Vol 13 No 2, February 2004
1009-1963/2004/13(02)/0229-05

Chinese Physics

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The pairing correlations in the phased t–U Hubbard model*

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(Received 27 June 2003; revised manuscript received 18 August 2003)

In this paper we have studied the phased t–U Hubbard model. Using the constrained path Monte Carlo method, we investigated the effects of phase factor on pairing correlation functions in the ground state, and we found that the long-range correlations are dependent on the choice of phase factor, and for some special values of phase factor there exist long-range pairing correlations only in the strong coupling region.

Keywords: Hubbard model, correlation function
PACC: 7110F, 0270

1. Introduction

The physics of the Hubbard model is quite rich, including magnetism, metal–insulator transition and heavy fermion behaviour. Over a long period of time, in search of an electronic model for high-temperature superconductivity, many researchers have studied Hubbard model and its various variants. They focused on the extent in which these models might exhibit superconductivity. Although they found pairing correlations in one-band as well as three-band Hubbard models [1–5] using the quantum Monte Carlo method, they also found that these correlations did not increase when the lattice size was increased. Both the $d_{x^2-y^2}$ wave and extended s-wave pairing correlations decayed quickly as functions of distance between pairs. These results suggest the absence of off-diagonal long-range order in the conventional t–U Hubbard model.

A possible way to improve this state might be to consider a modified Hubbard model in which the phase factor is present. For instance, for the simple t–U model, the phased Hamiltonian has the form

$$H = -t \sum_{<ij>,\sigma} (\mathrm{e}^{-\mathrm{i}\theta_{ij}} C^{\dagger}_{i\sigma} C_{j\sigma} + \mathrm{h.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

where $<ij>$ denotes the nearest neighbour sites i and j, θ_{ij} is the phase angle between them, t is the amplitude for hopping process between the corresponding lattice sites and $U > 0$ stands for the Coulomb repulsion of two electrons on the same lattice site. The operators $C^{\dagger}_{i\sigma}$ and $C_{i\sigma}$ create and destroy an electron with spin σ at site i. $n_{i\sigma} = C^{\dagger}_{i\sigma} C_{i\sigma}$ is the number operator for an electron with spin σ at lattice site i.

If we take all the phase angles to be zero, $\theta_{ij} = 0$, this phased Hubbard model is reduced to the conventional Hubbard model. If we carefully choose the phase factor, this model can be identical to the so-called d-p model. This model can be also considered at least as a modified version of the conventional t–U Hubbard model if we take the orbital coupling into account when the system is coupled with an external magnetic field.[6] In this case,

$$\theta_{ij} = \frac{e}{\hbar c} \int_{R_i}^{R_j} \mathrm{d}\boldsymbol{x} \cdot \boldsymbol{A}(\boldsymbol{x}),$$

and in order to investigate the effects of the phase factor, we ignore temporarily the Zeeman coupling which couples the spin with the magnetic field. Perhaps in some cases it is not impossible to regard the appearance of phase factor as the results of some "inner field" in the system in some sense; this "inner field" plays

*Project supported by the Natural Science Foundation of Henan Province and the National Natural Science Foundation of China (Grant Nos 60276004 and 60290083).

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a role in long-range correlations similar to the role of molecular field in a magnet. It is obvious that this model has richer mathematical structures and physics. Especially, there might exist the long-range pairing correlations in such a phased model. For example, if we consider the traditional square lattice and take phase angles as follows: (1) θ_{ij}=0 (or $2n\pi$) if the pair $< i,j >$ is parallel to the x axis, (2) θ_{ij}=0 (or $2n\pi$) if the pair $< i,j >$ is parallel to the y axis and the site number i is even, (3) $\theta_{ij} = (2n+1)\pi$ if the pair $< i,j >$ is parallel to the y axis and the site number i is odd, (n is any integer), we will find the results of the pairing correlations are encouraging.

