Physica C 469 (2009) 974–978

Contents lists available at ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

Interplay between antiferromagnetism and superconductivity in the Hubbard model with frustration

Kenji Kobayashi [a,*], Hisatoshi Yokoyama [b]

[a] Department of Natural Sciences, Chiba Institute of Technology, Shibazono, Narashino, Chiba 275-0023, Japan
[b] Department of Physics, Tohoku University, Sendai 980-8578, Japan

ARTICLE INFO

Article history:
Accepted 23 February 2009
Available online 31 May 2009

PACS:
71.10.Fd
74.20.Mn
74.25.Dw

Keywords:
Hubbard model
Variational Monte Carlo method
Superconductivity
Cuprate

ABSTRACT

Coexistence of and competition between antiferromagnetism (AF) and *d*-wave superconductivity (SC) are studied for a Hubbard model on the square lattice with a diagonal transfer t', using a variational Monte Carlo method. The following improvements are introduced into the trial function: (1) Coexistence of AF and *d*-wave singlet gaps that allows a continuous description of their interplay, (2) band renormalization effect, and (3) refined doublon–holon correlation factors. Optimizing this function for a strongly correlated value of U/t, we construct a phase diagram in the δ (doping rate)-t'/t space, and find that for $t'/t \geqslant -0.15$ a coexisting state is realized, whose range of δ extends as t'/t increases. In contrast, for $t'/t = -0.3$, AF and SC states are mutually exclusive, and a coexisting state does not appear. In connection with the "two-gap" problem, we confirm even for the present refined function that the gradient of momentum distribution function at the antinodal point mainly dominates the magnitude of the *d*-wave SC correlation function.

1. Introduction

Since the proximity of antiferromagnetic and superconducting phases is a feature universal to all cuprate superconductors, it is appropriate to consider that the origin of the two phases should be identical, probably the antiferromagnetic spin correlation. In most experiments of cuprates, however, these two phases are mutually exclusive and do not microscopically coexist [1]. Meanwhile, a recent NMR experiment for a multi-layered cuprate argued that the two phases coexist in a single CuO_2 (outer) plane owing to its extreme flatness as compared with other cuprates [2]. This discrepancy concerning the coexistence gives a key to mechanism of high-T_c superconductivity (SC), and is now actively investigated [3]. Another motivation of this study is the so-called "two gap" problem. Although it has been an orthodox interpretation that the pseudo gap is an incoherent singlet gap as a precursor of SC, recent experiments by different means found that the gap in the underdoped regime exhibits an opposite δ (hole doping rate) dependence between the nodal ($\mathbf{k} \sim (\pi/2, \pi/2)$) and antinodal ($\mathbf{k} \sim (\pi, 0)$) regions [4], leading to intensive arguments whether this different δ dependence is explained by a single gap or by two [5]. An important clue to this problem was provided by very recent experiments of angle-resolved photoemission spectroscopy and scanning tunneling microscopy [6], which found two kinds of (pseudo)gaps near the antinodal point. One of them is related to the SC gap, and the other may be of other origins such as charge inhomogeneity.

Previous theoretical studies on the coexistence using variational Monte Carlo (VMC) methods for the Hubbard and *t*-*J* models [7–10] drew conclusions that coexisting states are stabilized for small doping rates ($\delta \lesssim 0.1$). On the other hand, a recent study by cellular dynamical mean field calculations for the Hubbard model argued that at strong coupling ($U \gtrsim 8t$) the two phases do not mix [11]. Thus, it is important to clarify the stability of coexisting states as a function of U/t, t'/t and δ in theory. In this work, we consider the above two problems using a VMC method [12], which is useful to reliably treat a wide range of parameters in correlated systems. We adopt a wave function improved on a previous one [13] to properly describe the interplay between antiferromagnetism (AF) and SC, and applied it to the Hubbard model to link weak and strong coupling (*t*-*J* model) regimes. In a preceding publication [14], the present authors have checked U/t dependence of the stability of coexisting state for $t'/t = -0.3$ within the same formulation; for $U \lesssim 2W$ ($W \sim 8t$: band width), the pure AF state is more stable than the SC state, whereas for $U \gtrsim 2W$ an area of pure SC appears in the phase diagram. In this article, we focus on

* Corresponding author. Address: Department of Natural Sciences, Chiba Institute of Technology, 2-1-1, Shibazono, Narashino, Chiba 275-0023, Japan. Tel./fax: +81 47 454 9605.
E-mail address: koba@sun.it-chiba.ac.jp (K. Kobayashi).

