Magnetic Excitations in Strongly Correlated Electrons
J. Phys. Soc. Jpn. **69** (2000) Suppl. B. pp. 22–25

Stripe States in the Two-dimensional t-J Model

Masao OGATA *

Department of Basic Science, University of Tokyo, Komaba 3-8-1, Meguro-ku, Tokyo 153-8902, Japan

(Received December 27, 1999)

Stripe states in high-T_c superconductors are studied using the two-dimensional t-J model. The effect of strong correlation or the exclusion of doubly occupancies is taken into account via Gutzwiller approximation. The spatial dependence of the order parameters are obtained from the numerical diagonalization of the Bogoliubov-de Gennes equation derived in the Gutzwiller approximation. It is shown that there are two possibilities for the stripe pattern. One is the stripe state without $d_{x^2-y^2}$-wave superconductivity, which indicates the competition between the stripe state and superconductivity. However this state has a longer periodicity than that observed experimentally. The other is the stripe state in which the incommensurate antiferromagnetic correlation and $d_{x^2-y^2}$-wave superconductivity coexist. This state is consistent with experiments, but in order to stabilize it, some additional pinning potentials for holes are necessary.

KEYWORDS: stripe, t-J model, Gutzwiller approximation

§1. Introduction

Recently various experiments, especially neutron scattering have supported the existence of stripe state in some high-T_c cuprates.[1-5] This state has one-dimensional stripes containing holes (charge ordering) as well as the antiferromagnetic regions between the stripes (incommensurate antiferromagnetic spin ordering). In some cases, it has been argued that this type of stripe state coexists with superconductivity (SC).[2,4,5]

Theoretically the possibility of stripe states was discussed in the Hubbard model[6-11] and t-J model.[12-14] However the previous works considered only the incommensurate antiferromagnetism (ICAF) and charge ordering. The superconducting order parameters have not been taken into account. However one of the interesting problems is the interplay between the stripe state and $d_{x^2-y^2}$-wave SC. Actually Emery *et al* discussed that the stripe state is the origin of high-T_c superconductivity.[15] Therefore it is important to study whether the stripe state can coexist with the $d_{x^2-y^2}$-wave SC or not.

For this purpose the t-J model is the most appropriate model because this model represents the doped Heisenberg system and the AF and d-wave SC correlations can be studied on the equal footing. Since the main interaction in the t-J model is the superexchange interaction, there appear interesting phenomena relating to the magnetism in the superconducting state. Furthermore the two-dimensional t-J model is regarded as a realistic model for high-T_c superconductors,[16,17] and we can investigate the interplay between ICAF and d-wave SC as a function of hole-doping, which is important when compared with the actual high-T_c materials. This model takes the strong correlation into account through the Gutzwiller's projection operator prohibiting the double occupancy,[18] and thus we can elucidate the effect of strong correlation in addition to the doping dependences.[19-24]

Phase diagram of this model has been discussed from various viewpoints, i.e., slave boson mean-field theory,[25] variational Monte Carlo simulation,[19-21] Gutzwiller approximation[18,21] and high-temperature expansion.[26] All of these studies agree that the $d_{x^2-y^2}$-wave SC state is stabilized for finite doping region. The interplay between the AF near half-filling and d-wave SC was discussed in variational Monte Carlo simulations.[27,28] Although the state near half-filling is a coexistent state between AF and d-wave SC, the t-J model explains naturally the fact that the ground state changes from the AF to the SC state as the carrier density increases. In this paper we study the stripe state in the two-dimensional t-J model especially for the hole doping $\delta = 1/8$.

There are two possibilities for the stripe state in the t-J model. One is the coexistence between the d-wave SC and ICAF, as suggested by Emery *et al.*[15] In this case the d-wave order parameters are localized in the hole stripe regions and they are coupled two-dimensionally through the AF regions. We expect the spatial dependence of the d-wave order parameters: it is smaller in the AF region and larger in the hole stripe. The other possibility is the case where AF and d-wave SC compete each other. In this case we expect either a pure ICAF state or a pure d-wave SC state for the ground state.

We study these two possibilities in the t-J model using the Gutzwiller approximation (GA) in which the Gutzwiller projection is taken into account as a statistical weight.[18] Since the simple slave boson mean-field theory or Gutzwiller approximation gives a qualitatively wrong results when both the AF and the d-wave SC orders are considered, we use a modified GA. The spatial variation of the d-wave order parameter and AF order parameters around the stripe is determined self-

* address from April 2000, Department of Physics, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113-0033, Japan

consistently.