2. Pairing correlation functions

In our calculation periodic boundary conditions were imposed. We have computed the pairing correlation functions by using a constrained path Monte Carlo (CPMC) method [5,7] which is different from the ordinary Monte Carlo method [8,9] in working space. This method projects the ground state wavefunction $|\psi_0\rangle$ from a known initial wavefunction $|\psi_{\rm T}\rangle$ by a branching random walk in the Slater determinant space. Within the framework of this random walk, importance sampling and the constrained path approximation are imposed. We also use a population control procedure [10] and a numerical stabilization technique [11] in the random walk.

There are three wavefunctions in simulations. The first one is the importance wavefunction which is used to guide the random walkers. The second one is the constrained wavefunction which is used to constrain the random walker to one side of the nodal surface. The third one is the initial wavefunction. As is often the case, one can take the same trial wavefunctions $|\psi_{\rm T}\rangle$ as the three wavefunctions for convenience. The trial wavefunction can be either one in which the electrons with z component of spin are localized on sites $i_1^\sigma, \cdots, i_{N^\sigma}^\sigma$ or a filled Fermi sea, the correct ground state for $U = 0$. (N^σ is the number of fermions with spin σ). The unrestricted Hartree–Fock solution is also a good choice. However, we take the trial wavefunction as the combination of several Slater determinants in which each of them can be obtained from the methods mentioned above in order to improve the quality of Monte Carlo simulation.

We compute the pairing correlation functions as a function of the distance $\boldsymbol{R}$ between pairs. For the extended s-wave and the $d_{x^2-y^2}$ pairing functions we use

$$P_\alpha(\boldsymbol{R}) = \langle \Delta_\alpha^\dagger(\boldsymbol{R})\Delta_\alpha(0)\rangle,$$

where

$$\Delta_\alpha(\boldsymbol{R}) = \sum_\delta f_\alpha(\boldsymbol{\delta})(C_{R\uparrow}C_{R+\boldsymbol{\delta},\downarrow} - C_{R\downarrow}C_{R+\boldsymbol{\delta},\uparrow}),$$

and $\boldsymbol{\delta} = \pm\hat{x}, \pm\hat{y}$. For the extended s-wave pairing $f_{\rm s}(\boldsymbol{\delta}) = 1$ for all $\boldsymbol{\delta}$ and for the $d_{x^2-y^2}$ pairing, $f_{\rm d}(\boldsymbol{\delta}) = 1$ for $\boldsymbol{\delta} = \pm\hat{x}$ and $f_{\rm d}(\boldsymbol{\delta}) = -1$ for $\boldsymbol{\delta} = \pm\hat{y}$. We also investigate the "vertex contribution" to the correlation functions [1] defined as

$$V_\alpha(\boldsymbol{R}) = P_\alpha(\boldsymbol{R}) - \bar{P}_\alpha(\boldsymbol{R}).$$

$P_\alpha(\boldsymbol{R})$ has the contribution of dressed four-point Green functions of the form $\langle C_\uparrow^\dagger C_\uparrow C_\downarrow^\dagger C_\downarrow\rangle$. It is obtained in our simulations by calculating such four-point Green functions in a fixed auxiliary field first, then averaging over all auxiliary fields. $\bar{P}_\alpha(\boldsymbol{R})$ has terms like $\langle C_\uparrow^\dagger C_\uparrow\rangle\langle C_\downarrow^\dagger C_\downarrow\rangle$. In simulations, the dressed single-particle Green functions are obtained first, then the product of $\langle C_\uparrow^\dagger C_\uparrow\rangle\langle C_\downarrow^\dagger C_\downarrow\rangle$ is computed. It should be noted that over a few nearest neighbour distances, $P_\alpha(\boldsymbol{R})$ measures local correlations among spin and charge, giving little information about long-range pairing correlations, and even may give a "false positive" indication of enhanced pairing. So we will report neither the $\boldsymbol{k} = 0$ spatial Fourier transformation of $P_\alpha(\boldsymbol{R})$ nor its partial sums like $\sum_{R\le L} P_\alpha(\boldsymbol{R})$ as done in some author's works. Instead, as a measure of long-range order, we will report partial averages like

$$V_{\alpha-{\rm ave}}(R > L) = \frac{1}{N'}\sum_{R>L} V_\alpha(\boldsymbol{R}),$$

where $R = |\boldsymbol{R}|$, L is about two lattice spacings, and N' is the number of distances larger than L.

