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ScienceDirect
Physica C 463–465 (2007) 141–145
PHYSICA C
www.elsevier.com/locate/physc

Improved wave functions for Hubbard model: Superconductivity and Mott transition

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Accepted 26 January 2007
Available online 6 June 2007

Abstract

We extend the doublon–holon binding wave function, which was recently often used to consider Mott transitions and $d_{x^2-y^2}$-wave superconductivity, for the half-filled-band Hubbard model on square lattices with the diagonal hopping t'. We introduce two new features: (1) In the doublon–holon binding factor, more accurate configuration correlations are included. (2) The band renormalization effect owing to the electron correlation is introduced within the third-neighbor hopping, including the anisotropy between x- and y-directions in the nearest-neighbor hopping. Using an optimization variational Monte Carlo technique, we draw some definite answers to the topics concerning the above features.

PACS: 71.10.Fd; 71.30.+h; 74.20.Mn

Keywords: Hubbard model; Variational Monte Carlo method; Mott transition; Cuprate

1. Introduction

To study strongly-correlated electron systems like the cuprate superconductors, the optimization variational Monte Carlo (VMC) method is quite effective, because it can treat the local correlation accurately. To the Hubbard model, the famous Gutzwiller (on-site) projector $\mathscr{P}_G$ [1] has been applied for long time, and yielded some useful results. However, it was revealed that the single use of $\mathscr{P}_G$ sometimes leads to unphysical results [2,3]. Particularly at half filling, $\mathscr{P}_G$ cannot describe a Mott transition. Thanks to the recent rapid progress in optimization techniques for multiparameters in VMC calculations [4], the improved wave functions we propose have been practically feasible. By adopting a doublon–holon binding factor $\mathscr{P}_Q$ [5] in addition to $\mathscr{P}_G$, Mott transitions were successfully understood within the variation theory [6]. In contrast to the Brinkman-Rice transition [7], this transition is the first-order, and in the insulating regime the energy behaves as $\propto -t^2/U$, which is desirable in the strong-coupling theory. Furthermore, it was found that robust superconductivity (SC) occurs immediately below the Mott critical point U_c [8], if antiferromagnetism (AF) is excluded by some means.

In this study, we extend the wave function used in the previous study [8] for the two-dimensional Hubbard model with next-nearest-neighbor transfer, and solve it accurately using the optimization VMC method. Two features are newly introduced into the wave function: (1) In the doublon–holon binding factor, more accurate configuration correlations are considered. (2) Band renormalization effect owing to the electron correlation is considered within the third-neighbor hopping including the anisotropy between x- and y-directions in the nearest-neighbor hopping. Consequently, it is found that the doublon–multiholon binding is less advantageous than the doublon-to-single-holon binding. In the quasi-Fermi surface (effective Fermi surface

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doi:10.1016/j.physc.2007.01.067

of the renormalized band), the nesting condition is almost recovered in the insulating regime, and the anisotropy between x- and y-directions cannot be detected.

2. Method

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

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

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

In the following, we concentrate on the case of half-filled band ($n = N_{\rm e}/N_{\rm s} = 1$; $N_{\rm e}$: electron number and $N_{\rm s} = L \times L$: site number), and $t'/t = -0.4$; we adopt a somewhat large magnitude of t' for cuprate SC to emphasize the effect of frustration. Here, we chiefly consider the U/t dependence of ground-state properties. We use t as the unit of energy in the following.

To this model, we apply an optimization VMC method [4] that can correctly treat the local correlation in the whole range of U/t. As a variational wave function, we use a projected BCS state with d-wave pairing symmetry:

$$\Psi_{\rm d} = \mathscr{P}_Q \mathscr{P}_{\rm G} \Phi_{\rm d}, \quad (3)$$

where $\mathscr{P}_{\rm G}$ is the famous Gutzwiller (on-site) projector,

$$\mathscr{P}_{\rm G} = \prod_i [1 - (1-g)|\uparrow\downarrow_i\rangle\langle\uparrow\downarrow_i|], \quad (4)$$

and $|\gamma\rangle\langle\gamma|$ is a projection operator to extract the configuration γ. We extend the doublon–holon binding factor $\mathscr{P}_Q$ as follows:

$$\mathscr{P}_Q = \prod_{i,\ell} [1 - (1 - q_{n_{{\rm e},\ell}})|\uparrow\downarrow_i, n_{{\rm e},\ell}\rangle\langle\uparrow\downarrow_i, n_{{\rm e},\ell}|] \times [1 - (1 - q_{n_{{\rm d},\ell}})|0_i, n_{{\rm d},\ell}\rangle\langle 0_i, n_{{\rm d},\ell}|], \quad (5)$$

where $|\uparrow\downarrow_i, n_{{\rm e},\ell}\rangle$ represents a doubly occupied state at the site i with $n_{\rm e}$ empty sites (holons) in the four ℓ-th nearest neighbors, and $|0_i, n_{{\rm d},\ell}\rangle$ an empty state with $n_{\rm d}$ doubly-occupied sites (doublons) in the four ℓ-th nearest neighbors. Thus, $n_{\rm e}$, $n_{\rm d} = 0$, 1, 2, 3 or 4. The variational parameter