0921-4534/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.physc.2009.02.017

strongly correlated cases, fixing U at a typical value $30t$ (>2 W), and study the δ and t'/t dependence.

2. Method

We consider the Hubbard model on a square lattice with the next–nearest–neighbor transfer t',

$$\mathscr{H} = \mathscr{H}_{\rm kin} + \mathscr{H}_U = \sum_{\mathbf{k}\sigma} \varepsilon(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow}, \tag{1}$$

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

Eq. (1) with $t'/t < 0$ represents the hole-doped high-T_c cuprates, and electron-doped (more-than-half-filled) ones can be treated as less-than-half-filled systems with $t'/t > 0$ owing to a particle-hole transformation. We use t as the unit of energy and the lattice constant as the unit of distance. To this model, we apply an optimization VMC (or correlated measurement) method [15], which can effectively optimize the parameters in the whole range of U/t.

As a variational wave function, we use a Jastrow type, $\Psi = \mathscr{P}_Q \mathscr{P}_G \Phi$, where $\mathscr{P}_G$ is the Gutzwiller (on-site) projector, and $\mathscr{P}_Q$ the doublon–holon binding factor[16]. The following improvements are introduced into the wave function, as in the preceding work [14]: (1) coexistence of AF and d-wave singlet gaps to directly check the cooperation or competition between them [7–10], (2) band renormalization effect owing to electron correlation by adjusting hopping integrals in Φ, and (3) refined doublon–holon correlation factors, which control the effect of Mott transition near half-filling more precisely [16,17].

As the one-body part Φ in Ψ, we use a $d_{x^2-y^2}$-wave singlet state with a nearest–neighbor pairing gap $\tilde{\Delta}_d$ for N_e electrons

$$\Phi = \left(\sum_{\mathbf{k}} \varphi_{\mathbf{k}} b^\dagger_{\mathbf{k}\uparrow} b^\dagger_{-\mathbf{k}\downarrow} \right)^{\frac{N_e}{2}} |0\rangle, \tag{2}$$

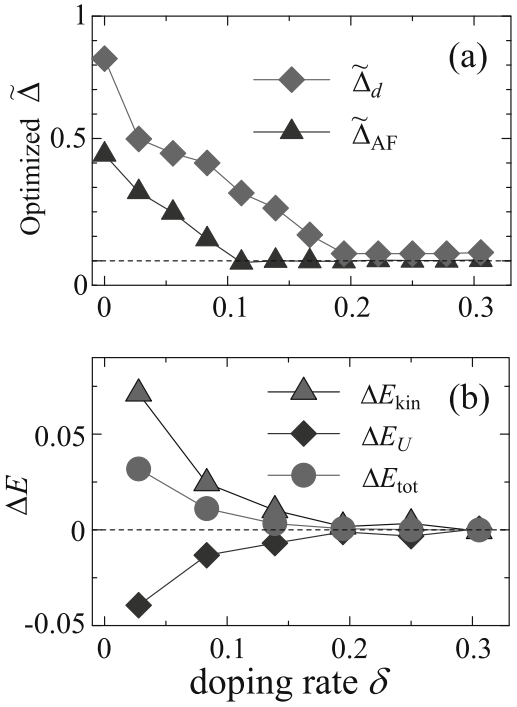

Fig. 1. (a) Optimized values of gap variational parameters in Ψ as a function of δ. (b) Difference in total energy between optimized gapped and non-ordered ($\tilde{\Delta}_d = \tilde{\Delta}_{\rm AF} = 0$) states [Eq. (3)], and its kinetic ($\Delta E_{\rm kin}$) and interaction (ΔE_U) components. The data in both panels are for $t'/t = 0$ and $U/t = 30$.