Figure 1 indicates the extended s-wave pairing correlations as a function of the displacement $\boldsymbol{R}$ between pairs. It can be found that even for some large distances the extended s-wave pairing correlations are not small. The same situation exists in the d-wave paring correlations which are shown in Fig.2. In contrast, in the conventional t–U model, both the pairing correlations in large distances are quite small.

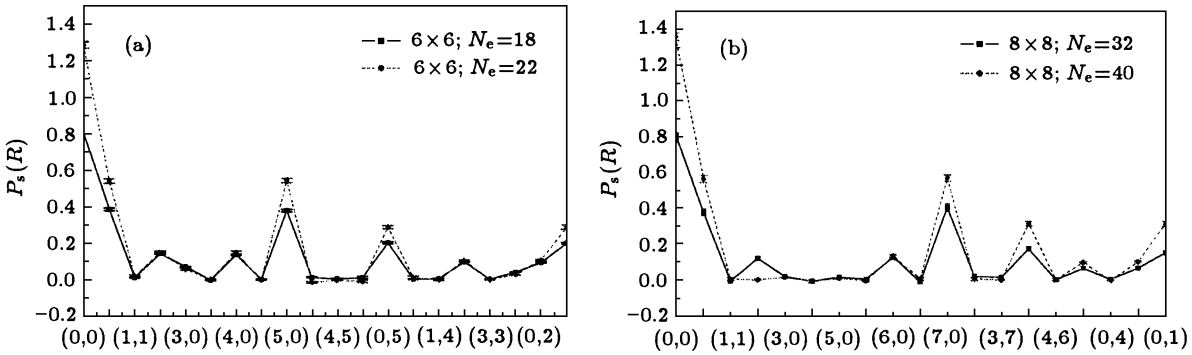


Fig.1. Extended s-wave pairing correlations as a function of the displacement $R = (R_x, R_y)$ between pairs, $U = 4$. (a) The lattice size is 6×6, (b) the lattice size is 8×8.

It can also be seen that the pairing correlations usually increase when electronic numbers increase. (N_e is the number of electrons). We can see from the above two figures that the pairing correlations do not decrease when the size of lattice is increased from 6×6 to 8×8.

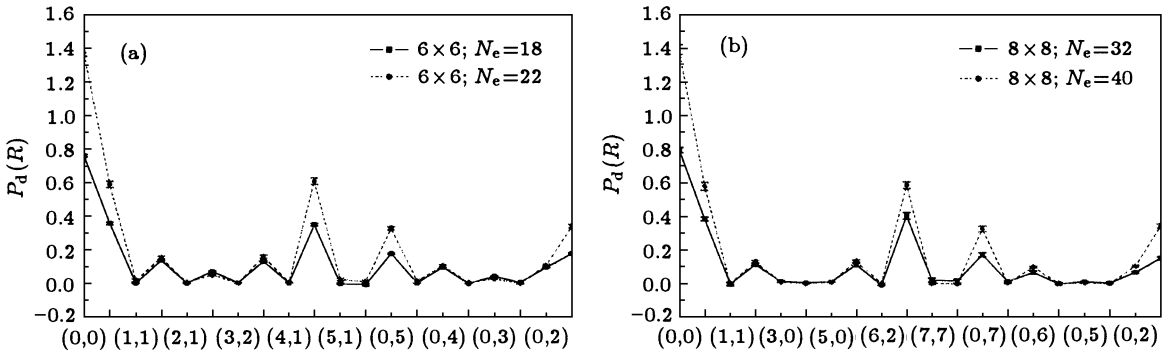


Fig.2. The d-wave pairing correlation as a function of the displacement $R = (R_x, R_y)$ between pairs, $U = 4$. (a) The lattice size is 6×6, (b) the lattice size is 8×8.

