Physica C 377 (2002) 85–88
PHYSICA C
www.elsevier.com/locate/physc

# Evidence of stripe formation tendency in $t$–$J$ model

Yongjin Jiang [a,b,*], Daosheng Deng [a,b], Ruibao Tao [c,d]

[a] Department of Physics, Surface Physics Laboratory (National key Laboratory), Fudan University, Shanghai 200433, China
[b] Center of Theoretical Physics, Fudan University, Shanghai 200433, China
[c] Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China
[d] Department of Physics, Fudan University, Shanghai 200433, China

Received 13 March 2001; received in revised form 10 September 2001; accepted 17 September 2001

**Abstract**

The d-wave RVB mean field theory for the $t$–$J$ model is generalized to the inhomogeneous case to incorporate harmonic hole modulation manifestly. Numerical results show that there are a monotonous decrease of ground state energy with the increase of amplitude of modulation. The form of this dependence strongly suggests the existence of a nontrivial stripe phase of $t$–$J$ model for different $t/J$, and doping values.


*PACS:* 74.20.Mn; 71.27.+a; 74.90.+n
*Keywords:* $t$–$J$ model; RVB pairing; Slave-boson transformation; Stripe phase

## 1. Introduction

The high $T_c$ superconductor is believed to be doped antiferromagnets shortly after its discovery [1]. Anderson argued in his pioneering work [2] that the ground state of superconductor is the RVB state. Since then, many efforts has been made based on such an idea [3,4]. Meanwhile, many other theoretical works have been suggested for the explanation of high $T_c$ mechanism. For understanding the high $T_c$ mechanism, the one of the most prominent experiments is the d-wave symmetry identification [6], which was successfully predicted by Koliar and Liu [4] for $t$–$J$ model based on the RVB mean field approximation. Recently the RVB theory is greatly improved by considering the gauge fluctuation [7,8]. Considering the long length/low energy gauge fluctuation exactly, the $2e$ charge unit [8] can be successfully derived. It comes from different microscopic mechanism compared to the usual BCS pairing. Experimental evidences of stripe correlation, either static or dynamic, in a wide class of strong correlated systems including cuprates and other systems are accumulating in the past few years [9–12]. There are many theoretical approaches to this interesting problem [13–21]. It is believed that a wise understanding of stripe phase will help to penetrate the core physics of high $T_c$ superconductivity, which is unclear up to now. Recently, through self-consistent approach alike that for one-dimensional phonon–electron polymer system, Matveenko and Mukhin have found ground state spin–charge

* Corresponding author. Address: Department of Physics, Surface Physics Laboratory (National key Laboratory), Fudan University, Shanghai 200433, China. Fax: +86-21-6510-4949.
*E-mail address:* jyjdy@263.net (Y. Jiang).

0921-4534/01/$ - see front matter 
PII: S0921-4534(01)01120-0

solitonic structure for Hubbard model as a function of hole doping [17]. The work of Machida group has related metal–insulator transition for an extended Hubbard model to the diagonal stripe phase to vertical stripe phase transition [18]. In this paper, however, we extend the usual d-wave RVB decoupling scheme for $t$–$J$ model to take into account the stripe structure explicitly. Numerical results show that modulated phase is more energetically favorable than homogeneous one for the ground state of $t$–$J$ model without long range Coulomb repulsion term. The ground state energy is monotonously decreasing with increase of the modulation amplitude of hole density. The result is generally true for a broad range of parameter values. This property of $t$–$J$ model obtained from the RVB framework is relevant to the mechanism of stripe phase now under hot research. Based on our calculation, we suggest that the stripe phase formation is an intrinsic tendency for the $t$–$J$ model even without long range Coulomb interactions which is in consistence with the results obtained by DMRG calculations [19].

## 2. Theoretical method

The Hamiltonian of $t$–$J$ model in the subspace of no doubly occupied sites is:

$$H = -t\sum_{\langle i,j\rangle s}(f_{is}^{\dagger}f_{is} + \text{h.c.}) + J\sum_{\langle i,j\rangle}\left(\mathbf{S}_i^{\dagger}\cdot\mathbf{S}_j - \frac{n_i n_j}{4}\right). \tag{1}$$

By a slave-boson transformation [22], we get

$$H = -t\sum_{\langle i,j\rangle s}(c_{is}^{\dagger}e_i e_j^{\dagger}c_{js} + \text{h.c.}) + J\sum_{\langle i,j\rangle}b_{ij}^{\dagger}b_{ij}. \tag{2}$$

The first term represents the boson–Fermi interaction, where the $e$ and $e^{\dagger}$ are holon of boson type, and $c$, $c^{+}$ are spinon of Fermi type. They must obey the constraint of the single-occupation identity: $e_i^{+}e_i + \sum_s c_{is}^{+}c_{is} = 1$ and

$$b_{ij}^{\dagger} = c_{i_\uparrow}^{\dagger}c_{j_\downarrow} - c_{i_\downarrow}^{\dagger}c_{j_\uparrow}. \tag{3}$$