We find that a stripe state is stabilized in which the period of the hole stripe is 8 lattice constant. In this case the ICAF is realized but the d-wave SC is completely suppressed. This indicates the competition between the d-wave SC and stripe state in the t-J model. On the other hand, the stripe state with 4 lattice periodicity can be stabilized only if the pinning potential for holes favoring the stripe pattern is introduced. In this case we find that the ICAF and d-wave SC coexist.

§2. t-J Model and Gutzwiller Approximation

We consider the two-dimensional t-J model on a square lattice:

$$\mathcal{H} = -t\sum_{\langle ij\rangle\sigma} P_G(c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.})P_G + J\sum_{\langle ij\rangle} \boldsymbol{S}_i\cdot\boldsymbol{S}_j, \quad (2.1)$$

where $\langle ij\rangle$ means the summation over nearest-neighbor pairs and $\boldsymbol{S}_i = c^\dagger_{i\alpha}(\frac{1}{2}\sigma)_{\alpha\beta}c_{i\beta}$. The Gutzwiller's projection operator P_G is defined as $P_G = \prod_i(1-\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$.

Since the constraint of no double occupancy is imposed on this Hamiltonian, it is difficult to carry out analytical calculations even in mean-field theories. Here we consider $T = 0$ variational theory. In order to study the electronic states in inhomogeneous systems, we assume site-dependent variational order parameters, $\Delta^{\rm V}_{ij}$, in the trial wavefunction

$$|\psi\rangle = P_G|\psi_0(\Delta^{\rm V}_{ij})\rangle, \quad (2.2)$$

where $|\psi_0(\Delta^{\rm V}_{ij})\rangle$ is a BCS-SDW mean-field solution. This wavefunction is a natural generalization of the RVB state.[16]

The variational parameters $\Delta^{\rm V}_{ij}$ are determined so as to minimize the variational energy

$$E_{\rm var} = \langle\psi|\mathcal{H}|\psi\rangle = \langle\psi_0(\Delta^{\rm V}_{ij})|P_G\mathcal{H}P_G|\psi_0(\Delta^{\rm V}_{ij})\rangle. \quad (2.3)$$

It is usually difficult to estimate $E_{\rm var}$ due to the Gutzwiller projection. Here we use a Gutzwiller approximation (GA),[18,21] in which the constraint is taken into account as a statistical average as

$$\langle\psi|\boldsymbol{S}_i\cdot\boldsymbol{S}_j|\psi\rangle = g_s\langle\boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle_0,$$
$$\langle\psi|c^\dagger_{i\sigma}c_{j\sigma}|\psi\rangle = g_t\langle c^\dagger_{i\sigma}c_{j\sigma}\rangle_0, \quad (2.4)$$

where $\langle\cdots\rangle_0$ represents the average in the wavefunction without Gutzwiller projection, $|\psi_0(\Delta^{\rm V}_{ij})\rangle$. This leads to

$$E_{\rm var} = \langle\mathcal{H}_{\rm eff}\rangle_0, \quad (2.5)$$

where the parameters t and J in $\mathcal{H}$ are replaced with

$$t^{\rm eff} = g_t t, \qquad J^{\rm eff} = g_s J, \quad (2.6)$$

in the effective Hamiltonian $\mathcal{H}_{\rm eff}$. It has been shown that the GA gives a fairly reliable estimation for the variational energy for the pure d-wave SC state when it is compared with the variational Monte Carlo results.[18,21]

As noted in §1, usual mean-field theories generally overestimate the AF long-range order. In the slave boson mean-field theory, the AF order is too overestimated and it extends up to unphysical doping rates (15∼20%).[29] In this scheme, we are unable to discuss the stripe state because it is stabilized near $\delta = 0.125$ doping. On the other hand, if the AF order parameter is taken into account in the GA, we obtain[30]

$$g_s = \left(\frac{2(1-\delta)}{1-\delta^2+4m^2}\right)^2, \quad (2.7)$$
$$g_t = \frac{2\delta(1-\delta)}{1-\delta^2+4m^2},$$

where m is the expectation value $m = \frac{1}{2}\langle n_{i\uparrow} - n_{i\downarrow}\rangle_0$. However it was shown that this GA does not give AF state even at half-filling.[18]

