Inhomogeneous superconductivity coexisting with SDW stripes in the two-dimensional Hubbard Model

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Abstract

The condensation energy of a spatially inhomogeneous d-wave superconducting (SC) state coexisting with spin-density wave (SDW) stripes is studied by using the Variational Monte Carlo (VMC) method. We calculate its hole-density dependence in the two-dimensional (2D) Hubbard model. With U=8t, it turns out that the coexistent state is the most stable state among other ordered states in the under-doped region. The obtained hole-density dependence of the incommensurability of the coexisting state is in good agreement with the neutron scattering data for $La_{2-x-y}Nd_ySr_xCuO_4$ in a wide region.

Key words: Hubbard model, Variational Monte Carlo, stripe, superconductivity, SDW

The problem of the coexistence of superconductivity (SC) and SDW stripes has attracted great interest. Recently, such a possibility has been experimentally investigated at low temperatures in the under-doped region of the high-T$_c$ superconductors. In the elastic and inelastic neutron scattering experiment with Nd doped $La_{2-x}Sr_xCuO_4$ [1], the incommensurate magnetic scattering spots around (π, π) were observed in the SC phase. It was shown that the incommensurability is proportional to the hole doping x in the low-doping region.

The SC coexisting with striped SDW structure has been theoretically proposed recently [2,3]. We showed that, in the under-doped region ($0.0833 \leq x \leq 0.125$), the SC state can coexist in the vertical stripe state as the ground state of the 2D Hubbard model by using VMC method [3]. We also found that, with decreasing hole doping rate, the decreasing tendency of the SC condensation energy is in accord with that estimated from the specific heat data [4] and the interval of stripes increases in accord with the change of incommensurability in the neutron scattering experiment. The same result was obtained from the calculation by using the d-p model [5]. In this paper, we examine the coexistent state in the 2D Hubbard model by using the VMC method in a wider doping region.

We now consider the 2D Hubbard model on a square lattice $H = -\sum_{i,j,\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + \text{h.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow}$ where the transfer energy $t_{ij} = t, t', 0$, if sites i and j are nearest neighbor, next-nearest neighbor and otherwise, 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, and U is the on-site Coulomb energy.

By using the VMC method, we calculate the variational energy in the coexistent state $E_{\text{coexist}} = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$. The trial wave functions is defined by $|\Psi\rangle = P_{N_e}P_{\text{G}}|\phi^{\text{MF}}_{\text{coexist}}\rangle$ where P_{G} is the Gutzwiller projection operator given by $P_{\text{G}} = \prod_i(1-(1-g)\hat{n}_{i\uparrow}\hat{n}_{i\downarrow})$ with g being a variational parameter in the range from 0 to unity, which controls the on-site electron correlation; P_{N_e} is a projection operator which extracts only the part with a fixed total electron number N_e, $|\phi^{\text{MF}}_{\text{coexist}}\rangle$ is a mean-field wave function for the coexisting superconductivity in a stripe state. The effective mean-field Hamiltonian for the coexistent state is

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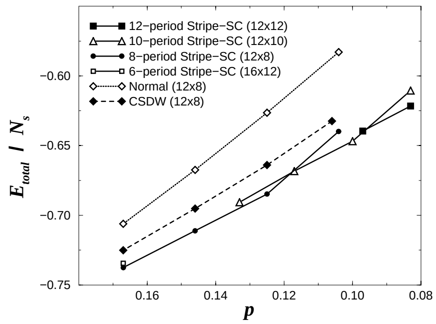

Fig. 1. The optimezed total energy per site as a function of hole density for $t' = -0.20$ and $U = 8$. Filled squares, open up-triangles, filled circles and open square denote the energy of coexistent state for 12-, 10-, 8- and 6-lattice period stripes with the SC state, respectively. Open and closed diamonds denote the normal state and commensurate SDW state, respectively. The error bars are smaller than the size of symbols.