Usually, in a mean field treatment [4,5], we simply set $e$, $e^{\dagger}$ to be $c$ number signifying complete boson condensation. In order to take into account the existence of stripe structure, we use a mean field decoupling with harmonic modulation of hole density in momentum space:

$$\begin{aligned}&\langle e_0^{\dagger}e_0\rangle = N\delta,\\ &\langle e_q^{\dagger}e_0\rangle = \langle e_0^{\dagger}e_q\rangle = \langle e_{-q}^{\dagger}e_0\rangle = \langle e_0^{\dagger}e_{-q}\rangle = N\Delta_{\mathrm{e}}.\end{aligned} \tag{4}$$

It reduces to $\langle e_i^{+}e_i\rangle = \delta + 4\Delta_{\mathrm{e}}\cos(\mathbf{q}\cdot\mathbf{r}_i)$, where $\delta$ is hole density and $4\Delta_{\mathrm{e}}$ the modulation amplitude. The average density of the spinon at site $i$ is $1 - \langle e_i^{+}e_i\rangle = (1-\delta) - 4\Delta_{\mathrm{e}}\cos(\mathbf{q}\cdot\mathbf{r}_i)$. The d-pairing RVB order parameter should be modulated with the same period $2\pi/q$. We assumed the condensation parameters of the spinon to be

$$\langle b_{ii\pm x}\rangle = \Delta(1 - p\cos(\mathbf{q}\cdot\mathbf{r}_i)), \tag{5}$$

$$\langle b_{ii\pm y}\rangle = -\Delta(1 - p\cos(\mathbf{q}\cdot\mathbf{r}_i)), \tag{6}$$

and choose $p$ as $4\Delta_{\mathrm{e}}/(1-\delta)$. After such mean field approximation, the effective mean field Hamiltonian becomes

$$H_{\mathrm{eff}} = H_1 + H_2 + \mu\sum_i c_i^{\dagger}c_i, \tag{7}$$

where

$$\begin{aligned}H_1 = &-t\sum_{\langle i,j\rangle s}\gamma(k)[\delta c_{ks}^{+}c_{ks} + \Delta_{\mathrm{e}}(c_{ks}^{+}c_{k+qs} + c_{k+qs}^{+}c_{ks}\\ &+ c_{k-qs}^{+}c_{k+qs} + c_{ks}^{+}c_{k-qs})],\end{aligned} \tag{8}$$

$$\gamma(k) = 2(\cos k_x + \cos k_y), \tag{9}$$

$$\begin{aligned}H_2 = &-J\sum_k(\cos k_x - \cos k_y)\{2\Delta[c_{k_\downarrow}c_{-k_\uparrow} - c_{k_\uparrow}c_{-k_\downarrow}\\ &+ \text{h.c.}] - \Delta p[c_{k_\downarrow}c_{-k-q_\uparrow} - c_{k_\uparrow}c_{-k-q_\downarrow} + c_{k_\downarrow}c_{-k+q_\uparrow}\\ &- c_{k_\uparrow}c_{-k+q_\downarrow}]\} + 4JN\Delta^2\left(1 + \frac{p^2}{2}\right).\end{aligned} \tag{10}$$

The chemical potential $\mu$ in the Hamiltonian can be determined by $1 - \delta = \frac{1}{2N}\langle\sum_{is}c_{is}^{+}c_{is}\rangle$,where $N$ is the number of lattice sites, and $\langle\cdots\rangle$ represents the average at ground state.

## 3. Numerical results and discussion

In the above formulation, we have discarded the normal Hartree–Fock terms which will affect the results quantitatively, but is not essential [23] for

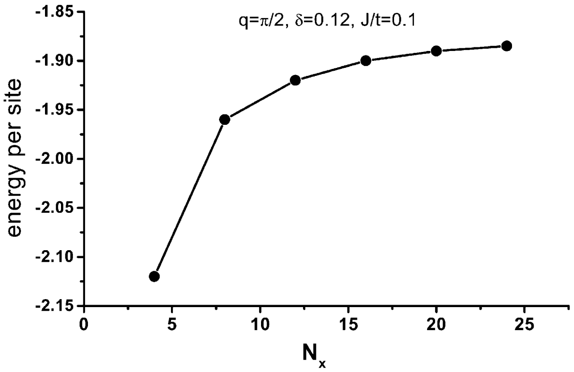


Fig. 1. The lattice size dependence of ground energy per site. Size $N_y$ is fixed to 8 and $N_x = 4$, 8, 12, 16, 20, 24 respectively. The modulated period is chosen as 4 lattice constants, doping density $\delta = 0.12$ and $J/t = 0.1$.

