

Diagonal Stripe States in the Light-doping Region in the Two-dimensional Hubbard Model

Mitake MIYAZAKI^{1,2}, Takashi YANAGISAWA² and Kunihiro YAMAJI²

¹Department of Physics and Mathematics, Aoyama Gakuin University, 5-10-1 Fuchinobe, Sagamihara, Kanagawa 229-8558

²National Institute of Advanced Industrial Science and Technology, 1-1-1 Tsukuba Central 2, Tsukuba, Ibaraki 305-8568

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We studied the ground state of the two-dimensional Hubbard model near half filling on the square lattice. 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 doping hole density x is as low as $x \simeq 0.06$. The inverse of stripe periodicity δ and the hole density x are observed to have the relationship $\delta \sim x$ ($\delta < x$) for the bond-centered diagonal stripe state (the vertical stripe state) in the light-doping region. These results are in good agreement with elastic neutron scattering experiments in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$.

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The influence of doping holes on the antiferromagnetic state such as in the parent materials of high- T_c superconductors is one of the most interesting problems for strongly correlated electrons. It is known that holes doped in a half-filled square lattice lead to an incommensurate spin- and charge-density wave (ISDW–ICDW) within the framework of the Hartree–Fock theory.¹⁾ In the elastic neutron scattering experiment on Nd-doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO) with a hole density of approximately $x \sim 0.125$, 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 a reciprocal space, respectively.²⁾ This result indicated the possibility of the ISDW–ICDW order stabilized at low temperatures. This state is now called the “vertical-stripe (VS) state” because the direction of the charge stripes is vertical to the 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 model⁵⁾ and the t - J model⁶⁾ in two dimensions (2D); all three models take the considerably strong correlation between electrons into account.

Recently, it has been experimentally found that the stripe order is stabilized in a wide underdoped region of LSCO at low temperature. From the experiment of resistivity in the light-doping region of LSCO, the system has a metallic behavior below the antiferromagnetic transition temperature, which is considered to originate in the formation of metallic charge stripes.⁷⁾ In addition, the spin-glass state in the insulating phase was found to have a 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, using

a similar computation as in the previous work⁴⁾ 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 moderate¹²⁾ 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,

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

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. $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the creation (annihilation) operator of the electron with spin σ (\uparrow or \downarrow) at sites i ($i = 1 \sim N_s$) and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. N_s is the number of sites. 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 $|\Psi_{\text{coexist}}\rangle = P_{N_e} P_G |\phi_{\text{coexist}}^{\text{MF}}\rangle$. P_G is the Gutzwiller projection operator given by $P_G = \prod_i (1 - (1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$, where g is the Gutzwiller 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 . $|\phi_{\text{coexist}}^{\text{MF}}\rangle$ is a mean-field wave function for the coexisting SC in a stripe SDW state. The mean-field Hamiltonian for $\phi_{\text{coexist}}^{\text{MF}}$ is given by

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

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

$$H_{ij\sigma} = -t_{ij} - \mu + \frac{U}{2} [n_i + \text{sgn}(\sigma)(-1)^{x_i+y_i} m_i] \delta_{r_i, r_j}, \quad (3)$$

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; $Y_l = \text{integer}$ (*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 terms of the d -wave SC gap as $F_{ij} = \sum_{\hat{e}} \Delta_{ij} \delta_{r_j, r_i + \hat{e}}$, 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 $\Delta_{i, i+\hat{y}} = -\Delta \cos(q_y(y_i - Y_l + \hat{y}/2))$. Here, $\mathbf{q} = (0, 2\pi\delta)$ 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 "antiphase" 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 $\Delta_{i, i+\hat{y}} = -\Delta |\cos(q_y(y_i - Y_l + \hat{y}/2))|$.^{4,6)}

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

$$\sum_j \begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F_{ji}^* & -H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} u_j^\alpha \\ v_j^\alpha \end{pmatrix} = E_\alpha \begin{pmatrix} u_i^\alpha \\ v_i^\alpha \end{pmatrix}, \quad (4)$$