Therefore in this paper we use the modified GA which gives the reasonable estimate of the AF correlation compared with the results in variational Monte Carlo simulations.[28,31] We found that the Gutzwiller factor g_s should depend on the direction of the quantization axis of the AF order,

$$\langle\psi|\boldsymbol{S}_i\cdot\boldsymbol{S}_j|\psi\rangle = g_s^{XY}\langle S^x_iS^x_j + S^y_iS^y_j\rangle_0 + g_s^Z\langle S^z_iS^z_j\rangle_0, \quad (2.8)$$

instead of eq. (2.4). The explicit forms of g_s^{XY}, g_s^Z are obtained by taking account of the intersite correlations [31]

$$g_s^{XY} = \left(\frac{2(1-\delta)}{1-\delta^2+4m^2}\right)^2 a^{-7}, \quad (2.9)$$
$$g_s^Z = g_s^{XY}\frac{1}{4m^2+X_2} \times\left[X_2 + 4m^2\{1+\frac{6X_2(1-\delta)^2}{1-\delta^2+4m^2}a^{-3}\}^2\right] \quad (2.10)$$

with

$$a = 1 + \frac{4X}{(1-\delta^2+4m^2)^2},$$
$$X = 2\delta^2(\Delta^2-\chi^2) + 8m^2(\chi^2+\Delta^2) + 2(\chi^2+\Delta^2)^2,$$
$$X_2 = 2(\chi^2+\Delta^2). \quad (2.11)$$

Here χ, Δ are expectation values for the hopping and superconductivity, respectively: $\chi = \langle c^\dagger_{i\sigma}c_{j\sigma}\rangle_0$ and $\Delta = \langle c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\rangle_0$. The Gutzwiller factor for the hopping term is given by

$$g_t = \frac{2\delta(1-\delta)}{1-\delta^2+4m^2}\,\frac{(1+\delta)^2-4m^2-2X_2}{(1+\delta)^2-4m^2}a. \quad (2.12)$$

The above expressions reproduce the results obtained in the variational Monte Carlo simulations.[31]

§3. Stripe States in the t-J Model

For studying inhomogeneous systems we use χ, Δ and m are local expectation values such as $\Delta_{ij} = \langle c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\rangle_0$ etc. Thus the Gutzwiller factors g_s^{XY}, g_s^Z and g_t depend on the bond (ij). Minimizing $E_{\rm var}$ in eq. (2.3), we obtain a Bogoliubov-de Gennes equation and a set of self-consistent equations in a similar way to the BCS mean-field theory:[28]

$$\begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F^*_{ji} & -H_{ji\downarrow}\end{pmatrix}\begin{pmatrix} u^\alpha_j \\ v^\alpha_j\end{pmatrix} = E^\alpha\begin{pmatrix} u^\alpha_i \\ v^\alpha_i\end{pmatrix}, \quad (3.1)$$

with

$$H_{ij\sigma} = -\sum_{\tau} \left(t_{ij}^{\text{eff}} + J_{ij}^{\text{eff}} \chi_{ji}^{\text{V}}\right) \delta_{j=i+\tau} + \left(\sigma \sum_{\tau} h_{ii+\tau}^{\text{eff}} - \mu\right) \delta_{ij},$$
$$F_{ij} = -\sum_{\tau} J_{ij}^{\text{eff}} \Delta_{ij}^{\text{V}} \delta_{j=i+\tau}, \tag{3.2}$$

where τ runs as vectors pointing to the nearest-neighbor sites and

$$t_{ij}^{\text{eff}} = g_{t,ij} t,$$
$$J_{ij}^{\text{eff}} = \frac{1}{2} g_{s,ij}^{XY} J + \frac{1}{4} g_{s,ij}^{Z} J,$$
$$h_{ij}^{\text{eff}} = \frac{1}{2} g_{s,ij}^{Z} J m_j + \frac{\partial \langle H_{ij} \rangle}{\partial m_i}. \tag{3.3}$$

