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Variational Monte Carlo Indications of d-Wave Superconductivity in the Two-Dimensional Hubbard Model

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The possibility of superconductivity in the ground state of the two-dimensional Hubbard model was investigated by means of the variational Monte Carlo method. With slight hole doping on the 6×6 and 10×10 lattices, a clear minimum was obtained on the curve of the total energy versus the amplitude of the d-wave gap function for large on-site Coulomb energies. Superconducting pair correlations were observed to be well developed. The-next-nearest-neighbor transfer was found to appreciably affect the minimum depth.

KEYWORDS: two-dimensional Hubbard model, variational Monte Carlo method, superconductivity, d-wave

Recently the mechanisms of superconductivity in high-temperature cuprate superconductors and organic superconductors have been extensively studied using various two-dimensional models of electronic interactions. The two-dimensional Hubbard model is the simplest and one of the most fundamental ones among such models. Early numerical studies of this model showed the existence of an attractive interaction for an anisotropic pairing.[1,2] However, by means of further numerical investigations using quantum Monte Carlo (M.C.) methods, some authors concluded that the enhanced superconducting correlation does not develop into the predominant one at low temperatures or in the ground state in this model.[3-5] However, since the investigated parameter space, *e.g.*, the ranges of on-site Coulomb energy U and temperature, was restricted due to the methods, whether or not this model has a ground state with predominant superconducting correlation in any parameter region is still a fundamental problem. Although for the t-J model evidence of the occurrence of superconductivity has been obtained,[6-9] the transformation of the Hubbard model to the t-J model is only valid at the first expansion term in the canonical transformation, so it is highly desirable to investigate this problem directly.

In the above-mentioned studies concerning this model, the most severe restriction was that to U. U had to be, at most, half the bandwidth in the quantum M.C. calculations. The cluster size was rather small. We have applied the variational Monte Carlo method, which is more flexible concerning these restrictions, for the search of superconductivity in the model of the title. Very recently there appeared two preprints suggesting the occurrence of the d-wave superconductivity in this model.[10,11] However, these projection M.C. studies are still restricted to U less than half the bandwidth. The present study gives much clearer indications of d-wave superconductivity in the strong correlation region where the above-mentioned studies could not access. Because we consider that next-nearest-neighbor (n.n.n) transfer energy t' affects the occurrence of superconductivity for a reason given later, we have included it in our model and confirmed the effect.

Our model is the two-dimensional Hubbard model defined by

$$H = -t \sum_{\langle jl \rangle, \sigma} (c^{\dagger}_{j\sigma} c_{l\sigma} + \text{H.c.}) + U \sum_{j} c^{\dagger}_{j\uparrow} c_{j\uparrow} c^{\dagger}_{j\downarrow} c_{j\downarrow}, \quad (1)$$

where $c^{\dagger}_{j\sigma}$ ($c_{j\sigma}$) is the creation (annihilation) operator of an electron with spin σ at the jth site; the sites form a rectangular lattice; t is the transfer energy between the nearest-neighbor (n.n.) sites; t is our energy unit; $\langle jl \rangle$ denotes summation over all the n.n. bonds. U is the on-site Coulomb energy. Later on in this paper, we also study the effect of t' between n.n.n. sites by including

$$H_{nnn} = -t' \sum_{\langle\langle jl \rangle\rangle, \sigma} (c^{\dagger}_{j\sigma} c_{l\sigma} + \text{H.c.}) \quad (2)$$

in the Hamiltonian; in the above equation $\langle\langle jl \rangle\rangle$ means summation over the n.n.n. pairs.

Our trial wavefunction is a Gutzwiller-projected BCS-type wavefunction defined as:

$$\Psi_{\text{s}} = P_N P_{\text{G}} \psi_{\text{BCS}}, \quad (3)$$

$$\psi_{\text{BCS}} = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow}) |0\rangle, \quad (4)$$

where P_{G} is the Gutzwiller projection operator given by

$$P_{\text{G}} = \prod_{j} (1 - (1-g) n_{j\uparrow} n_{j\downarrow}); \quad (5)$$

g is a variational parameter in the range from 0 to unity and j labels a site in the real space. P_N is a projection operator which extracts only the states with a fixed total electron number N. Coefficients $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ appear in our calculation only in the ratio defined by

$$v_{\boldsymbol{k}}/u_{\boldsymbol{k}} = \Delta_{\boldsymbol{k}}/(\xi_{\boldsymbol{k}} + \sqrt{\xi^2_{\boldsymbol{k}} + \Delta^2_{\boldsymbol{k}}}), \quad (6)$$