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

$$\begin{aligned} \gamma_{\alpha\uparrow} &= u_i^\alpha c_{i\uparrow} + v_i^\alpha c_{i\downarrow}^\dagger & (E_\alpha > 0) \\ \gamma_{\bar{\alpha}\downarrow} &= u_i^{\bar{\alpha}} c_{i\uparrow} + v_i^{\bar{\alpha}} c_{i\downarrow}^\dagger & (E_{\bar{\alpha}} < 0), \end{aligned} \quad (5)$$

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

$$P_G P_{N_e} |\phi_{\text{coexist}}^{\text{MF}}\rangle \sim P_G \left(\sum_{ij} (U^{-1}V)_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger \right)^{N_e/2} |0\rangle, \quad (6)$$

with $(U)_{ij} = u_j^i$ and $(V)_{ij} = v_j^i$ with $i, j = 1, 2, \dots, N_s$.

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 letter, we choose the system parameters $t' = -0.20$ and $U = 8$ suitable for cuprate superconductors such as LSCO. The periodic boundary condition is used in the x -direction, and antiperiodic 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 .

In Fig. 1, we show the minimized total energy per site, E_{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 underdoped 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. The error bars are smaller than the size of symbols. The period of the minimum energy state switches from 12-lattice through to 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 δ for the most stable stripe state tends to deviate to smaller values from the relation of $\delta = x$ as x decreases; when $\delta = x$ is maintained, the hole density along a stripe is equal to $1/2$ per unit length. 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_{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. In this doping region, the total energy of the DS

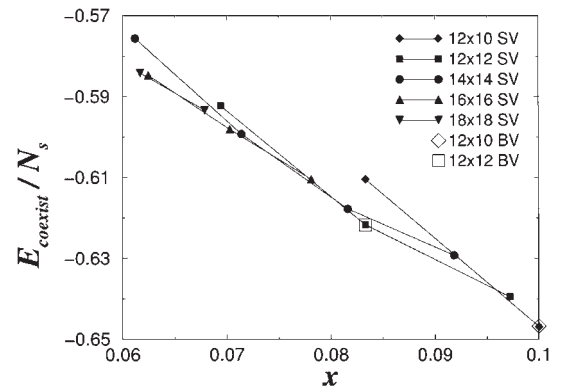


Fig. 1. Total energy of coexistence state of the VS state and d -wave SC as a function of hole-density x for $U = 8$ and $t' = -0.20$. Filled symbols denote the cases of site-centered VS type (SV). The bond-centered VS cases (BV) are represented by open symbols. $n \times m$ denotes the cluster size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

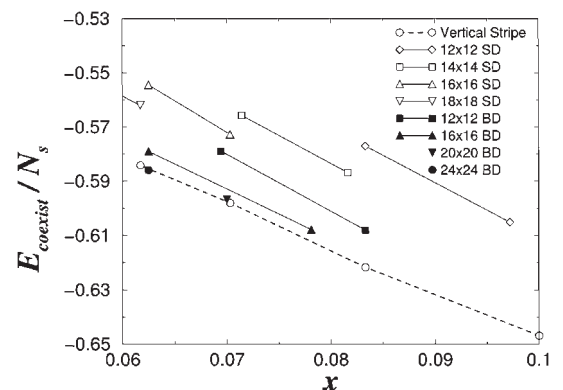


Fig. 2. Total energy per site of the coexistence state of DS and d -wave SC as a function of hole-density x for $U = 8$ and $t' = -0.20$. Open symbols denote for the cases of site-centered DS type (SD). The bond-centered DS cases (BD) are represented by filled symbols. The value of the minimum energy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

state with larger stripe period is lowered. The bond-centered DS state with a 24-lattice period is most stable at $x = 1/16$. The total energy is definitely lower than that for the VS curve by more than the error bar. 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. We also found that the total energy for the bond-centered type is lower than that for the site-centered type for the same stripe's period.