Here $\langle H_{ij} \rangle$ is defined as the local energy,

$$\langle H_{ij} \rangle = -2\text{Re}\left[t_{ij}^{\text{eff}} \chi_{ij}\right] - J_{ij}^{\text{eff}} \left(|\Delta_{ij}|^2 + |\chi_{ij}|^2\right) + \frac{1}{2} g_{s,ij}^{Z} J m_i m_j, \tag{3.4}$$

and the partial derivative of $\langle H_{ij} \rangle$ with respect to m_i is only applied to the Gutzwiller factors, $g_{t,ij}, g_{s,ij}^{XY}$ and $g_{s,ij}^{Z}$. Self-consistent equations are

$$\Delta_{ij}^{\text{V}} = \Delta_{ij} - \frac{1}{J_{ij}^{\text{eff}}} \frac{\partial \langle H_{ij} \rangle}{\partial \Delta_{ij}^*},$$
$$\chi_{ij}^{\text{V}} = \chi_{ij} - \frac{1}{J_{ij}^{\text{eff}}} \frac{\partial \langle H_{ij} \rangle}{\partial \chi_{ij}^*}, \tag{3.5}$$

with

$$\Delta_{ij} = \langle c_{i\uparrow}^{\dagger} c_{j\downarrow}^{\dagger} \rangle_0 = -\frac{1}{4} \sum_{\alpha} (u_i^{\alpha *} v_j^{\alpha} + u_j^{\alpha} v_i^{\alpha *}) \tanh \frac{\beta E^{\alpha}}{2},$$
$$\chi_{ij} = \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle_0 = -\frac{1}{4} \sum_{\alpha} (u_i^{\alpha *} u_j^{\alpha} - v_j^{\alpha} v_i^{\alpha *}) \tanh \frac{\beta E^{\alpha}}{2}. \tag{3.6}$$

We solve numerically the Bogoliubov-de Gennes equation and carry out an iteration until the self-consistent equation for $\Delta_{ij}^V, \chi_{ij}^V$ is satisfied. Thus we obtain the fully quantum results. In Fig. 1, the self-consistent solution for $\delta = 1/8$ and $J/t = 0.3$ is shown. We have used a unit cell of the size 16×2 which is compatible with various stripe states. The stripe state in Fig. 1 is the vertical stripe and has the 8 lattice periodicity for the hole density, which does not coincide with that observed experimentally. We did not find any self-consistent solution of the stripe state with 4 lattice periodicity, but we will show shortly that such a stripe state is stabilized by pinning potential for holes (Fig. 2).

As apparent from Fig. 1, the phase of the AF region changes π when it crosses the hole stripe as predicted. However the AF moment is not so large in the AF region and there is not rapid change of the hole density. Furthermore in this state the d-wave SC order parameters are completely suppressed. This suggests the competition between ICAF and d-wave SC in the t-J model. Actually we find another local-minimum solution with uniform d-wave SC order parameters without any AF moment. Comparing the variational energies E_{var} (eq. (2.3)), we find that the stripe state in Fig. 1 has the lower energy than the pure d-wave SC state. But the energy difference is only $\Delta E_{\text{var}} = 0.005t$.

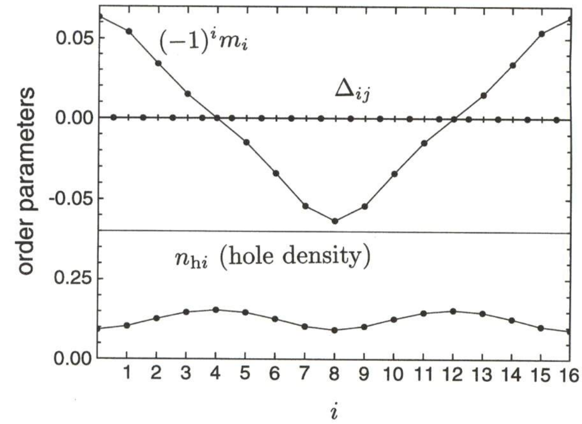

Fig. 1. Stripe state with 8 lattice periodicity found in the t-J model with the hole doping $\delta = 1/8$ and $J/t = 0.3$. The d-wave SC order parameters Δ_{ij} are completely suppressed.

