Diagonal Stripe States in the Light-Doping region in the Two-Dimensional Hubbard Model

Mitake MIYAZAKI[1,2], Takashi YANAGISAWA[2] and Kunihiko YAMAJI[2]

[1]*Department of Physics, Aoyama Gakuin University, Fuchinobe, Sagamihara-shi, Kanagawa 229-8568*
[2]*National Institute of Advanced Industrial Science and Technology, Tsukuba Central 2, 1-1-1, Tsukuba-shi, Ibaraki 305-8568*

(Received February 10, 2004)

We studied the ground state of the two-dimensional Hubbard model near half filling on the square-lattice. By using Variational Monte Carlo method, we show that the diagonal stripe state of bond-centered type, in which the domain wall is located between two sites, becomes more stable than the vertical stripe state when the doped hole density x is as low as $x \simeq 0.06$. Inverse of stripe periodicity δ and the hole density x are observed to keep relationship $\delta \sim x$ ($\delta < x$) for the bond-centered diagonal stripe state (the vertical stripe state) in the light-doped region. These results are in good agreement with elastic neutron scattering experiments in $La_{2-x}Sr_xCuO_4$.

KEYWORDS: two-dimensional Hubbard model, variational Monte Carlo, diagonal stripe, high-Tc

The influence of doped holes on the anti-ferromagnetic state such as in the parent materials of high-T_c superconductors is one of the most interesting problems on strongly correlated electrons. It is known that holes doped into the half-filled square-lattice lead to an incommensurate spin- and charge-density wave (ISDW-ICDW) within the framework of Hartree-Fock theory.[1)] In the elastic neutron scattering experiment on Nd-doped $La_{2-x}Sr_xCuO_4$ (LSCO) with hole density around $x \sim 0.125$, Tranquada *et al.* observed incommensurate magnetic and charge peaks at $(1/2, 1/2 \pm \delta)$ or $(1/2 \pm \delta, 1/2)$ and $(2 \pm 2\delta, 0)$ or $(0, 2 \pm 2\delta)$ in the reciprocal space, respectively.[2)] This result indicated the possibility of the ISDW-ICDW order stabilized at low temperatures. This state is now called "vertical stripe (VS) state" because charge stripes are vertical to the horizontal crystal axis. It was shown by Variational Monte Carlo (VMC) studies that the coexistent state of the VS order and d-wave superconductivity (SC) is obtained as the ground state in the doping region around $x = 0.125$ not only in the Hubbard model[3,4)] but also in the d-p model[5)] and the t-J model[6)] in two dimensions (2D); all three models take account of considerably strong correlation between electrons.

Recently, it was experimentally found that the stripe order is stabilized in a wide under-doped region of LSCO at low temperature. From the experiment of resistivity in the light-doping region of LSCO, the system holds metallic behavior below the anti-ferromagnetic transition temperature, which is considered to originate in formation of metallic charge stripes.[7)] In addition, the spin-glass state in the insulating phase was found to have well-developed stripe-like correlation.[8)] The elastic neutron scattering experiment of LSCO in the light-doping region, $0.03 < x < 0.07$, revealed that the position of incommensurate magnetic peaks changed from $(1/2, 1/2 \pm \delta)$ to $(1/2 \pm \delta', 1/2 \pm \delta')$ as x becomes less than 0.06.[9,10)] This means that the stripe direction rotates by 45°, becoming diagonal, at this transition. In the "diagonal stripe (DS) state", the magnetic peaks were observed to keep a relationship $\delta \simeq x$ which is held in the VS state in the low doping region.

Our purpose in this paper is to examine if the relationship $\delta \sim x$ is obtained in the lower doping region or not and if the DS state is obtained in the further lower doping region, in the similar computation as in the previous work[4)] by the VMC study on the ground state of the 2D Hubbard model. This model is more appropriate than the t-J model for cuprates since on site coulomb energy U is considered to be moderate[12)] and this model gives the SC condensation energy close to the experimental one.[12)] We will show that the bond-centered DS state is more stable than the VS state when $x \leq 1/16$ and that this state holds $\delta \sim x$ as well as in $1/16 < x < 1/8$. Here, the bond-centered state implies that the center of the stripe runs between two sites while the conventional stripe running on the sites is called site-centered type.