In Figs.3 and 4 is shown the vertex contribution to the pairing correlation as a function of the displacement $\boldsymbol{R}$ between pairs for the same lattice sizes and electron densities as in Figs.1 and 2. We can see again that the vertex contributions to pairing correlations do not decrease when the size of lattice is increased. These contributions are not small even for some large distances of pairs.

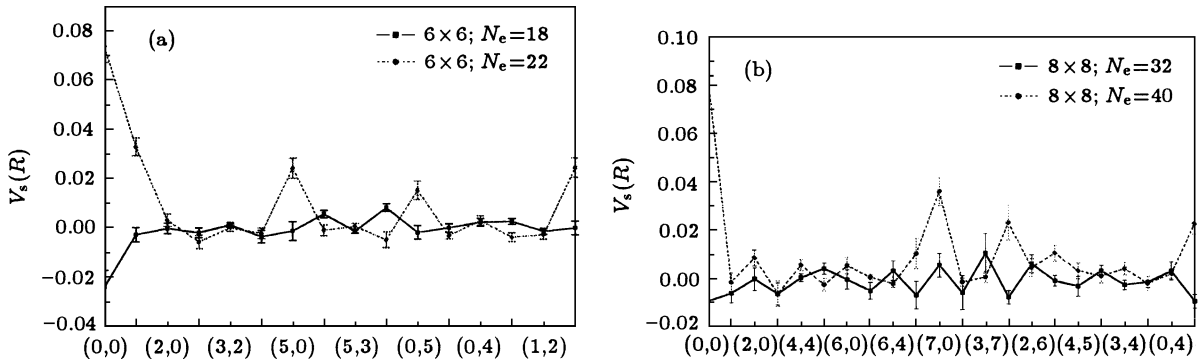


Fig.3. Vertex contribution to the extended s-wave pairing correlations as a function of the displacement $R = (R_x, R_y)$ between pairs. $U = 4$. (a) The lattice size is 6×6, (b) The lattice size is 8×8.

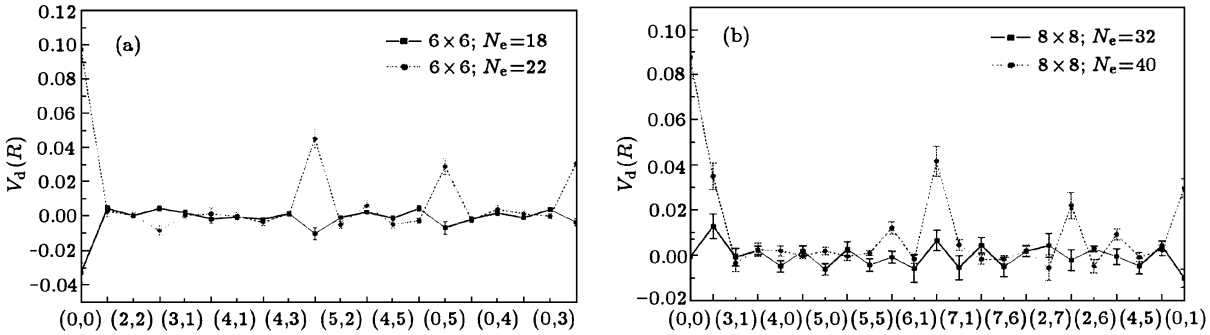


Fig.4. Vertex contribution to the d-wave pairing correlations as a function of the displacement $R = (R_x, R_y)$ between pairs. $U = 4$. (a) The lattice size is 6×6, (b) the lattice size is 8×8.