$$\xi_{\boldsymbol{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu, \quad (7)$$

where μ is the chemical potential and $\Delta_{\boldsymbol{k}}$ is a $\boldsymbol{k}$-dependent gap function defined later; $c_{\boldsymbol{k}\sigma}$ is the Fourier

transform of $c_{j\sigma}$. Neglecting constant factors, $\Psi_{\rm s}$ can be rewritten as

$$\Psi_{\rm s} \sim P_N P_{\rm G} \exp(\sum_{\boldsymbol{k}} (v_{\boldsymbol{k}}/u_{\boldsymbol{k}}) c^\dagger_{\boldsymbol{k}\uparrow} c^\dagger_{-\boldsymbol{k}\downarrow})|0\rangle, \quad (8)$$

$$= P_N P_{\rm G} \exp(\sum_{j,l} a(j,l) c^\dagger_{j\uparrow} c^\dagger_{l\downarrow})|0\rangle, \quad (9)$$

$$\sim P_{\rm G} (\sum_{j,l} a(j,l) c^\dagger_{j\uparrow} c^\dagger_{l\downarrow})^{N/2}|0\rangle, \quad (10)$$

$$= P_{\rm G} \sum_{j_1,..,j_{N/2},l_1,..,l_{N/2}} A(j_1,..,j_{N/2};l_1,..,l_{N/2})$$

$$\times\ c^\dagger_{j_1\uparrow} c^\dagger_{j_2\uparrow} \cdots c^\dagger_{j_{N/2}\uparrow} c^\dagger_{l_1\downarrow} c^\dagger_{l_2\downarrow} \cdots c^\dagger_{l_{N/2}\downarrow}|0\rangle, \quad (11)$$

where $a(j,l)$ is defined by

$$a(j,l) = (1/N_{\rm s}) \sum_{\boldsymbol{k}} (v_{\boldsymbol{k}}/u_{\boldsymbol{k}}) \exp\{{\rm i}\boldsymbol{k}\cdot(\boldsymbol{R}_l - \boldsymbol{R}_j)\}, \quad (12)$$

with $N_{\rm s}$ being the number of sites and

$$A(j_1, j_2, \cdots, j_{N/2}; l_1, l_2, \cdots, l_{N/2}) =$$

$$\begin{vmatrix} a(j_1,l_1) & a(j_1,l_2) & \ldots & a(j_1,l_{N/2}) \\ a(j_2,l_1) & a(j_2,l_2) & \ldots & a(j_2,l_{N/2}) \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & \ldots\ldots \\ a(j_{N/2},l_1) & a(j_{N/2},l_2) & \ldots & a(j_{N/2},l_{N/2}) \end{vmatrix}. \quad (13)$$

Then the ground state energy

$$E_{\rm g} = \langle H\rangle \equiv \langle\Psi_{\rm s}|H|\Psi_{\rm s}\rangle / \langle\Psi_{\rm s}|\Psi_{\rm s}\rangle \quad (14)$$

is obtained using a M.C. procedure.[12,13] We optimize this energy with respect to g, $\Delta_{\boldsymbol{k}}$ and μ. Our programs were made by modifying previous ones used for the two-chain Hubbard model.[14] We tested our programs using exact diagonalization results for small systems.

We studied the cases of the d-, extended s- (s^*-) and s-wave gap functions as follows.

$$\begin{array}{ccccc} d & \Delta_{\boldsymbol{k}} & = & \Delta(\cos k_x - \cos k_y), \\ s^* & \Delta_{\boldsymbol{k}} & = & \Delta(\cos k_x + \cos k_y), \\ s & \Delta_{\boldsymbol{k}} & = & \Delta \end{array} \quad (15)$$

The sizes of the lattice we treated are 6×6 and 10×10 having electron density close to unity with slight hole doping to the half-filled state.

Results indicating the occurrence of the d-wave superconductivity were obtained even for the case of electron number $N_{\rm e} = 32$ on a 6×6 lattice with the periodic and the antiperiodic boundary conditions (b.c.'s) for the x- and the y-direction, respectively. This set of b.c.'s was chosen so that $\Delta_{\boldsymbol{k}}$ does not vanish for any $\boldsymbol{k}$ points possibly occupied by electrons. The result is shown in Fig. 1 with $U = 8$ and $t' = 0$. Ground state energy $E_{\rm g}$ divided by site number $N_{\rm s}$ is plotted as a function of Δ defined in eq. (15). g and μ are optimized for each value of Δ by turns until optimization is sufficient. The value of $E_{\rm g}$ was obtained as the average of ten independent M.C. calculations each with 5×10^7 M.C. steps for the optimized g and μ. The error bar shows the standard deviation. Clearly $E_{\rm g}/N_{\rm s}$ is minimized at $\Delta \approx 0.10$. Here $g = 0.3038$ and $\mu = -0.48$. We can estimate the energy gain due to the gap formation as ~ 0.00028/site from the difference between the minimum and the intercept of the curve with the ordinate.

