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Journal of Physics and Chemistry of Solids 62 (2001) 237–241

JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS

www.elsevier.nl/locate/jpcs

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

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Abstract

The variational Monte Carlo calculations give a finite bulk-limit value of superconducting (SC) condensation energy E_{cond} in the 2D Hubbard model with next-nearest-site transfer energy t' when electron density $\rho \geq 0.84$ 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_{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_{cond} increased moderately while the SDW E_{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_{cond} is finite whereas that for the SDW vanishes. The SC E_{cond} obtained in both ways around the optimal doping is in fair agreement with the experimental value ~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_{cond} is overwhelmingly larger than the SC E_{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.

Keywords: D. Superconductivity; D. Thermodynamical properties

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 supported 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_{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 $\rho = 0.80$, 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_{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

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0022-3697/00/$ - see front matter
PII: S0022-3697(00)00136-0

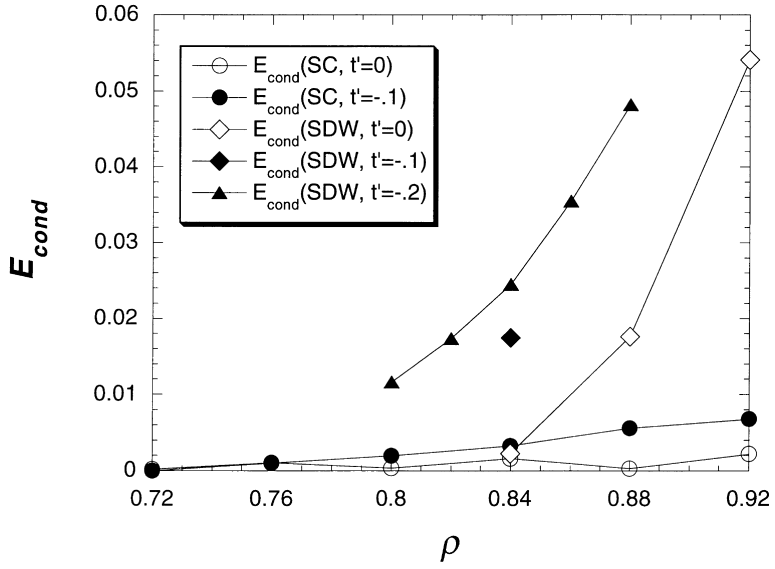

Fig. 1. SC and SDW condensation energies E_{cond} as functions of electron density ρ calculated by the unmodified variational M.C. method for the 10×10 lattice with a few values of t' indicated by the labels shown in the inset.

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 $YBa_2Cu_3O_7$, 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 $YBa_2Cu_3O_7$ [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_{cond}, the SDW E_{cond} was

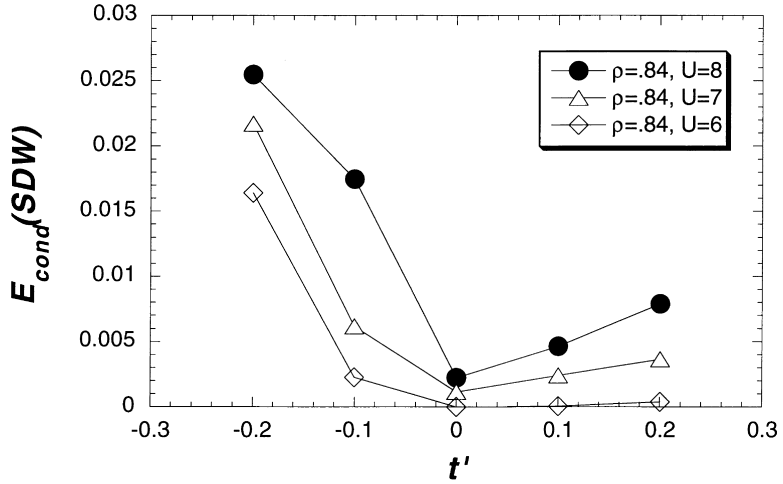

Fig. 2. t'-dependence of the SDW E_{cond} in the case of $\rho = 0.84$ and the 10×10 lattice for three values of U.