We start from the 2D Hubbard model,

$$H = -\sum_{i,j,\sigma} \frac{1}{2} t_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

where the transfer energy $t_{ij} = t, t'$, if sites i and j are nearest neighbors and next-nearest neighbors, respectively. In the following we take t as the unit of energy. $c^\dagger_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of the electron with spin σ ($\uparrow$ or $\downarrow$) at site i ($i = 1 \sim N_s$) and $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$. N_s is the number of sites. By using the VMC method, we calculate the variational total energy in the coexistent state, $E_{\text{coexist}} = \langle \Psi_{\text{coexist}} | H | \Psi_{\text{coexist}} \rangle / \langle \Psi_{\text{coexist}} | \Psi_{\text{coexist}} \rangle$. We use the trial wave function $\Psi_{\text{coexist}}\rangle$ as defined by $|\Psi_{\text{coexist}}\rangle = P_{N_e} P_G |\phi^{\text{MF}}_{\text{coexist}}\rangle$. P_G is the Gutzwiller projection operator given by $P_{\text{G}} = \prod_i (1 - (1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$, where g is the Gutwiller variational parameter in the

range from 0 to unity, which controls the on-site electron correlation. Projector P_{N_e} assures a fixed total electron number N_e. $|\phi^{\rm MF}_{\rm coexist}\rangle$ is a mean-field wave function for the coexisting SC in a stripe SDW state. The mean-field Hamiltonian for $\phi^{\rm MF}_{\rm coexist}$ is given by

$$H_{\rm MF} = \sum_{ij}(c^\dagger_{i\uparrow}\ c_{i\downarrow}) \begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F^*_{ji} & -H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c^\dagger_{j\downarrow} \end{pmatrix}, \quad (2)$$

where diagonal terms describe the mean field due to ISDW-ICDW as

$$H_{ij\sigma} = -t_{ij} - \mu + \frac{U}{2}\left[n_i + {\rm sgn}(\sigma)(-1)^{x_i+y_i} m_i\right]\delta_{\boldsymbol{r}_i,\boldsymbol{r}_j}, \quad (3)$$

where μ is the chemical potential. Following Giamarchi et al.,[5] we assume charge density n_i and spin density m_i are spatially modulated as $n_i = 1 - \sum_l \alpha/\cosh((y_i - Y_l)/\xi_c)$ and $m_i = m\prod_l \tanh((y_i - Y_l)/\xi_s)$, respectively. Here amplitude α is fixed by $\sum_i n_i = N_e$. Y_l denotes the position of the domain wall, where the hole density is maximal; Y_l = *integer* (*half-integer*) corresponds to the site- (bond-) centered stripe state. Stripes extend along the x-direction. The meanings of m, ξ_c, and ξ_s are apparent. The DS state can be treated in the same way by replacing y_i by $x_i - y_i$. On the other hand, the off-diagonal terms in eq. (2) are defined in term of the d-wave SC gap as $F_{ij} = \sum_{\hat e}\Delta_{ij}\delta_{\boldsymbol{r}_j,\boldsymbol{r}_{i+\hat e}}$, where $\hat e = \pm\hat x, \pm\hat y$ are unit vectors. We consider the spatially inhomogeneous SC state so that the SC amplitude takes the maximum on the stripes as $\Delta_{i,i+\hat x} = \Delta\cos(q_y(y_i - Y_l))$ and $\Delta_{i,i+\hat y} = -\Delta\cos\left(q_y(y_i - Y_l + \hat y/2)\right))$. Here $\boldsymbol{q} = (0, 2\pi\delta)$ and δ is a incommensurability given by the stripe's period in the y direction with regard to the spin in the VS case. Note the period in charge distribution is half of the spin period. The sign of the SC gap is opposite between neighboring stripes. It was already confirmed that this "anti-phase" configuration is more stable than the state where the SC gap is given by $\Delta_{i,i+\hat x} = \Delta|\cos(q_y(y_i - Y_l))|$ and $\Delta_{i,i+\hat y} = -\Delta|\cos\left(q_y(y_i - Y_l + \hat y/2)\right))|$.[4,6]