The normal state value of $E_{\rm g}/N_{\rm s}$ was also calculated by a similar variational M.C. procedure. We obtained $E_{\rm g} = -0.6535$ at $g = 0.30$. In the case of s-wave pairing in eq. (15), the $E_{\rm g}/N_{\rm s}$-vs-Δ curve was found to have a sharp positive slope, and was extrapolated to ~ -0.65351 for $\Delta = 0$, which is very close to the normal state value, as expected. The extrapolated value of the d-wave state $E_{\rm g}/N_{\rm s} \sim -0.65495$ for $\Delta = 0$ is lower by ~ 0.0014 than the above values. This difference is understood to be due to a size effect in the following way. At the minimum of the d-wave curve $\mu = -0.48$ lies between the filled and the empty $\boldsymbol{k}$-point energies in the $U = 0$ picture. For $\Delta = 0.01 \sim 10^{-9}$, μ increased to ~ -0.20 which slightly exceeds the energy of the lowest empty $\boldsymbol{k}$ points, i.e., point A and its equivalents in Fig. 2. Therefore, in the limit of small Δ, coefficient $v_{\boldsymbol{k}}$ is dominatant over $u_{\boldsymbol{k}}$ even for $\boldsymbol{k}$ belonging to the A group, as for the occupied $\boldsymbol{k}$ points shown by filled circles in Fig. 2, and the part of the d-wave wavefunction excluding the Gutzwiller projector in eq. (8) does not satisfy the closed shell condition. It contains components in which a BCS-like pair of electrons are excited to the A-group $\boldsymbol{k}$ points from the C and equivalent $\boldsymbol{k}$ points in Fig. 2. The ratios of these components to the closed shell component are finite even in the limit of $\Delta = 0$. These components lower $E_{\rm g}$ given by eq. (14) since their coefficient has a sign opposite to that of the main component. If we neglect the effect of the Gutzwiller projection, we get the energy gain of about 0.0013/site which is in a good agreement with the above-mentioned difference. This gain of $E_{\rm g}$ occurred due to the $\boldsymbol{k}$-dependent sign of $v_{\boldsymbol{k}}/u_{\boldsymbol{k}}$ with the asymmetrical distribution of discrete $\boldsymbol{k}$ points. This effect does not occur for the s- or s^*-wave wavefunctions.

The calculation was extended to the 10×10 lattice. The results for $N_{\rm e} = 84$ on this lattice with periodic and antiperiodic b.c.'s for the x- and y-directions are shown in Fig. 3 for the case of $U = 8$ and $t' = 0$. Here $E_{\rm g}/N_{\rm s}$ is plotted as a function of Δ for the three types of gap functions given in eq. (15). At each value of Δ shown in Fig. 3, $g = 0.30$ was chosen as the initial value of g, on the basis of preliminary survey, and then the optimal value of μ was found by the least squares fit of $E_{\rm g}$ as a function of μ to a parabola. Using this value of μ, g was optimized again. Since $E_{\rm g}$ was a smooth function of g, the obtained optimal g and μ are sufficiently accurate. Using these values, $E_{\rm g}$ was obtained as the average of the results of eight M.C. calculations each with 5×10^7 steps at $\Delta = 0.01$, 0.04 and 0.08 for the d-wave. The standard deviations were less than 0.00011. At other points, the numbers of M.C. calculations and steps were different but their error bars were within 0.00015. The diamond shows the normal state value, -0.73585 ± 0.00024, obtained from 20 M.C. calculations each with 10^7 steps.