represented by

$$H_{\rm MF} = \sum_{ij} \begin{pmatrix} c^{\dagger}_{i\uparrow} & c_{i\downarrow} \end{pmatrix} \begin{pmatrix} H_{ij\uparrow} & F_{ij} \\ F^{*}_{ji} & -H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c^{\dagger}_{j\downarrow} \end{pmatrix}, \quad (1)$$

where the diagonal terms describe the stripe state with $H_{ij\sigma} = -t_{ij} - \mu + \frac{U}{2}\left[n_i + {\rm sgn}(\sigma)(-1)^{x_i+y_i} m_i\right]\delta_{i,j}$ where μ is the chemical potential. The vertical stripe state is denoted by the charge density n_i and the spin density m_i spatially modulated as $n_i = 1 - \sum_l \alpha/\cosh\left((y_i - Y_l)/\xi_c\right)$ and $m_i = m \prod_l \tanh\left((y_i - Y_l)/\xi_s\right)$ where Y_l denotes the position of a vertical stripe [6]. Amplitude α is fixed by $\sum_i n_i = N_e$. On the other hand, the off-diagonal terms in eq. (1) define the d-wave SC state with $F_{ij} = \sum_{\hat{e}} \Delta_{ij}\delta_{j,i+\hat{e}}$ where $\hat{e} = \pm\hat{x}$ or $\pm\hat{y}$ is a unit vector; we treat the spatially inhomogeneous SC state [2,3] in which the SC amplitude takes the maximum on the stripes and the sign of the parameter Δ_{ij} changes between the nearest stripes, i.e. $\Delta_{i,i+\hat{x}} = \Delta\cos\left(q_y(y_i - Y)\right)$ and $\Delta_{i,i+\hat{y}} = -\Delta\cos\left(q_y\left(y_i - Y + \hat{y}/2\right)\right)$; here $q_y = 2\pi\delta$ and δ is a incommensurability given by the stripe's periodicity in the y direction with regard to the spin. Note the periodicity in charge distribution is half of the spin periodicity. In actual calculations, variational parameters are μ, m, g, ξ_c, ξ_s and Δ. In this paper, we choose the system parameters $t' = -0.20$ and $U = 8$ suitable for cuprate superconductors. The Periodic boundary condition is used in the x-direction, and the anti-periodic one in the y-direction.

In Fig. 1, we show the $E_{\rm coexist}$ per site as a function of hole density p. We evaluate the optimized energy of 6-, 8-, 10- and 12-lattice-period stripe on the 16×12, 12×8, 12×10 and 12×12 lattices, respectively. As a reference, we show the energies of the normal state and the commensurate SDW state without considering the SC ordering in Fig. 1. We find that the periodicity δ of the minimum energy state switches as a function p, being approximately proportional to the doping rate in $1/12 \leq p \leq 1/8$, while the total energy of the 8-lattice period stripe's case (which hardly changes even in the case of 12×16 lattices) is more stable than that of the 6-lattice period stripe's case for $p = 1/6$. This result is in good agreement with the neutron scattering data [1] where the incommensurability is proportional to the Sr concentration x in the range of $0.07 < x < 0.125$ and saturates at $\delta \sim 0.125$ beyond $x \sim 0.12$. We find also that the crossing point of the normal state's line and the 8-lattice period stripe state's line by linear fitting is $p \sim 0.22$. The hole density of the point decreases for smaller U with the stripe's condensation energy decreasing, which was confirmed in the case of $U = 7$ and $t' = -0.20$. This value is close to an intriguing critical point near $x \sim 0.19$ suggested from the specific heat and NMR experiment in the SC phase [4]. In this calculation, however, the size effect cannot be disregarded. The calculation of the size dependence is now in progress.

In conclusion, we have studied the coexistent state of the SC and stripes as the ground state of the 2D Hubbard model in a wide parameter range. The SC phase at very low temperatures of the under-doped region is understandable by the picture of the coexistent state of the inhomogeneous d-wave superconductivity and vertical stripes. The homogeneous d-wave SC state without coexisting with stripe structure is indicated to be realized in the overdoped region [7].

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