The Ground and Low Lying Excited States of the Two-Dimensional Hubbard Model

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We have studied the ground state of the two-dimensional (2D) Hubbard model by using a quantum Monte Carlo method paying special attention to the shell structure effect on finite size clusters. Our calculations show there is a gap for spin excitations in the ground state and incommensurate peaks at \((\pi \pm \delta, \pi)\) and \((\pi, \pi \pm \delta)\) in the spin correlation function for a low lying excited state. In the ground state, the long range part of the \(d\) wave superconducting correlation function is enhanced and the momentum distribution function at the Fermi level \((\pi, 0)\) is rounded. The gap in spin excitations and the momentum distribution function rounding is consistent with opening a \(d\) wave superconducting gap in the ground state.

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The low temperature properties and ground state of the doped two-dimensional (2D) Hubbard model have been intensively studied. This activity increased rapidly after the discovery of the high-\(T_c\) cuprate, because it is widely believed that the single band model of the 2D \(CuO_2\) plane is the essential model for the high-\(T_c\) mechanism. Although some novel scenarios have been proposed for the low temperature state and the ground state of the doped 2D Hubbard model, little is known with any degree of certainty. One fact which is exactly known is that no superconducting \(O(D)\) long range order (ODLRO) exists at any finite temperature. However it is not known if there is superconducting ODLRO in the ground state.

The auxiliary field quantum Monte Carlo methods have been applied to the doped 2D Hubbard model. The results obtained so far by using the ground state algorithms have not been sufficient to create a consensus whether or not there is superconducting ODLRO in the ground state of the model. The difficulty partly comes from the negative sign problem of quantum Monte Carlo methods, which prohibits one from studying the ground state of the doped 2D Hubbard model in wider classes of physical parameter ranges, carrier densities, band structures, and lattice sizes. Algorithms have been proposed trying to reduce the negative sign ratio.

We have studied the ground state of the doped 2D Hubbard model by using the recently developed adaptive sampling quantum Monte Carlo (ASQMC) method, with which the negative sign ratio can be greatly reduced. To simulate the Fermi degeneracy among \(k\) points around the Fermi level which may be indispensable to enhance the \(d\) wave superconducting correlation on the finite size lattices, we have carefully tuned the non-interacting band structure as well as the carrier density. We found keeping the pseudo degeneracy around the Fermi level is quite essential to our results. This is a difficult requirement for the standard quantum Monte Carlo methods.

The Hubbard model we studied has the next-nearest hopping term and the third nearest hopping term in addition to the nearest neighbor hopping term: \(H = -t \sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + H.C. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} - t' \sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma}^\dagger c_{j\sigma} + H.C. \right) + t'' \sum_{\langle i,j \rangle, \sigma} \left( c_{i\sigma} c_{j\sigma} + H.C. \right)\), where the \(t\), \(t'\), and \(t''\) terms are the nearest neighbor hopping, the next nearest neighbor hopping, and the third nearest neighbor hopping terms and the \(U\) term is the on-site Coulomb repulsion term. We fixed \(t = 1\) and it is the unit of energy. Only the \(S_z = 0\) subspace was studied.

We have studied the Hubbard model on 6 \(\times\) 6 and 10 \(\times\) 10 lattices. Non-interacting band structure and the filling are tuned such that the energy gap between the lowest unoccupied level (LUL) close to \((0.4\pi, 0.4\pi)\) and the highest occupied level (HOL) at \((\pi, 0)\) is less than \(0.04\). The following two cases were studied: (i) 6 \(\times\) 6 lattice with \(t' = -0.1667\), and \(t'' = 0.2\). The number of electron is 28, (ii) 10 \(\times\) 10 lattice with \(t' = -0.2\), and \(t'' = 0.05\). The number of electron is 84. In both cases, we introduced anisotropy \(\pm 0.0001\) on the \(x\) and \(y\) components of \(t\) and \(t''\). The band structures obtained with these parameter values may correspond to those of high-\(T_c\) cuprates. It should be noted that the fillings do not necessarily correspond to those of real high-\(T_c\) cuprate and were chosen for the sake of tuning \(\Delta_{\text{LUL-HOL}}\). We have studied both cases with \(U = 4\). The \(U = 6\) case was also studied in (i) and some other smaller values of \(U\) were adopted to check the consistency of our results. We used periodic boundary condition in the \(x\) and \(y\) directions.

In the case of (i) with \(U = 4\), we found there are the two quasi-degenerate states with the lowest energies. These two states were obtained by using two different trial wavefunctions; the non-interacting wavefunction and spin polarized Unrestricted Hartree-Fock (UHF) wavefunction. The energy difference is about 0.01. Holes are doped around \((\pi, 0)\) and its symmetric points in the ground state and they are doped around \((0.33\pi, 0.33\pi)\) and its symmetric points in the excited state. The spin...
correlation function $<S(q)> = 1/N \sum_{i,j} \exp(-q \cdot (\vec{r}_i - \vec{r}_j)) <\vec{S}_i \cdot \vec{S}_j>$ has a broad peak at $Q = (\pi, \pi)$ in the ground state but it has incommensurate peaks at $(\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$ in the excited state.

Similar results were obtained in the case of (ii) with $U = 4$. The energy gap is calculated to be 0.04. The spin correlation functions are shown in Fig. 1. The broad peak of spin correlation function at $Q$ suggests strong quantum and/or dynamical fluctuation induced by the doped hole in the ground state. The incommensurability $\delta$ in the excited state is calculated to be about 0.1π when the electron density $\rho = 0.84$. The real space spin correlations $<\vec{S}_0^2, \vec{S}_R^2>$ and their magnitude $|<\vec{S}_0^2, \vec{S}_R^2>|$ in the ground and the excited state are plotted in Fig. 2. In the ground state, the magnitude of the spin correlation decays exponentially, while that of the excited state does not. This suggests there is a gap in spin excitations in the ground state.

