = a_k + b_k$, are degenerate (superscript), and the mode $x_{k3} = a_k - b_k$ (subscript). The energy $E_k$ is

$$E_k^2 = [J_1 + \lambda \{3R - R\cos 2k_x - 2R\cos k_y\}] \times [J_1 + \lambda \{3R - (R + J_1)\cos 2k_x - 2(R \pm J_1 \mp J_2)\cos k_y \pm 2J_2 \cos k_y \cos 2k_x\}] . \tag{6b}$$

The domain of stability ($E_k^2 > 0$ for all $k_x$ and $k_y$) for $\lambda = 1$ is given by the inequalities

$$\frac{1}{2}J_1 \leqslant J_2 \leqslant J_1, \quad \text{or} \quad J_2 \leqslant \frac{1}{2}J_1 + R, \qquad R \geqslant \frac{1}{3}J_1 .$$

This domain is shown in Fig. 2 by the horizontal hatching.

The expansion in $\lambda$ to first order corresponds to a quadratic form in the spin operators and apparently corresponds to the results of the mean-field theory. Since the spin excitation spectrum has a gap inside the hatched regions, allowance for the next corrections in the interaction does not disrupt the phase stability. Since the boundaries of the regions have a gapless spectrum, it is expected that the logarithmic corrections to the magnon interaction amplitude would lead to a dynamic mass generation and to a displacement of the stability boundary.[5] Our results show that the phase in Fig. 1a is preferable.

Zero-point fluctuations require the ground state of the system to be redefined; specifically, the adjacent dimers acquire a spin correlation. The order parameter, which corresponds to the VBS phase and which is given by $\langle S_{2i-1}S_{2i}\rangle - \langle S_{2i}S_{2i+1}\rangle$, remains nonzero, however. For the neighboring dimers situated on the $x$ axis, for example, we have

$$\langle S_i S_{i-1}\rangle = \frac{1}{4\pi^2}\int_{-\pi/2}^{\pi/2} dk_x \int_{-\pi}^{\pi} dk_y \left(\frac{v_k^2 \cos 2k_x}{u_k^2 + v_k^2}\right),$$

where $v_k$ and $u_k$ are the coefficients of the $u - v$ transformation. Estimate of this expression in the second order in $\lambda$ gives $\langle S_i S_{i-1}\rangle \sim -(\lambda^2/8)[(2J_2 - J_1)/J_1]^2$ for Fig. 1a and $\langle S_i S_{i-1}\rangle \sim -(\lambda^2/8)(J_1 - J_2)/J_1$ for Fig. 1b.

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