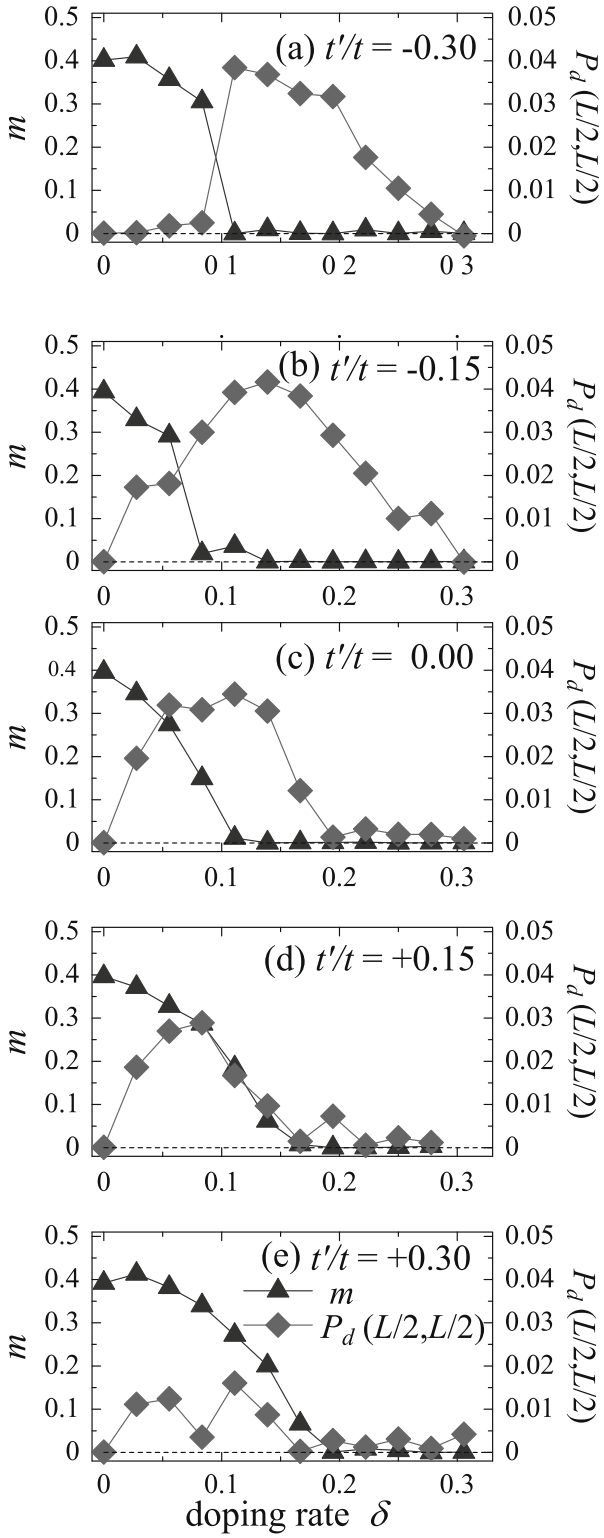

Fig. 2. By using the optimized Ψ, the expectation values of staggered magnetization m (triangles) and d-wave nearest-neighbor pair correlation function $P_d(\mathbf{r})$ for the farthermost distance $\mathbf{r} = (L/2, L/2)$ (diamonds) are plotted as a function of δ for $U/t = 30$. The values of t'/t differ among the five panels.

where

$$\varphi_{\mathbf{k}} = \frac{\Delta_d(\mathbf{k})}{\tilde{\varepsilon}_{\mathbf{k}} - \tilde{\zeta} + \sqrt{(\tilde{\varepsilon}_{\mathbf{k}} - \tilde{\zeta})^2 + |\Delta_d(\mathbf{k})|^2}},$$