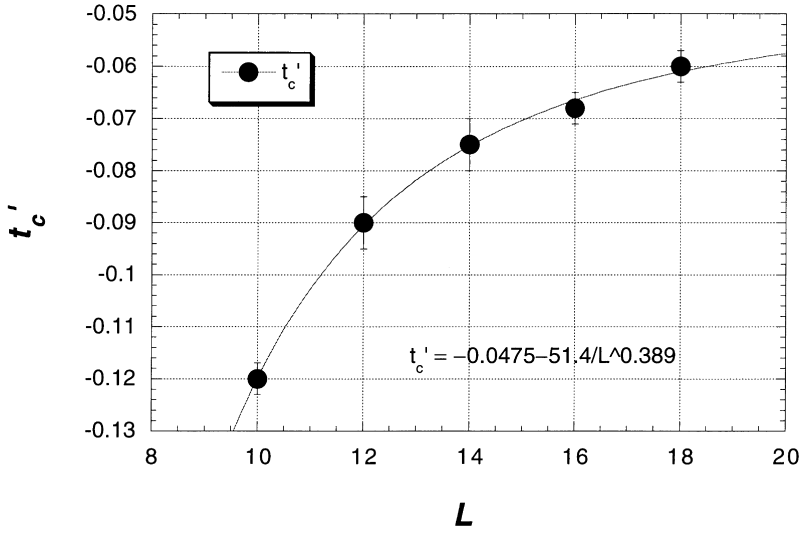

Fig. 3. Critical value $t_c{}'$ of t' as a function of length L of the edge of the lattice calculated by the modified variational M.C. method which introduces n.n. correlation parameter h. The fitting curve is defined by the equation in the figure and gives the bulk-limit $t_c' = -0.0475$.

much larger than the SC E_{cond} (Fig. 1). Also we found that the SDW E_{cond} increases quite sharply with an increase of the absolute value of negative t' (Fig. 2). This tendency is contrary to our previous observation [10]; this difference came from the present slightly modified SDW trial wave function in which the electron filling to the **k**-points was improved. Generally, in the highly doped region the SDW disappears but this boundary is close to that where the bulk-limit SC E_{cond} vanishes. Another prominent feature is that the SDW E_{cond} increases with decreasing doped hole density more sharply than the SC E_{cond}. Since both boundaries are not identical, we have been looking for a parameter region where the SC E_{cond} is larger than the SDW E_{cond}.

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_{cond} increased moderately while the SDW E_{cond} decreased so much that there appeared a good prospect of getting a parameter region where the bulk-limit SC E_{cond} dominates the SDW E_{cond}. 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

$$\Psi_{\mathrm{s}} = P_{N_{\mathrm{e}}} \prod_{\langle ij \rangle} h^{n_i n_j} P_{\mathrm{G}} \psi_{\mathrm{BCS}}, \tag{1}$$

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

$$\Delta_{\mathbf{k}} = \Delta(\cos k_x - \cos k_y), \tag{2}$$

with Δ being a variational parameter; ψ_{BCS} contains another variational parameter μ, chemical potential, P_{G} is the Gutzwiller projection operator defined by

$$P_{\mathrm{G}} = \Pi_l (1 - (1 - g) n_{l\uparrow} n_{l\downarrow}), \tag{3}$$

where g is a variational parameter in the range from 0 to unity and $n_{l\sigma}$ is the number operator for site l and spin state σ; 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; $P_{N_{\mathrm{e}}}$ is a projection operator which extracts only the states with a fixed total electron number N_{e}. The ground state energy

$$E_{\mathrm{g}} = \langle H \rangle \equiv \langle \Psi_{\mathrm{s}} | H | \Psi_{\mathrm{s}} \rangle / \langle \Psi_{\mathrm{s}} | \Psi_{\mathrm{s}} \rangle \tag{4}$$