In order to diagonalize the Hamiltonian, eq. (2), it is necessary to solve the Bogoliubov-de Gennes equation,

$$\sum_j \begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F^*_{ji} & -H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} u^\alpha_j \\ v^\alpha_j \end{pmatrix} = E_\alpha \begin{pmatrix} u^\alpha_i \\ v^\alpha_i \end{pmatrix}, \quad (4)$$

with $i = 1, 2, \cdots, N_s$. Here we obtain N_s positive eigenvalues E_α ($\alpha = 1 \sim N_s$) with their eigenvectors (u^α_i, v^α_i). While, N_s negative eigenvalues $E_{\bar\alpha}$ are obtained with eigenvectors ($v^{\bar\alpha}_i$,$u^{\bar\alpha}_i$). The coefficients u^α_i and v^α_i determine the Bogoliubov transformation,

$$\begin{aligned} \gamma_{\alpha\uparrow} &= u^\alpha_i c_{i\uparrow} + v^\alpha_i c^\dagger_{i\downarrow} \qquad (E_\alpha > 0) \\ \gamma_{\bar\alpha\downarrow} &= u^{\bar\alpha}_i c_{i\uparrow} + v^{\bar\alpha}_i c^\dagger_{i\downarrow} \qquad (E_{\bar\alpha} < 0), \end{aligned} \quad (5)$$

where the $\gamma_{\alpha\uparrow}$ and $\gamma_{\bar\alpha\downarrow}$ are quasi-particle annihilation operators, which satisfy the anti-commutation relations. Then we obtain the expression of the trial function,[4,6]

$$P_{\rm G}P_{N_e}|\phi^{\rm MF}_{\rm coexist}\rangle \sim P_{\rm G}\Big(\sum_{ij}(U^{-1}V)_{ij}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\Big)^{N_e/2}|0\rangle, \quad (6)$$

with $(U)_{ij} = u^i_j$ and $(V)_{ij} = v^i_j$ with $i, j = 1, 2, \cdots, N_s$.

In actual calculations, variational parameters are μ, m, g, ξ_c, ξ_s and Δ. Main efforts are made on such clusters where there are two stripes. In this paper, we choose the system parameters $t' = -0.20$ and $U = 8$ suitable for cuprate superconductors such as LSCO. Periodic boundary condition is used in the x-direction, and anti-periodic one in the y-direction. The correlated measurements and Newton method were used for optimization of the total energy. In each Newton step, the number of total Monte Carlo steps was greater than 6×10^6.

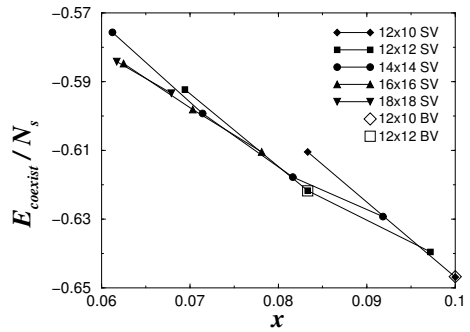

Fig. 1. Total energy of coexistence state of the VS state and d-wave SC as a function of hole-density x for $U = 8$ and $t' = -0.20$. Filled symbols denote for the cases of site-centered VS type (SV). The bond-centered VS cases (BV) are represented by open symbols. $n \times m$ denotes the cluster size of n in the x- and m in the y-direction. m is equal to the stripe's period.

In Fig. 1, we show the minimized total energy per site, $E_{\rm coexist}/N_s$, of the coexistent state of the VS and d-wave SC as a function of hole density, x. We performed the numerical calculation in the under-doped region of $0.06 < x \leq 0.1$ where the coexisting state of vertical ISDW and SC state was observed in LSCO.[10] Filled symbols represent values for site-centered VS states with 12-,14-,16- and 18-lattice periods on square-lattices. Error bars are smaller than the size of symbols. The period of the minimum energy state switches from 12-lattice through 18-lattice as x decreases. This behavior is basically the same as that in the previous calculation for $1/12 \leq x \leq 1/8$.[4] However, the hole density dependence of the incommensurability for the most stable stripe state tends to deviate to smaller values δ from the relation of $\delta = x$ as x decreases; when $\delta = x$ is hold, the hole density along a stripe is equal to 1/2 per unit lenght. Such a deviation from $\delta = x$ was reported in the inelastic neutron scattering experiment by Yamada *et al.*[13] We found also that the total energy of the bond-centered VS state is very close to that of site-centered one. This closeness is in agreement with the result from density matrix renormalization group calculations by White *et al.*[14]