In Fig.5 with the specific phase we chose above, we show the effects of changing U on the vertex contributions to the d-wave pairing correlations. Comparing with the conventional Hubbard model which corresponds to zero phase angle, we can find some obvious differences between these two models. In the region of strong coupling ($U > 4$) the long-range vertex contribution in phased model is not suppressed with the increase of lattice size from 6×6 to 8×8 system. These facts are consistent with the current points of view that high-T_c superconductivity is related to the effect of strong correlations. In contrast, in the conventional t–U model the long-range behaviour is suppressed from the intermediate to strong coupling region.[5] We also compare the long-range vertex contributions to the phased model with those to the conventional model in the case of $U = 4$ in Table 1. We make the electron densities in the third row as close as possible to those in the second row in order to compare the existing results of the ordinary model with our results.

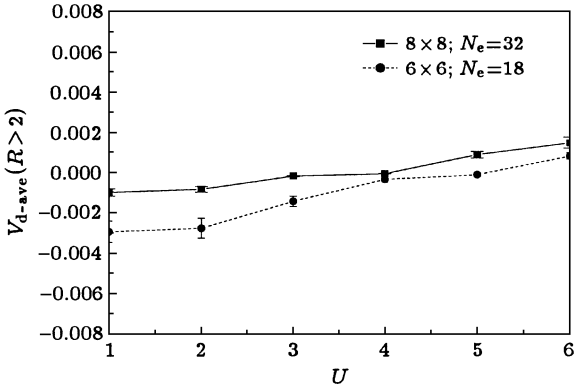


Fig.5. Long-range vertex contribution to the d-wave pairing correlations as a function of U for the 6×6 and 8×8 systems.

We can find from Table 1 that the long-range vertex contributions to s-wave pairing correlations do not decrease with the increase of lattice size in the phased model, while the long-range vertex contributions to d-wave pairing correlations decrease (slowly) with the increase of lattice size in the phased model (the second row). On the other hand, in the conventional model the long-range vertex contributions decrease more quickly with the increase of lattice size in the same case.

Table 1. The long-range vertex contributions.

$V_{s\text{-ave}}(R>2)$		$V_{d\text{-ave}}(R>2)$	
(6×6, N_e=22)	(8×8, N_e=40)	(6×6, N_e=22)	(8×8, N_e=40)
2.32×10^{-4}	1.48×10^{-3}	2.54×10^{-3}	1.50×10^{-3}
		*(6×6, N_e=26)	*(8×8, N_e=42)
		5.8×10^{-3}	1.5×10^{-3}

*Means in ordinary model[5].

3. Conclusion and discussion

Using the CPMC method, we have simulated the two-dimensional phased Hubbard t–U model to investigate the effects of the phase factor. As we know, the scaling behaviour with the lattice size of long-range vertex contributions in the conventional Hubbard model means no long-range off-diagonal order can be observed. However, in the phased Hubbard model, the scaling behaviour with the lattice size is satisfactory. These results suggest there might exist long-range pairing correlations (only) in the strong coupling region in the phased model. It is well known that strongly correlated effect and strongly magnetic coupling effect are the key part to understand many anomalous properties of high-T_c superconductors. In the phased Hubbard model, we can regard the action of the phase factor as the action of equivalently effective field. It is its coupling that can strongly influence the behaviour of long-range correlation.

This is the first time (to our knowledge) that the effects of phase factor on long-range correlations are

discussed for such strongly correlated systems. Although our discussion is restricted to a special phase factor which corresponds to the case that the "inner" or "external" magnetic field is parallel to the z axis (the relationship between the long-range pair correlations and the general phase angles is not a trivial problem in CPMC, which will be reported elsewhere), it still gives a positive indication of long pairing correlations.

We have also studied the Zeeman coupling using the same magnetic field corresponding to the phase factor chosen in the above case of phased Hubbard model, and we find that the Zeeman coupling does not change our above results qualitatively. Our results suggest that the phase factor may play some role in realizing long-range order in such models.

Acknowledgments

Liu P would like to express her appreciation to Professor Lin H Q and Dr. Huang Z B for their help.

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