Superconducting and SDW condensation energies in the 2D Hubbard model and the meaning to the stripe phase

K. Yamaji*, T. Yanagisawa, S. Koike

Electrotechnical Laboratory, 1-1-4 Umezono, Tsukuba 305-8568, Japan

Abstract

The variational Monte Carlo calculations give a finite bulk-limit value of superconducting (SC) condensation energy $E_{\text{cond}}$ in the 2D Hubbard model with next-nearest-site transfer energy $t'$ when electron density $n \equiv 0.84$ with $-0.25 \leq t' \leq -0.10$; our energy unit is the transfer energy between the nearest-neighbor (n.n.) sites. However, the SDW $E_{\text{cond}}$ computed by the same method is larger than the SC one in such a region. This suggests that the SC region is very restricted, if it exists. When we improved the trial wave function taking into account the n.n.-site correlation, the SC $E_{\text{cond}}$ increased moderately while the SDW $E_{\text{cond}}$ decreased considerably. With this modified variational Monte Carlo method we have found a set of parameter values for which the bulk-limit SC $E_{\text{cond}}$ is finite whereas that for the SDW vanishes. The SC $E_{\text{cond}}$ obtained in both ways around the optimal doping is in fair agreement with the experimental value $\sim 0.26$ meV/site for YBCO estimated from the specific heat and the critical magnetic field, in contrast to the case of the $t-J$ model which gives a value larger by almost two orders of magnitude. In the low-doping region the SDW $E_{\text{cond}}$ is overwhelmingly larger than the SC $E_{\text{cond}}$. Further, the striped SDW state seems more stable here. This is considered to be the energetic origin of the stripe features and presumably of the consequent pseudogap in the underdoped region. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

In the context of the mechanism of superconductivity in high-temperature cuprate superconductors and organic superconductors, the 2D Hubbard model is one of the most fundamental ones. Early numerical studies of this model showed the existence of an attractive interaction for an anisotropic pairing [1]. However, this possibility has been notoriously controversial [2–8]. Some authors support it by numerical results using the variational Monte Carlo (M.C.) method [4] and the quantum M.C. methods [5,6]. Some authors have asserted from quantum M.C. results that the enhanced superconducting (SC) correlation does not develop into the predominant one at low temperatures or in the ground state of this model [2,3,7,8].

2. Our preceding results

In preceding works [9–11] we have studied this problem by means of the variational M.C. method, since this method allows us to treat moderate-to-large values of on-site Coulomb energy $U$, important in the consideration of realistic situations, and also allows us to treat large lattice sizes so that we can obtain bulk-limit properties. We computed the energy gain in the $s$-, extended $s$- and $d$-wave SC states in reference to the normal state, i.e. SC condensation energy (condensation energy per site is denoted as $E_{\text{cond}}$). Only the $d$-wave SC state proved to have a positive energy gain. The energy gain was found to become largest around $U = 7$ (our energy unit is the nearest-neighbor (n.n.) transfer energy $t$). It was also found to increase sharply when the next n.n. transfer energy $t'$ takes an appropriate negative value in accordance with a preceding work [5]. In order to investigate the system size dependence of the result, we have extended such calculations to the lattices of $8 \times 8 \sim 22 \times 22$ sites with fixed electron density $n \equiv 0.80, 0.84$ and 0.86 with $t' = -0.25$ to 0 for fixed $U = 8$ [11]. The obtained energy gain per site in the SC state in reference to the normal state, i.e. SC $E_{\text{cond}}$, was found to be linearly fitted with the inverse of the number of lattice sites in the main cases and to be extrapolated to a finite value in the bulk limit; in

* Corresponding author. Tel.: +81-298-61-5368; fax: +81-298-61-5099.
E-mail address: yamaji@etl.go.jp (K. Yamaji).