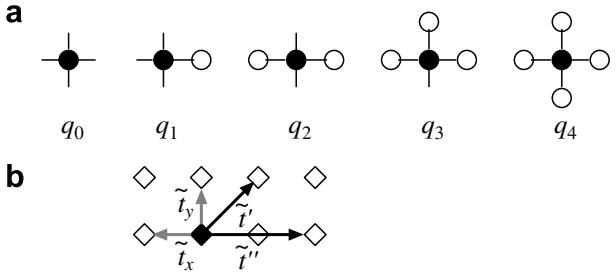

Fig. 1. (a) Weight of doublon–holon binding projector q_n according to local electron configuration. Closed [open] circles indicate doubly-occupied sites (doublons) [empty sites (holons)], and open bonds indicate singly occupied sites or doublons. (b) Hopping terms which are optimized in $\tilde{\varepsilon}_{\mathbf{k}}$ in the variational wave function to allow for the band renormalization effect.

q_γ controls the probability weight of the configuration γ, as shown in Fig. 1a. For example, q_3 with $\ell = 2$ indicates the probability weight of the doublon (holon) site with three holon (doublon) sites in the four next–nearest–neighbors. Because at half filling the relation between a doublon and a holon is symmetric, the weights for a doublon site and a holon site are identical, $q_{n_{\rm e}} = q_{n_{\rm d}} (\equiv q_n)$ in Eq. (5), if $n_{\rm e} = n_{\rm d}$. In the present work, q_n ($n = 0, \ldots, 4$) are independently optimized for $\ell = 1$, 2, namely, for the nearest and second (diagonal) neighbors. In the previous studies [5,6,8,9], $q_1 = q_2 = q_3 = q_4 = 1$ and only q_0 is optimized with the relation to the present notation as $q_0 = 1 - \mu$.

Regarding a one-body part, we adopt a singlet wave function in a form of the BCS function with a $d_{x^2-y^2}$-wave gap [$\Phi_{\rm d}$ in Eq. (3)]:

$$\Phi_{\rm d} = \left(\sum_{\mathbf{k}} \varphi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \right)^{\frac{N_{\rm e}}{2}} |0\rangle, \quad (6)$$

$$\varphi_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{\tilde{\varepsilon}_{\mathbf{k}} - \tilde{\zeta} + \sqrt{(\tilde{\varepsilon}_{\mathbf{k}} - \tilde{\zeta})^2 + \Delta^2_{\mathbf{k}}}}, \quad (7)$$

with

$$\tilde{\varepsilon}_{\mathbf{k}} = -2(\tilde{t}_x \cos k_x + \tilde{t}_y \cos k_y) - 4\tilde{t}' \cos k_x \cos k_y - 2\tilde{t}''[\cos(2k_x) + \cos(2k_y)], \quad (8)$$

and $\Delta_{\mathbf{k}} = \tilde{\Delta}(\cos k_x - \cos k_y)$. Here, $\tilde{\zeta}$, $\tilde{\Delta}$, $\tilde{t}_x$, $\tilde{t}_y$, $\tilde{t}'$, and $\tilde{t}''$ are variational parameters to be optimized. $\tilde{\zeta}$ corresponds to the chemical potential in the BCS theory. Although the parameter $\tilde{\Delta}$ indicates the magnitude of the d-wave gap, it does not necessarily mean the realization of SC; in the insulating phase, $\tilde{\Delta}$ is related to the pseudo gap [10]. In this study, we take account of a renormalization effect of the quasi-Fermi surface owing to the electron correlation. In a previous study for an anisotropic triangular lattice [9], conspicuous renormalization of $\tilde{t}'$ has been observed in the insulating regime. In this study, in addition to the contribution of $\tilde{t}'$, we include that of $\tilde{t}''$ in $\Phi_{\rm d}$. Furthermore, we allow for the asymmetry between the nearest-neighbor hoppings in x- and y-directions through $\tilde{t}_x$ and $\tilde{t}_y$, which may result in a quasi one-dimensional state [11]. In Fig. 1b, we summarize the renormalized hopping parameters.

We then have the following 17 variational parameters: (i) the Gutzwiller projection g, (ii) 10 four-body parameters on the doublon–holon binding q_0, q_1, q_2, q_3, and q_4 for $\ell = 1$, 2, respectively, and (iii) six one-body parameters in $\Phi_{\rm d}$; $\tilde{\zeta}$, $\tilde{\Delta}$, $\tilde{t}_x$, $\tilde{t}_y$, $\tilde{t}'$, and $\tilde{t}''$. Using optimization VMC techniques, we compute energy expectation values and minimize the energy by searching for the optimal set of variational parameters above. As pilot calculations, we have fixed the system size at 10×10 with periodic–antiperiodic boundary conditions.

3. Results and discussion

To begin with, let us look at the optimized values of the variational parameters in $\Psi_{\rm d}$, which are plotted in Fig. 2.