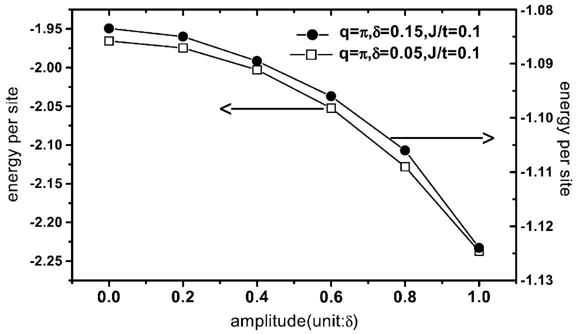


Fig. 2. The hole modulation amplitude dependence of ground state energy. The modulation amplitude is in units of hole density $\delta$. The monotonous decreasing behavior is characteristic of intrinsic tendency of stripe forming.

superconductivity. The order parameter $\Delta$ is determined by minimizing the ground state energy. We use the general formulation of Bogoliubov transformation to diagonalize the Hamiltonian for small lattices with sizes: $8N_x$, $N_x = 4$, 8, 12, 16, 20, 24. In Fig. 1, we have fixed the modulated period to be 4 lattice constant, $J/t = 0.1$ and hole density $\delta = 0.12$. The size dependent ground state energy is calculated and shown in Fig. 1. One can see that the convergence of the ground state energy is quite good. The value of the $8 \times 16$ lattice almost reaches to the convergent limit, so all the following calculations are for $8 \times 16$ lattice only. We vary $\Delta_e$ of Eq. (4), hence the modulation amplitude of hole density. The ground state energy is decreasing as the stripe becomes more "clear" as shown in Fig. 2. It corresponds to a general tendency of stripe formation. We extrapolate that the more "sharp" striped structure, such as stripe phase with far separated thin hole lines, will be more stable. Some authors [15] argue that phase separation of *t–J* model is ubiquitous phenomena in the limit of small doping, and it is because of long range Coulomb interaction which frustrates the local tendency to the phase separation that drives the formation of stripe phase. However, based on the DMRG calculations, White et al. [19] argue that the Coulomb interaction is not necessary to form stripes which is consistent with our extended mean field calculation. In real systems, the stripe formation will break electroneutrality microscopically, taking into account the extra Coulomb energy will only stabilize the stripe structure considering the phase separation arguments [15,16].

Furthermore, we have calculated the $q$ dependence of $E_g$ shown in Fig. 3. From the figure, it is clear that the modulated phases is more energetically favorable than homogeneous one. Meanwhile, the most stable phase of the ground state is in period 2 It is not well consistent with most experimental periods that can be changed [11].This reflects the underlying antiferromagnetism which is dominant in our harmonic decoupling. However, the existence of more stable nontrivial stripe phase in *t–J* model based on the extended RVB theory is qualitatively clear.

From physics point of the view, the *t–J* model is a coupled field of spinons and holons after slave boson transformation, and the system is two

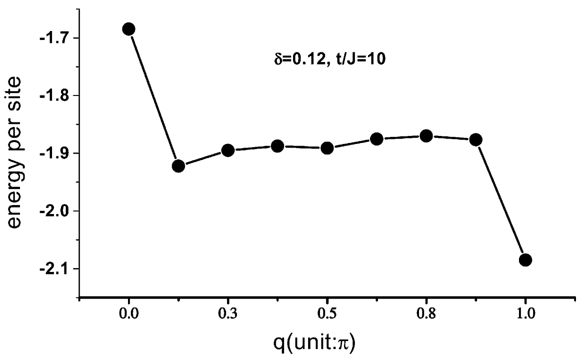


Fig. 3. The ground state energy as a function of the modulation period. The horizontal axis is wave vector $q$ in units of $\pi$.

dimensional. The "nesting property" of Fermi surface in light doping region leads to the instability toward some modulated structure. It is very similar to the two-dimensional electron–phonon field which often shows modulated phase behavior due to the intrinsic instability. The analogy suggest that the mechanism of the stripe phase in $t$–$J$ model may be from the two dimensionality and the coupling of spinon (fermion) and holon (boson) fields.

In summary, the d-wave RVB mean field theory [4] is extended to the inhomogeneous case, we compare the ground state energy of different periodic phases and homogeneous one and find that the modulated phases always have a lower energy. The overall decreasing tendency of ground state energy with the increase of modulation amplitude strongly suggests the existence of a nontrivial stripe-like phase that is closely related to the experimental findings. In this harmonic modulation scheme, we cannot derive quantitatively good results by extended RVB mean field approximation. The lowest energy corresponds to the period-2 stripe in our calculation which is not quantitatively agree with experimental results. However, the monotonous decreasing behavior of ground state energy tells much about the intrinsic physics in $t$–$J$ model to form stripe, which is not completely known yet.