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Fig. 1. SC and SDW condensation energies $E_{\text{cond}}$ as functions of electron density $\rho$ calculated by the unmodified variational M.C. method for the $10 \times 10$ lattice with a few values of $t'$ indicated by the labels shown in the inset.

particular, 0.00117/site in the case of electron density $\rho = 0.86$ with $t' = -0.20$ (Fig. 1 in Ref. [11]). The bulk-limit was found to remain finite in the cases where electron density $\rho \geq 0.84$ and $-0.25 \leq t' \leq -0.10$. The above-mentioned theoretical SC condensation energy is equal to 0.60 meV if we note $t \sim 0.5$ eV [12], which is remarkably close to the experimental value for the optimally doped YBa$_2$Cu$_3$O$_{7-y}$, i.e. 0.26 meV/[Cu site], obtained from the critical magnetic field $H_c$ [13] and 0.17 meV/[Cu site] from specific heat data [14]. The above-mentioned values of $U$ and $t'$ are close to the appropriate ones for YBa$_2$Cu$_3$O$_7$ [12]. This agreement strongly indicates the relevance of the 2D Hubbard model as the model of high-$T_c$ cuprate superconductors. On the other hand, it questions the validity of the corresponding $t$–$J$ model, at least around the optimal doping. This model gives a value larger than the experimental one by almost two orders of magnitude [15,10].

3. Competition with the SDW

It is known that in the hole-doped region the SDW state extends to quite a wide region. We have checked the competition between the SC state obtained in the above-mentioned way and the SDW state, computing the SDW condensation energy similarly by the variational M.C. method. In the cases with $\rho \geq 0.84$ and $-0.25 \leq t' \leq -0.10$, where we obtained a finite bulk-limit SC $E_{\text{cond}}$, the SDW $E_{\text{cond}}$ was

Fig. 2. $t'$-dependence of the SDW $E_{\text{cond}}$ in the case of $\rho = 0.84$ and the $10 \times 10$ lattice for three values of $U$. 
Fig. 3. Critical value $t'_c$ of $t'$ as a function of length $L$ of the edge of the lattice calculated by the modified variational M.C. method which introduces n.n. correlation parameter $h$. The fitting curve is defined by the equation in the figure and gives the bulk-limit $t'_c = -0.0475$.

4. Improvement of the trial wave functions taking into account the n.n. correlation

When we improved the trial wave function by taking into account the n.n-site correlation, the total energy of the system lowered appreciably and the value of the SC $E_{\text{cond}}$ increased moderately while the SDW $E_{\text{SDW}}$ decreased so much that there appeared a good prospect of getting a parameter region where the bulk-limit SC $E_{\text{cond}}$ dominates the SDW $E_{\text{SDW}}$. Our model and method are basically the same as in the preceding works [9–11]. The model is the 2D Hubbard model that has both the n.n. and next n.n. transfer terms with coefficients $-t$ and $-t'$, respectively, as well as the Coulomb interaction term with $U$. Our trial wavefunction for the SC state is a Gutzwiller-projected BCS-type wavefunction defined by

$$\Psi_{\text{BCS}} = P_N \Pi_{\gamma \neq 0} P_G \psi_{\text{BCS}}, \quad (1)$$

where $\psi_{\text{BCS}}$ is the standard BCS-type wavefunction given in, e.g. Ref. [10], with a $k$-dependent gap function $\Delta_k$ defined by

$$\Delta_k = \Delta (\cos k_x - \cos k_y), \quad (2)$$

with $\Delta$ being a variational parameter; $\psi_{\text{BCS}}$ contains another variational parameter $\mu$, chemical potential, $P_G$ is the Gutzwiller projection operator defined by

$$P_G = \Pi_l (1 - (1 - g)n_l n_{\bar{l}}), \quad (3)$$

where $g$ is a variational parameter in the range from 0 to unity and $n_{\bar{l}}$ is the number operator for site $l$ and spin state $\sigma$; the second factor is a newly introduced Gutzwiller-like operator allowing the occupancy of the n.n. sites to be modified by adjusting $h$ in the range between 0 and 1; $P_{N_h}$ is a projection operator which extracts only the states with a fixed total electron number $N_e$. The ground state energy

$$E_g = \langle H \rangle = \langle \Psi_s | H | \Psi_s \rangle = \langle \Psi_s | \Psi_s \rangle \quad (4)$$

is calculated using a M.C. procedure. The boundary conditions along the $x$- and $y$-axes are periodic and anti-periodic, respectively; the allowed $k$-points are $(\pm 2\pi j/L, \pm 1/mL)$ with $j = 0, 1, \ldots, L/2 - 1$ and $l = 1, 3, \ldots, L - 1$ for the $L \times L$ lattice ($L$ is assumed even). We minimized $E_g$ while optimizing the variational parameters, $g$, $h$, $\Delta$, and $\mu$, by means of the correlated measurements method and finally calculated $E_g$ for the optimal set of values with $\sim 2 \times 10^8$ M.C. steps.