Next, in Fig. 2, we show $E_{\rm coexist}/N_s$ in the cases of both site- and bond-centered DS states as functions of x. As a reference, the minimum values of the VS state obtained from Fig. 1 are plotted by open circles. We calculated in the cases of 12-, 16-, 20- and 24-lattice period DS states on square-lattices. We found that the total energy for the bond-centered type is definitely lower than that for the site-centered type for the same stripe's period by more than the error bar. This result clearly differs from that in the VS case. In this doping region, the total energy of the DS state with larger stripe period

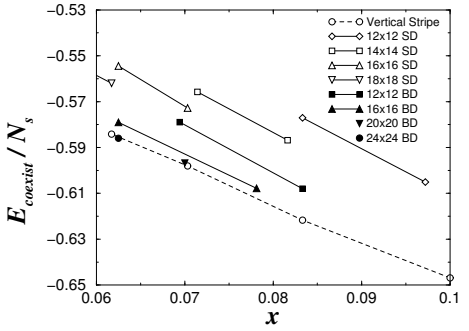

Fig. 2. Total energy per site of the coexistence state of DS and d-wave SC as a function of hole-density x for $U = 8$ and $t' = -0.20$. Open symbols denote for the cases of site-centered DS type (SD). The bond-centered DS cases (BD) are represented by filled symbols. The value of the minimum energy for the VS state as shown in Fig. 1 are also plotted by open circles.

is lowered. The bond-centered DS state with 24-lattice period is most stable at $x = 1/16$. It lies lower than the VS curve. Although the possibility of the DS state with a larger stripe period is not excluded, the 24-lattice period state is very probable to be the lowest energy state at $x = 1/16$, since the energy difference between the successive periodicity states are quickly decreasing and close to zero for the 24-lattice period state.

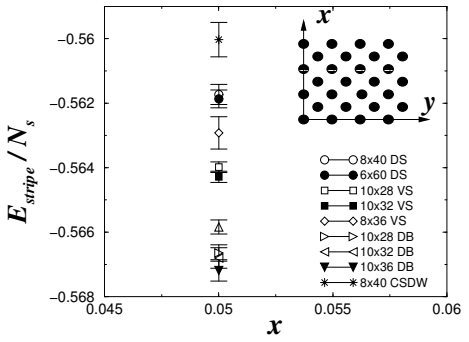

Fig. 3. Total energy for VS (square) state and bond-centered (circle) and site-centered (triangle) DS state against $x = 0.05$. The inset shows the lattice configuration used only in numerical calculations for DS state. Periodic boundary conditions are used in both the x- and y-direction in the inset. The lattice of the inset is labeled 4×8 denoting the cluster size of 4 in the x-direction and 8 in the diagonal-direction. The latter number is equal to the stripe's period with regard to the spin. Two stripes are extend along the x direction. The total energy for commensurate SDW state is also plotted by diamond.

When we calculated the total energy for the DS state, we have employed the square-lattice because the boundary condition with the periodic spin arrangement is needed in both x and y direction. However, the numerical calculation of lattices larger than 24×24 sites requires too much CPU time. We now employ the rectangular lattice (we called this configuration "diagonal-lattice" in this paper) cutting a square-lattice along the diagonal direction as shown in the inset of Fig. 3, which enables us to evaluate the variational energy of the DS state in lower-doping region. Moreover, we set the SC gap parameter at zero because this SC condensation energy is much smaller than that for the stripe SDW part in the present small x region.[4] The following arguments are not influenced by the choice of the cluster lattice. We checked that close total energies of DS states were obtained by both diagonal-and square-lattices of 16×16 sites, lying in the range of the statistics error bar. We show the total energies per site of DS states for various stripe-periods with $x = 0.05$ in Fig. 3. The calculations for the VS state were performed on the square-lattice as in Fig. 1 and 2. We found that the bond-centered DS state with the 36-lattice period in spin along the diagonal direction of the inset is the most stable. This period is closer to the relation, $\delta = x$, rather than $\delta = x/2$ because δ is defined as the inverse of the stripe interval in the direction perpendicular to the DS; $1/\delta = 36/\sqrt{2} \simeq .039$. The total energy is higher in the case of the site-centered DS states than both in the VS and bond-centered DS cases. Incidentally, the DS state with the 60-lattice period $(1/\delta = 60/\sqrt{2})$ is the most stable in the site-centered type. In this case, it seems that the relation of $\delta \sim x/2$ is satisfied. On the other hand, the site-centered VS state is most stable when the period is 32-lattice in square-lattices, in which $\delta = x$ is not maintained.