Clearly, $E_{\rm g}/N_{\rm s}$ is minimum at a finite value of $\Delta \approx 0.08$ in the case of the d-wave gap parameter. The optimal parameter values at $\Delta = 0.08$ are $g = 0.3037$ and $\mu = -0.4263$. The least squares fit of d-wave data points to a parabola gave the minimum position at $\Delta \cong 0.0766$. The curves of $E_{\rm g}/N_{\rm s}$ for the s- and s^*-wave gap functions

have definite positive slopes at small Δ and are extrapolated to ~ -0.7354 and ~ -0.7353, respectively, which are practically equal. Again these values are slightly higher than the extrapolated value ~ -0.73605 for the d-wave. The normal state value of $E_{\rm g}/N_{\rm s} = -0.73585$ lies between the two groups of extrapolated values. This value was obtained from the Gutzwiller-projected Fermi sea in which $(\pi/6, 7\pi/10)$ and $(-\pi/6, -7\pi/10)$ are fully occupied but $(\pi/6, -7\pi/10)$ and $(-\pi/6, 7\pi/10)$ are unoccupied. The differences are explained as follows. In the limit of $\Delta = 0$ the four points are equally occupied in the s-, s^*- and d-state wavefunctions. These wavefunctions give an expectation value of the on-site Coulomb term that is larger than the normal state wavefunction. This difference is equal to $4U/N_{\rm s}^2$ per site. It would be diminished by the effect of the Gutzwiller projection in the variational calculation, and become closer to the observed difference between the normal state value and the s- and s^*-state values in the limit of $\Delta = 0$. Furthermore, for the same reason as in the case of $N_{\rm s} = 6 \times 6$, $E_{\rm g}/N_{\rm s}$ of the d-wave state becomes lower than that of the s- and s^*-state values in the limit of $\Delta = 0$. In this d-state, low-energy BCS pairs are excited to the four partially occupied $\boldsymbol{k}$ points. The calculated energy gain was in fair agreement with the difference between the $E_{\rm g}/N_{\rm s}$ values of the d-state and the s- and s^*-states in the limit of $\Delta = 0$.

The energy gain in the d-wave state is ~ 0.0015/site. This gain per site is nearly equal to the expected superconducting condensation energy $\sim$ (state density) $\times \Delta^2$. It is five times larger than that for $N_{\rm e} = 32$ and $N_{\rm s} = 36$. This suggests that the size effect is still appreciable in the latter system and that the energy gain per site would remain finite in the bulk limit.

In order to check the superconducting nature of the ground state with a finite value of Δ, the correlation functions of BCS pair operators were calculated. Superconducting pair correlation functions $D_{\alpha\beta}(l), \alpha, \beta = x, y$, are defined as:

$$D_{\alpha\beta}(l) = \langle \Delta_\alpha^\dagger(i+l, j)\Delta_\beta(i, j)\rangle, \tag{16}$$

where $\Delta_\alpha(i, j), \alpha = x, y$, denote the annihilation operators of singlet electron pairs staying on n.n. sites as:

$$\Delta_x(i, j) = c_{ij\downarrow}c_{i+1,j\uparrow} - c_{ij\uparrow}c_{i+1,j\downarrow}, \tag{17}$$

$$\Delta_y(i, j) = c_{ij\downarrow}c_{i,j+1\uparrow} - c_{ij\uparrow}c_{i,j+1\downarrow}, \tag{18}$$

where $c_{ij\sigma}$ means the annihilation operator at site (i, j). The average $\langle \ldots \rangle$ is defined in eq. (14). The result for a state close to the minimum $E_{\rm g}$ point in Fig. 3, i.e., $\Delta = 0.078$, $\mu = -0.428$ and $g = 0.30$, is shown in Fig. 4. The long range parts are enlarged. The correlation extends over the lattice as expected, showing a clear contrast to the normal state. The d-wave nature appears in the negative sign of $D_{xy}(l)$ for $l = 2 \sim 5$.

In the case of $U = 4$ the minimum of the $E_{\rm g}$-vs-Δ curve lies at $\Delta \sim 0.01 - 0.02$ and is much shallower for both 6×6 and 10×10 lattices. In the case of $U = 16$ the minimum of around $\Delta \sim 0.12$ is as deep as that for $U = 8$. However, $U = 16$ is much larger than bandwidth 8 and may be too large for the Gutzwiller wavefunction to be justified.