When we calculated the total energy for the DS state, we employed the square-lattice because q boundary condition with periodic spin arrangement is needed in both the x - and y -directions. 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 letter) 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 the 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 Figs. 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; $1/\delta = 36/\sqrt{2} \simeq 0.039$. The total energy is higher in the case of the

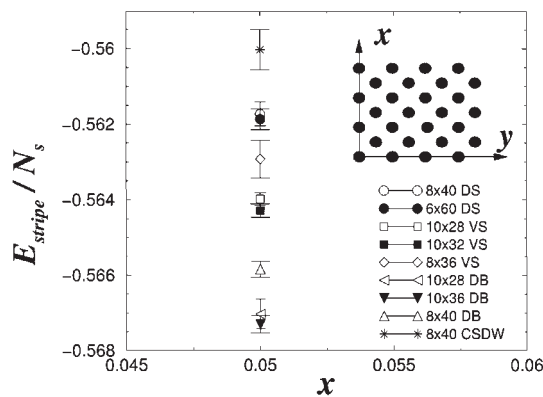


Fig. 3. Total energy for VS (square) state and bond-centered (circle) and site-centered (triangle) DS state against $x = 0.05$. The inset shows the lattice configuration used only in numerical calculations for DS state. Periodic boundary conditions are used in both the x - and y -directions in the inset. 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 as a star.

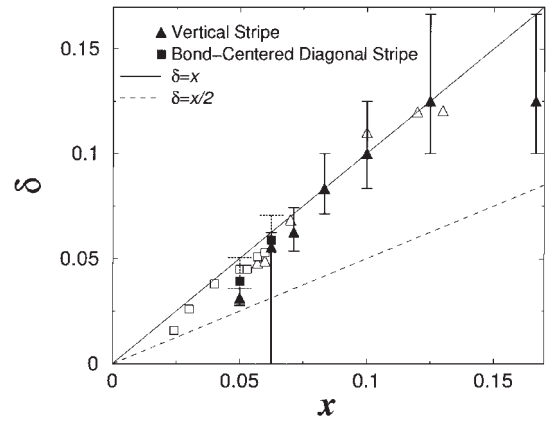


Fig. 4. Incommensurability δ depending on the hole density x for $U = 8$ and $t' = -0.2$. Previous results for $x = 1/6, 1/8, 1/10$ and $1/12$ are included.¹⁵⁾ The numerical result for the VS and the bond-centered DS state are represented by filled triangle and square symbols, respectively. Open triangles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

site-centered DS states than in both 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 a square lattice, in which $\delta = x$ is not maintained.

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 squares and triangles 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 $x_{critical}$ 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 $x_{critical}$: it is thought that the DS state is stabilized in the 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 hand, Giamarchi *et al.* showed that the DS state is stabler when U is larger.³⁾ Therefore, the value of $x_{critical}$ 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 the introduction.¹⁶⁾

We now discuss the relative stability of the bond-centered and site-centered-type 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 the 12-lattice period with $x = 1/12$. In this case the VS state is more stable than the DS

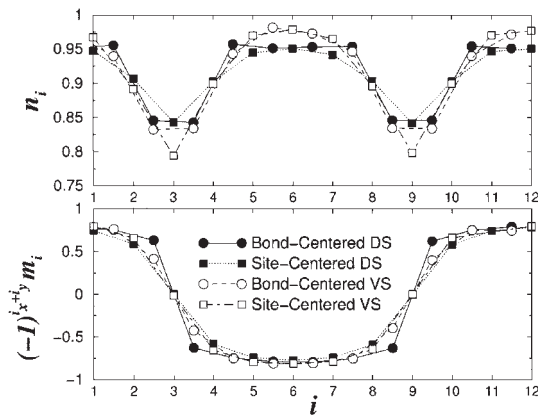


Fig. 5. Charge density n_i and staggered magnetization m_i along the y -direction for 12-lattice period stripes. The stripe center of the bond-centered type is adjusted to that of the site-centered one.

state. Note that calculated values for bond-centered DS and VS states are shifted by 0.5 along the y -direction in order to make it easy to compare with those of the site-centered-type states. n_i and m_i for both the bond-centered and the site-centered VS states take very similar distributions, respectively, which implies that the 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 of the bond-centered VS state as if it tended to earn the kinetic energy. In addition, the magnetic domains outside the stripe region are extended more than those of the site-centered DS state and also more 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 differ from the site-centered one? There is a possibility that these differences result from the effective hopping energy along the 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). The difference between site- and bond-centered-type VS states may be smaller than that between the site- and bond-centered-type DS states 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

particularly 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.

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