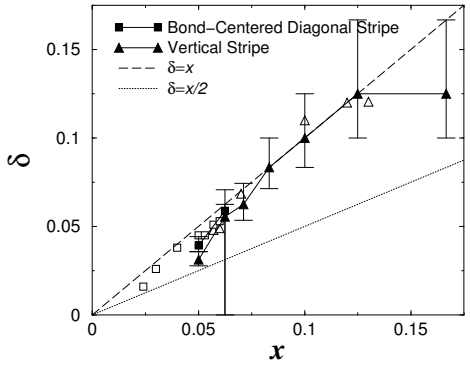

Fig. 4. Incommensurability δ depending on the hole density x for $U = 8$ and $t' = -0.2$. Previous results for $x = 1/6$, $1/8$, $1/10$ and $1/12$ are included.[15] The numerical result for the VS and the bond-centered DS state are represented by filled square and down-triangle symbols, respectively. Open squares and triangles show the results of the vertical and diagonal ISDW order observed from neutron scattering measurements, respectively.[10]

In Fig.4, we show the incommensurability of the most stable stripe state as a function of x by using the results obtained above. Open squares and triangles are values for diagonal and vertical ISDW's obtained in the elastic neutron scattering experiment on LSCO, respectively. Filled down-triangle and squares show our results for the DS and the VS states, respectively. Error bars present possible deviations due to the fact the stripe state with intermediate periods was not treated by our calculation. While, in the light-doping region, δ starts to deviate from the relation $\delta = x$ in the VS state, the relationship is approximately held there in the DS state. These results are in a good agreement with experimental data. We also found that the phase boundary $x_{\rm critical}$ between DS and VS state lies at or above 0.0625 in the case of $U = 8$ and $t' = -0.2$. The following factors may give rise to slight changes of calculated $x_{\rm critical}$: it is thought that the DS state is stabilized in low-temperature-orthorhombic (LTO) phase in LSCO. We confirmed that the DS state stabilizes further by forming a line along larger next-

nearest hopping direction due to the anisotropic t' generated by the Cu-O buckling in the LTO phase. On the other hands, Giamarchi et al showed that the DS state is stabler when U is larger.[3] Therefore, the value of $x_{\rm critical}$ is larger as U increases or in the LTO phase. Taking these effects into consideration, a slightly smaller value of U is considered to be more appropriate as noted in introduction.[16]

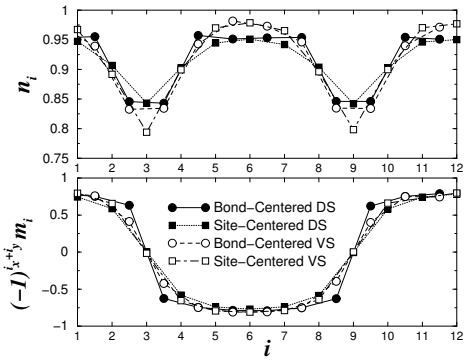

Fig. 5. Charge density n_i and staggered magnetization m_i along y direction for 12-lattice period stripes. The stripe center of the bond-centered type is adjusted to that of the site-centered one.

We now discuss about the relative stability of the bond-centered and site-centered types of VS and DS states. Figure. 5 shows the expectation values of the charge density $n_i = n_{i\uparrow} + n_{i\downarrow}$ and the staggered magnetization $m_i = (-1)^{i_x+i_y}(n_{i\uparrow} - n_{i\downarrow})$ along the y direction for the case of 12-lattice period with $x = 1/12$. In this case the VS state is more stable than the DS state. n_i and m_i for both the bond-centered and the site-centered VS states take very similar distributions, respectively, which implies that VS states of two types have very close gains of kinetic and magnetic energies. On the other hand, the charge amplitude of the site-centered DS state is smaller than that of the site-centered VS state. On the contrary, in the bond-centered DS state, the charge distribution near the domain wall is close to that for the bond-centered VS state as if it tended to earn the kinetic energy. In addition, the magnetic domains outside the stripe region is extended than those of the site-centered DS state and also than that in the VS state, which is considered to be advantageous in the light-doping region because the loss of the SDW formation energy caused by hole-concentrated stripes keep smaller. Why does the bond-centered DS state differs from the site-centered one? There is a possibility that these differences result from the effective hopping energy along diagonal stripe direction. While holes move on one charge stripe by next-nearest-site hopping energy t' in the case of site-centered DS state, holes in the bond-centered one can zigzag on the ladder-like charge stripes by nearest-site hopping energy t (where local spin densities are ferromagnetically arranged). In the VS state, the difference of site- and bond-centered type may be smaller than that for the DS state because both of charge stripes are oriented in the vertical direction with nearest-site hopping energy t.