## Acknowledgements

This work is supported by National Natural Science Foundation of China and Shanghai Research Center of Applied Physics.

## References

[1] J.A. Bednoedz, K.A. Müller, Z. Phys. B 64 (1986) 189.
[2] P.W. Anderson, Science 235 (1987) 1196.
[3] G. Baskaran, Z. Zhou, P.W. Anderson, Solid State Commun. 63 (1987) 973;
I. Affleck, J.B. Marston, Phys. Rev. B 37 (1988) 3774;
Y. Suzumura, Y. Hasegawa, H. Fukuyama, J. Phys. Soc. Jpn. 57 (1988) 2768.
[4] G. Kotliar, Phys. Rev. B 37 (1988) 3664;
G. Koliar, J.L. Liu, Phys. Rev. B 38 (1988) 5142.
[5] Z. Zhou, P.W. Anderson, Phys. Rev. B 37 (1988) 627.
[6] Z.X. Shen et al., Phys. Rev. Lett. 70 (1993) 1553;
J. Kane, Q. Chen, K.-W. Ng, H.-J. Tao, Phys. Rev. Lett. 72 (1994) 128.
[7] P.A. Lee, X.G. Wen, Phys. Rev. Lett. 78 (1997) 4111;
P.A. Lee, N. Nagaosa, T.-K. Ng, X.-G. Wen, Phys. Rev. B 57 (1998) 6003;
P.A. Lee, 1998. Available from cond-mat/9812226.
[8] D.H. Lee, 1999. Avaliable from cond-mat/9909111.
[9] S.W. Cheong et al., Phys. Rev. Lett. 67 (1991) 1791;
S.M. Hayden et al., Phys. Rev. Lett. 68 (1992) 1061;
C.H. Chen et al., Phys. Rev. Lett. 71 (1993) 2461.
[10] J.M. Tranquada et al., Phys. Rev. Lett. 73 (1994) 1003.
[11] J.M. Tranquada et al., Phys. Rev. B 54 (1996) 7489;
J.M. Tranquada et al., Phys. Rev. Lett. 78 (1997) 338.
[12] J.M. Tranquada, J. Phys. Chem. Solids 59 (1998) 2150;
H. Hwang, S.W. Cheong, Nature 389 (1997) 942;
S. Mori, C. Chen, S.W. Cheong, Nature 392 (1998) 473;
Y.S. Lee et al., Available from cond-mat/9902157;
Wakimoto et al., Available from cond-mat/9902319.
[13] J. Zaanen, O. Gunnarsson, Phys. Rev. B 40 (1989) 7391;
D. Poiblanc, T.M. Rice, Phys. Rev. B 39 (1989) 9749;
H.J. Schulz, Phys. Rev. Lett. 64 (1990) 1445.
[14] V.J. Emery, S.A. Kivelson, J.M. Tranquada, 1999. Available from cond-mat/9907228.
[15] S.A. Kivelson, V.J. Emery, in: K.S. Bedell, et al. (Eds.), Proceedings of Strongly Correlated Electronic Materials: The Los Alamos Symposium 1993, Addison Wesley, Redwood, 1994, p. 619;
V.J. Emery, S.A. Kivelson, Physica C 209 (1993) 594;
C. Hellberg, E. Manousakis, Phys. Rev. Lett. 78 (1997) 4609;
C. Hellberg, E. Manousakis, J. Phys. Chem. Solids 59 (1998) 1818.
[16] V.J. Emery, S.A. Kivelson, O. Zachar, Phys. Rev. B 56 (1997) 6120.
[17] S.I. Matveenko, S.I. Mukhin, Phys. Rev. Lett. 84 (2000) 6066.
[18] M. Ichioka, K. Machida, Physica B 281 (2000) 804;
M. Ichioka, K. Machida, J. Phys. Soc. Jpn. 68 (12) (1999) 4020;
K. Machida, M. Ichioka, J. Phys. Soc. Jpn. 68 (7) (1999) 2168.
[19] S.R. White, D.J. Scalapino, Phys. Rev. Lett. 80 (1998) 1272;
S.R. White, D.J. Scalapino, Phys. Rev. Lett. 81 (1998) 3227;
S.R. White, D.J. Scalapino, Phys. Rev. B 61 (2000) 6321.
[20] W. Zheng, 2000. Available from cond-mat/0002233.
[21] L.P. Pryadko, S.A. Kivelson, V.J. Emery, Y.B. Bazaliy, E.A. Demler, 1999. Available from cond-mat/9905146.
[22] S.E. Barnes, J. Phys. F 6 (1976) 1375, 7 (1977) 2637;
P. Coleman, Phys. Rev. B 29 (1984) 3035.
[23] G. Baskaran, Z. Zhou, P.W. Anderson, Solid State Commun. 63 (1987) 973.