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 $(\pm 2\pi j/L,\ \pm l\pi/L)$ 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, Δ and μ, 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]

$$\Psi_{\mathrm{SDW}} = \prod_{\langle ij \rangle} h^{n_i n_j} P_{\mathrm{G}} \psi_{\mathrm{SDW}}, \tag{5}$$

$$\psi_{\mathrm{SDW}} = \prod_{\mathbf{k}} (u_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}+\mathbf{Q}\uparrow}) \times \prod_{\mathbf{k}'} (u_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}'\downarrow} - v_{\mathbf{k}'} c^{\dagger}_{\mathbf{k}'+\mathbf{Q}\downarrow}) 0\rangle, \tag{6}$$

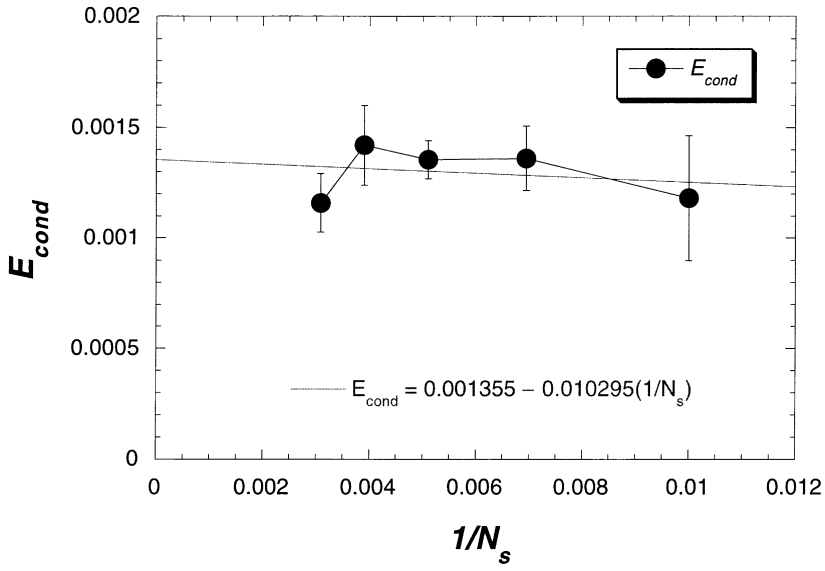

Fig. 4. SC E_{cond} for the $\rho = 0.82$, $U = 7$ and $t' = -0.045$ is plotted as a function of the inverse of the number N_s of sites. The fitting curve is defined by the equation in the figure and gives the bulk-limit $E_{\mathrm{cond}} = 0.001355$.

$$u_{\mathbf{k}} = \left[\frac{(1 - w_{\mathbf{k}}/\sqrt{w_{\mathbf{k}}^2 + M^2})}{2} \right]^{1/2}, \tag{7}$$

$$v_{\mathbf{k}} = \left[\frac{(1 + w_{\mathbf{k}}/\sqrt{w_{\mathbf{k}}^2 + M^2})}{2} \right]^{1/2}, \tag{8}$$

$$w_{\mathbf{k}} = \frac{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{Q}})}{2}, \tag{9}$$

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y. \tag{10}$$

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

This approximation scheme increased the SC E_{cond}, e.g. in the case of $\rho = 0.84$, $U = 8$, $t' = -0.1$ for the 10×10 lattice from 0.0033 to.0051, while it decreased the SDW E_{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 10×10 lattice. When t' is slightly larger than the bulk-limit $t_c{}'$, the SC E_{cond} takes considerable values and a finite bulk-limit SC E_{cond} looks possible. In fact for $t' = -0.045$ the bulk-limit of the SC E_{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_{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 δ_c existing around the optimal doping level. In the region below δ_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.

Acknowledgements

The computations were performed mainly on the massively parallel computer of University of Tsukuba and partly on a facility provided by the ACT-JST.

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