Figure 2 shows the stripe state with 4 lattice periodicity, which is stabilized when the pinning potential for holes is applied. This state corresponds to the stripe state experimentally observed. We have included the pinning potential

$$\sum_i V_i (1 - \hat{n}_i - \delta), \tag{3.7}$$

in the t-J model, where $\delta = 1/8$ is the average hole density. In Fig. 2, we have chosen $V_i = 0.1t$ for $i = 4n (n = \text{integer})$ and $V_i = -0.1t$ for $i = 4n + 2$. In this case the d-wave SC order parameters Δ_{ij} do not vanish inside the AF region. Stabilization of this stripe state indicates that the ICAF and d-wave SC can coexist if the charge ordering is stabilized by other mechanisms such as

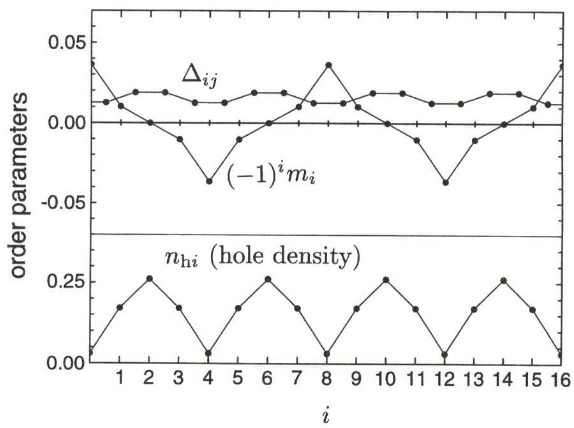

Fig. 2. Stripe state with 4 lattice periodicity found in the t-J model with the hole doping $\delta = 1/8$ and $J/t = 0.3$. This state is stabilized only with the pinning potential for holes. The d-wave SC order parameters do not vanish inside the AF region.

impurity pinning etc. We also studied the dependence of the amplitude of the pinning potential V_i. We find that the stripe state in Fig. 2 is stabilized when $|V_i| > 0.05t$. If we chose $|V_i| < 0.05t$, the self-consistent solution is either uniform d-wave SC state without AF order or the stripe state as in Fig. 1.

§4. Summary and Discussions

In this paper we have shown that there are two possibilities for the stripe state in the two-dimensional t-J model. One is the case where ICAF and d-wave SC coexist as shown in Fig. 2. This stripe state corresponds to the state observed experimentally. However this state is realized only when the charge ordering is stabilized by other mechanisms outside of the t-J model. We expect that impurity potential, instability to the LTT lattice distortion etc. will cause the formation of the stripe state. If the ICAF is more enhanced than in Fig. 2, the d-wave SC looses its phase coherence and thus the SC transition is suppressed.

Another possibility for the stripe state is that shown in Fig. 1. This state has 8 lattice periodicity of the hole density and the d-wave SC order parameters are suppressed. This corresponds to the stripe states found in the Hubbard model.[6-11] It is interesting that the d-wave SC can coexist only in the stripe state with 4 lattice periodicity (Fig. 2).

The difference between the above two stripe states becomes apparent when we look at the local density of states (DOS). In the stripe state without d-wave SC, the local DOS has a characteristic feature of the soliton band just above the Fermi energy. On the other hand, in the other stripe state with d-wave SC, the local DOS is close to the DOS for the d-wave SC state (V-shape DOS). In the region where the AF moment is large or close to half-filling, the local DOS looks like the DOS for the underdoped region (i.e., larger SC gap). Therefore if the scanning tunneling spectroscopy is carried out, it is possible to distinguish the two kinds of stripe states.

Recently stripe states with shorter periodicity have been discussed in some extended models.[14,32] Thus it is interesting to see the interplay with the d-wave SC in the models with nearest neighbor repulsion and/or hopping terms. The doping dependences of the present stripe states as well as the effect of additional terms are under investigation and will be published elsewhere. As for the interplay between the AF and d-wave SC, another interesting problem is the possibility of an antiferromagnetic vortex core which was expected in the SO(5)-symmetric theory.[33,34] Since the d-wave superconducting order parameter is suppressed inside the core, the antiferromagnetic local moment may show up inside the core. We studied this possibility using the modified GA where the antiferromagnetic local moment is taken into account.[35]

Acknowledgements. The author wishes to thank H. Fukuyama, Y. Endoh, K. Yamada, Y. Koike, H. Yokoyama and K. Kobayashi for their useful discussions.