The momentum distribution function $<n_k>$ of the excited state is qualitatively similar to that of the non-interacting model. It has a sharp drop at the Fermi level. In the ground state, the drop of $<n_k>$ at the Fermi level $(\pi, 0)$ and $(0, \pi)$ is smeared out and transferred to $(0.4\pi, 0.4\pi)$ and its symmetric points as shown in Fig. 3. $<n_k>$ is therefore similar to the momentum distribution function in the d-wave superconducting state.

We have calculated the d-wave superconducting correlation function: d-wave($\vec{R}$) = $<O_0 O_0^{\dagger} \vec{R}>$, where $O_0^{\dagger} = \frac{1}{\sqrt{2}} (c_{\vec{R}}^\dagger c_{\vec{R}+\vec{x}} - c_{\vec{R}}^\dagger c_{\vec{R}+\vec{y}}) - \frac{1}{\sqrt{2}} (c_{\vec{R}}^\dagger c_{\vec{R}+\vec{y}} - c_{\vec{R}}^\dagger c_{\vec{R}+\vec{x}})$. In the ground states of the cases (i) and (ii), we found enhancement of d-wave($\vec{R}$) at large distances due to $U$. d-wave($\vec{R}$) in the ground state of the case (i) is plotted against $r$ in Fig. 4, where $\vec{R} = (3, r)$. The d-wave correlation function of $U = 4$ is enhanced against that of $U = 0$ at the largest distance. We observed the enhancement is persistent up to $U = 6$. d-wave($\vec{R}$) in the ground state (a) and the excited state (b). The system and the parameter values are the same as the previous figures.
state of the case (ii) with $U = 4$ is plotted against $r$, where $\mathbf{R} = (4, r)$ in the same figure. The d-wave correlation function is enhanced at the two largest distances. Therefore the enhancement due to $U$ is persistent against increase of lattice size. The gap in spin excitations and the reduction of the momentum distribution function at $(\pi, 0)$ found in the ground state are also consistent with a d-wave superconducting ground state.

We have studied the shell structure and/or the band structure effects on d-wave($\mathbf{R}$) on the $6 \times 6$ and $10 \times 10$ lattices. The parameter $t'$ in (i) and (ii) is changed as a variable. We put $U = 4$. The enhancement of d-wave($\mathbf{R}$) is obtained when $t' \leq -0.16$ in the case of (i). The region shrinks to $-0.2007 \leq t' \leq -0.1997$ in the case of (ii). While the width of the flat region of the non-interacting band dispersion near $(\pi, 0)$ in the case (i) is about $\pi/3$, that of the case (ii) is almost zero. This may be the primary reason why the enhancement is achieved in a limited region in the case of (ii). This suggests that the instability of the d-wave superconducting state is largely influenced by the non-interacting band dispersion near $(\pi, 0)$ and hence $t'/t$ and $t''/t$.

**FIG. 4.** The d-wave superconducting correlation function $d$-wave($\mathbf{R}$) of the ground states of the $6 \times 6$ (a) and the $10 \times 10$ (b) lattices in the case of (i) and (ii) as a function of $r$, where $\mathbf{R} = (x, r)$. $U$ is taken as a variable and denoted in the legends of figures. $x = 3$ in (a) and $x = 4$ in (b). Open circles, closed squares, and closed triangles are results obtained with $U = 0, 4$, and 6, respectively.

Implications of our results may be summarized as follows: (1) The energy difference between the lowest excited state with the incommensurate spin correlation and the d-wave superconducting ground state is very small. The stabilities of these states are changed by the non-interacting band structure and the filling. We cannot rule out a possibility that these two states may coexist in a phase separated region in a high-$T_c$ sample. This possibility is also a matter of experimental and theoretical concern today. (2) In the flat band region near $(\pi, 0)$, doped holes may lose their phase coherence due to $U$ and may not be able to remain itinerate and hence they become unstable. To restore the phase coherence, they form Cooper pairs and become stabilized. This scenario for superconductivity in the cuprate is consistent with our numerical results and has also been discussed on the basis of a scaling theory. The reduction of $< n_h >$ at $(\pi, 0)$ due to $U$ is also consistent with this mechanism.

It should be noted that $\Delta_{LUL-HOL}$ implicitly used in most previous studies, which are often done at closed shell fillings, is still too large. Such a situation makes it hard for superconductivity to have ODLRO in the ground state. Small $\Delta_{LUL-HOL}$ were adopted by the present author and also by Kuroki and Aoki (KA). KA studied the small $U/t$ region ($U/t \approx 1$). In the small $U/t$ region, they observed enhancements of the d-wave superconducting correlation at large distances. The results obtained with larger value of $U/t$ ($U/t \approx 4$ and 6) here may be consistent with their results.

In conclusion, we have studied the 2D Hubbard model with special attention to the shell structure on the finite size lattice by using the recently proposed ASQMC method. We found two quasi-degenerate states with the lowest energies. In the low lying excited state, there are incommensurate peaks of the spin correlation function at $(\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$. In the ground state, there is a gap in spin excitations and reduction of the momentum distribution function near $(\pi, 0)$. We observed enhancements of the d-wave superconducting correlation function in the ground state. The gap in spin excitations and the momentum distribution function rounded at the Fermi level are consistent with a d-wave ground state.

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