The trial wave function for the SDW state is given by [10]

$$\Psi_{\text{SDW}} = \Pi_{\gamma \neq 0} h^{n_{\gamma \neq 0}} P_G \psi_{\text{SDW}}, \quad (5)$$

$$\psi_{\text{SDW}} = \Pi_k (u_k c^\dagger_k + v_k c^\dagger_{-k+Q}) \times \Pi_k (u_k c^\dagger_k - v_k c^\dagger_{-k+Q}), \quad (6)$$
Fig. 4. SC $E_{\text{cond}}$ for the $\rho = 0.82$, $U = 7$ and $t' = -0.045$ is plotted as a function of the inverse of the number $N_s$ of sites. The fitting curve is defined by the equation in the figure and gives the bulk-limit $E_{\text{cond}} = 0.001355$.

$$u_k = \left(1 - w_k / \sqrt{w_k^2 + M^2}\right)^{1/2}$$

$$v_k = \left(1 + w_k / \sqrt{w_k^2 + M^2}\right)^{1/2}$$

$$w_k = \frac{\epsilon_k - \epsilon_{k+0}}{2}$$

$$\epsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$$

Product over $k$ and $k'$ is performed over the filled $k$-points. $u_k$ and $v_k$ for $k$-points in the upper-band above the SDW gap are modified to $\tilde{u}_k = v_k$ and $\tilde{v}_k = -u_k$, respectively. The procedure to get the lowest total energy is similar. In this work we fixed $Q = (\pi, \pi)$.

This approximation scheme increased the SC $E_{\text{cond}}$, e.g. in the case of $\rho = 0.84$, $U = 8$, $t' = -0.1$ for the $10 \times 10$ lattice from 0.0033 to 0.0051, while it decreased the SDW $E_{\text{cond}}$, e.g. in the same case from 0.0175 to 0.0037. The SDW region was found to get a clear-cut boundary even in the bulk limit, as is shown in Fig. 3 for the critical value $t_c'$ as a function of the length $L$ of the square edge in the case of $\rho = 0.82$, $U = 7$ and $10 \times 10$ lattice. When $t'$ is slightly larger than the bulk-limit $t_c'$, the SC $E_{\text{cond}}$ takes considerable values and a finite bulk-limit SC $E_{\text{cond}}$ looks possible. In fact for $t' = -0.045$ the bulk-limit of the SC $E_{\text{cond}}$ was found to be finite as in Fig. 4. Further, when we brought in a finite n.n.-site Coulomb interaction, its detrimental effect was found to be stronger on the SDW than the SC state, favoring the SC phase to the SDW phase. This situation encourages our expectation that outside the SDW-dominating region we have a considerably wide SC region where the bulk-limit SC $E_{\text{cond}}$ is larger than that for the SDW.

5. Reasoning on the SC phase in the underdoped region

The above results indicate that a uniform pure superconducting phase is possible only in the highly doped region beyond a critical degree of doping $\delta_c$ existing around the optimal doping level. In the region below $\delta_c$ we expect to have an SDW phase, which has an overwhelmingly larger condensation energy. Furthermore, this commensurate SDW state is known to be dominated by the striped SDW state in the low-doping region at least up to 0.10 (e.g. Ref. [16]). However, we have a superconducting phase in the region from the optimal doping level to a quite low-doping level. Energetic consideration gives ground to a hypothesis that in this region the dominant electronic structure is striped SDW, may it be static or dynamically fluctuating, and that the current-carrying channels along the stripes become superconducting. Anomalies in the underdoped region in both the anomalous metallic and SC regions are considered to arise in such a spatially non-uniform situation.

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References