1) J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nagure **375**, 561 (1995) and J. M. Tranquada *et al*, Phys. Rev. B **54**, 7489 (1996).
2) J. M. Tranquada, J. D. Axe, N. Ichikawa, A. R. Moodenbaugh, Y. Nakamura, and S. Uchida, Phys. Rev. Lett. **78**, 338 (1997).
3) K. Yamada, C. H. Lee, K. Kurahashi, J. Wada, S. Wakimoto, S. Ueki, H. Kimura, Y. Endoh, S. Hosoya, G. Shirane, R. J. Birgeneau, M. Greven, M. A. Kastner, and Y. J. Kim, Phys. Rev. B **57**, 6165 (1998).
4) H. Kimura, K. Hirota, H. Matsushita, K. Yamada, Y. Endoh, S-H. Lee, C. F. Majkrzak, R. Erwin, G. Shirane, M. Greven, Y. S. Lee, M. A. Kastner, and R. J. Birgeneau, Phys. Rev. B **59**, 6517 (1999).
5) S. Wakimoto, G. Shirane, Y. Endoh, K. Hirota, S. Ueki, K. Yamada, R. J. Birgeneau, M. A. Kastner, Y. S. Lee, P. M. Gehring, and S. H. Lee, Phys. Rev. B **60**, 769 (1999) and cond-mat/9902319.
6) D. Poilblanc and T. M. Rice, Phys. Rev. B **39**, 9749 (1989).
7) K. Machida, Physica C **158**, 192 (1989) and M. Kato, K. Machida, H. Nakanishi and M. Fujita, J. Phys. Soc. Jpn. **59**, 1047 (1990).
8) H. J. Schulz, Phys. Rev. Lett. **64**, 1445 (1990) and J. Phys. France **50**, 2833 (1989).
9) J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989).
10) T. Giamarchi and C. Lhuillier, Phys. Rev. B **42**, 10641 (1990).
11) K. Machida and M. Ichioka, cond-mat9812398.
12) S. R. White and D. J. Scalapino, Phys. Rev. Lett. **80**, 1272 (1998).
13) C. S. Hellberg and E. Manousakis, Phys. Rev. Lett. **83**, 132 (1999).
14) K. Kobayashi and H. Yokoyama, Physica B **259-261**, 506 (1999) and to appear in J. Low Temp. Phys.
15) V. J. Emery, S. A. Kivelson and O. Zachar, Phys. Rev. B **56**, 6120 (1997) and S. A. Kivelson, E. Fradkin and V. J. Emery, Nature **393**, 550 (1998).
16) P. W. Anderson, Science **235**, 1196 (1987).
17) F. C. Zhang and T. M. Rice: Phys. Rev. B **37**, 3759 (1988).
18) F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
19) H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 3570 (1987) and J. Phys. Soc. Jpn. **57**, 2482 (1988).
20) C. Gros, Phys. Rev. B **38**, 931 (1988) and Ann. Phys. (N.Y.) **189**, 53 (1989).
21) H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. **65**, 3615 (1996).
22) A. Himeda, M. Ogata, Y. Tanaka and S. Kashiwaya, J. Phys. Soc. Jpn. **66**, 3367 (1997).
23) Y. Tanuma, Y. Tanaka, M. Ogata and S. Kashiwaya, J. Phys. Soc. Jpn. **67**, 1118 (1998) and Phys. Rev. B **60**, 9817 (1999).
24) H. Tsuchiura, Y. Tanaka, M. Ogata and S. Kashiwaya, J. Phys. Soc. Jpn. **68**, 2510 (1999).
25) T. Suzumura, H. Hasegawa and H. Fukuyama, J. Phys. Soc. Jpn. **57**, 401 (1988).
26) W. O. Putikka, M. U. Luchini and T. M. Rice, Phys. Rev. Lett. **68**, 538 (1992).
27) T. Giamarchi and C. Lhuillier, Phys. Rev. B **43**, 12943 (1991).
28) A. Himeda and M. Ogata, Phys. Rev. B **60**, R9935 (1999).
29) M. Inaba, H. Matsukawa, M. Saitoh and H. Fukuyama, Physica C **257**, 299 (1996).
30) T. Ogawa, K. Kanda and T. Matsubara, Prog. Theor. Phys. **53**, 614 (1975).
31) M. Ogata and A. Himeda, in preparation.
32) K. Machida and M. Ichioka, private communication.
33) S. C. Zhang, Science **275**, 1089 (1997).
34) D. P. Arovas, A. J. Berlinsky, C. Kallin and S. C. Zhang, Phys. Rev. Lett. **79**, 2871 (1997).
35) M. Ogata, Proceedings of the 12th International Symposium on Superconductivity (ISS'99), to be published in *Advances in Superconductivity XII.*