More recently, it was shown by using the Hartree-Fock theory that the diagonal stripe structure varies from the site-centered one to the bond-centered one as hole density decreases from $x = 0.05$ when the period is fixed at 40-lattices.[17] However, the strong electron correlations should be taken into consideration in the doped Mott insulator. It is especially important in cuprates with an inhomogeneous charge distribution.

In conclusion, we performed the VMC calculation to the 2D Hubbard model for $U = 8$ and $t' = -0.2$. The VS state switches to the bond-centered DS state as the hole density decreases from $x \leq 1/16$. In the lower doping region, the relationship of the hole density and the incommensurability, $\delta \sim x$, is satisfied in the case of the bond-centered DS state while $\delta < x$ in the VS state. These results are in good agreement with the experiments in the light-doped LSCO. This supports the validity of the 2D Hubbard model for cuprates and also the soundness of the VMC method. The result provides the basis for clarifying the remaining problems in the light-doping region. It would also help one understand the stability of the static diagonal stripe in the nickel system.

Acknowledgments

One of authors (M.M.) was supported by a Grant-in-Aid for 21st COE Program from the MEXT of the Japanese Government. VMC calculations were performed on *Aoyama Plus systems*, CP-PACS of University of Tsukuba, the TACC facility of AIST as well as on the group's facility.

References

1) See, for example, J. Ichioka and K. Machida: J. Phys. Soc. Jpn. **68** (1999) 4020. and references therein.
2) J. M. Tranquada, J. D. Axe, N. Ichikawa, Y. Nakamura, S. Uchida and B. Nachumi: Pys. Rev. B **54** (1996) 7489.
3) T. Giamarch and C. Lhuillier: Phy. Rev. B **42** 10641.
4) M. Miyazaki, K. Yamaji and T. Yanagisawa: J. Phys. Chem. Solid **63** (2002) 1403.
5) T. Yanagisawa, S. Koike and K. Yamaji: J. Phys. Condens. Matter **12** (2002) 21.
6) A. Himeda, T. Kato and M. Ogata: Phys. Rev. Lett. **88** (2002) 117001.
7) Y. Ando, A. N. Lavorv, S. Komiya, K. Segawa and X. F. Sun: Phys. Rev. Lett. **87** (2001) 017001.
8) B. J. Sternlieb, G. M. Luke, Y. J. Uemura, T. M. Riseman, J. H. Brewer, P. M. Gehring, K. Yamada, Y. hidaka, T. Murakami, T. R. Thurston, and R. J. Birgeneau: Phys. Rev. B **41** (1990) 8866.
9) M. Matsuda, M. Fujita, K. Yamada, R. J. Birgeneau, M. A. Kastner, H. Hiraka, Y. Endoh, S. Wakimoto and G. Shirane: Phys. Rev B **62** (2000) 9148.
10) M. Fujita, K. Yamada, H. Hiraka, P. M. Gehring, S. H. Lee, S. Wakimoto and G. Shirane: Phys. Rev. B **65** (2002) 064505.
11) R. Coldea, S. M. Hayden, G. Aeppli, T. G. Perring, C. D. Frost, T. E. Mason, S. W. Cheong and Z. Fisk: Phys. Rev. Lett. **86** (2001) 5377.
12) K. Yamaji, T. Yanagisawa, T. Nakanishi and S. Koike: Physica C **304** (1998) 225.
13) K. Yamada, C. H. Lee, K. Kurahashi, J. Wasa, S. Wakimoto, S. Ueki, H. Kimura, Y. Endoh, S. hosoya, G. Shirane, R. J. Bergeneau, M. Greven, M. A. Kastner and Y. J. Kim: Phys. Rev. B **57** (1998) 6165.
14) S. R. White and D. J. Scalapino: Phys. Rev. Lett. **80** (1998) 1272.
15) M. Miyazaki, K. Yamaji and T. Yanagisawa: Physica C **388-389** (2003) 82.
16) K. Yamaji, T. Yanagisawa and M. Miyazaki: preprint.

17) E. Kaneshita, M. Ichioka and K. Machida: J. Phys. Soc. Jpn.
72 (2003) 2441.