The Δ-dependence of $E_{\rm g}/N_{\rm s}$ for the d-wave state in the case of the periodic b.c.'s for both directions were found to have similar features as those in the preceding case of the periodic and the antiperiodic b.c.'s. In the present case, the d-wave $\Delta_{\boldsymbol{k}}$ is zero for some $\boldsymbol{k}$ values, which gives rise to a difficulty related to the factor $v_{\boldsymbol{k}}/u_{\boldsymbol{k}}$ in eq. (6). To prevent this difficulty, we replaced $\Delta_{\boldsymbol{k}}$ with $\Delta_c = 10^{-7}$ when $|\Delta_{\boldsymbol{k}}| < \Delta_c$. In the range of Δ_c from 10^{-9} to 10^{-3}, no dependence of resulting $E_{\rm g}$ on Δ_c was found beyond data scattering. The depth of the minimum in the $E_{\rm g}/N_{\rm s}$-vs-μ curve for d-wave pairing in the case of $N_{\rm s} = 10 \times 10$ and $N_{\rm e} = 86$ was close to that in the case of periodic and antiperiodic b.c.'s with $N_{\rm s} = 10 \times 10$ and $N_{\rm e} = 84$ mentioned above. The depth of the minimum in the case of these b.c.'s with $N_{\rm s} = 6 \times 6$ and $N_{\rm e} = 30$ was ~ 0.00069, which is twice as large as that in the preceding case with $N_{\rm s} = 6 \times 6$ and $N_{\rm e} = 32$.

In the two-dimensional Hubbard and d-p models, the state density around the van Hove singularities located in the neighborhood of $(0, \pi)$ and $(\pi, 0)$ is known to develop with the increase of electron correlation, as the single-particle dispersion along the lines from these points to $(0, 0)$ becomes anomalously weak.[15] The increased state density around the singularity has been argued to enhance the $T_{\rm c}$ of the d-wave superconductivity.[16] When t' is negative, the van Hove singularity moves toward the Fermi energy in the hole-doped systems, which should further increase $T_{\rm c}$. We have examined the t'-dependence of the minimum of the $E_{\rm g}$-vs-Δ curve, including H_{nnn} in (2) in our model. In the case of $N_{\rm e} = 32$ on the 6×6 lattice with the periodic and antiperiodic b.c.'s, the energy minimum became slightly deeper with the change of t' from zero to -0.25, but at $t' = 0.25$ the minimum became shallower by a factor of 2. In the case of $N_{\rm e} = 84$ on the 10×10 lattice with the same b.c.'s, the minimum clearly became deeper with the increase of t' in the negative direction from zero to -0.1 and -0.25. With a positive value of $t' = 0.1$, the minimum became shallow. It nearly vanished when $t' = 0.25$. Thus, a negative value of t' stabilizes the d-wave superconductivity in the hole-doped case in the Hubbard model, at least up to $t' = -0.25$, which is in qualitative agreement with ref. 17.

In summary, the variational M.C. calculation on the two-dimensional Hubbard model gave a clear minimum of the total energy as a function of the amplitude of the d-wave gap function. In this energy minimum state, the superconducting correlation extends over finite-size systems. The energy gain increases with increase of U up to $8t \sim 16t$. The preceding negative results are considered to mainly be due to the restriction of the computation method to small or moderate values of U. Next-nearest-neighbor transfer t' increases the energy gain with increase of $|t'|$ when t' is negative.

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Fig. 1. Computed ground state energy per site E_g/N_s is plotted against Δ, amplitude of the d-wave superconducting gap function, for the case of 32 electrons on the 6×6 lattice with periodic and antiperiodic b.c.'s for the x- and the y-direction. $U = 8$ and $t' = 0$. The unit of energy is transfer energy t.

Fig. 2. Doubly occupied $\boldsymbol{k}$ points are shown by filled circles in the two-dimensional $\boldsymbol{k}$ space for the case of 32 electrons on the 6×6 lattice with periodic and antiperiodic b.c.'s for the x- and the y-direction, respectively, in the limit of $U = 0$ with $t' = 0$. Open circles are empty $\boldsymbol{k}$ points. Dotted open circles at $k_x = -\pi$ are equivalent to open circles at $k_x = \pi$. Here the unit of length is the lattice constant.

Fig. 3. Computed ground state energy per site E_g/N_s is plotted against Δ for the case of 84 electrons on the 10×10 lattice with periodic and antiperiodic b.c.'s for the x- and the y-direction. $U = 8$ and $t' = 0$. Filled circles are for the d-wave gap function with g and μ optimized for each Δ. Filled squares and triangles are for the s^*- and s-wave gap functions, respectively. The diamond shows the normal state value.

Fig. 4. Parts of the correlation functions of superconducting pair operators for the case of 84 electrons on the 10×10 lattice with periodic and antiperiodic b.c.'s for the x- and the y-directions. The abscissa is the distance l between the x-coordinates of the positions of two pair operators. $U = 8$ and $t' = 0$. The closed symbols denote the superconducting pair correlations in the energy minimum state. They are the average of four M.C. calculations each with 3×10^7 M.C. steps. The error bars are standard deviations. The open symbols are for the normal state. Since we focus on the long-range parts, the parts for $l = 1$ are omitted.