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System-parameter dependence of the metallic phase of the non-doped 2D Hubbard model

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ABSTRACT

Naito et al. reported that some non-doped T′-214-type compounds drive high-T_c superconductivity. The compounds are considered to be metallic since on-site Coulomb energy U is moderate and the Fermi surface is much deformed in these compounds. In order to confirm this picture and extract electronic structure information, we have examined the phase diagram of the metallic state of the 2D Hubbard model as a function of U and t' (with t'' we fixed at $-t'/2$ here; t' and t'' are the second- and third-neighbor transfer energies, respectively) by means of the variational Monte–Carlo method. We employed a Jastrow-type Gutzwiller trial wave function. In the studied range of $U = 2$–12, the boundary value for $|t'|$ at which SDW disappears increases almost linearly with U. Jump-wise transition to the Mott insulator state was not observed. Using the boundary curve and experimental band parameter values, we estimate $U \sim 5$ for T′-214 compounds. Preceding works are discussed in the last part.

1. Introduction

The Naito group published several experimental reports [1] showing that non-doped T′-214-type compounds of many varieties of compositions drive high-T_c superconductivity instead of the insulating state at low temperatures. Although they are not yet successful to completely exclude a possibility of electron doping due to oxygen deficiency, their results strongly indicate that in the ground state most non-doped intrinsic T′-214-type compounds are not a Mott insulator but a superconductor so that their on-site Coulomb energy U is in the intermediate- or moderate-coupling regime. In terms of the Hubbard model incorporating a 2D tight-binding band, the metal-insulator transition is understandable in the way that due to sizable t' and t'' (second- and third-neighbor transfer energies, respectively, on the square lattice) the 2D Fermi surface is so much deformed from a simple square-like form that the upper and lower bands on both sides of the SDW insulating gap are apt to overlap, leading to the collapse of the insulating state and the appearance of the metallic state. To confirm this interpretation and obtain electronic structure information, we have examined the phase diagram of the metallic state as a function of U and t' (with t'' fixed at $-t'/2$) using the variational Monte Carlo method [2]. We employed a Jastrow-type Gutzwiller wave function [2b] taking account of the electron correlations of both on-site and nearest-neighbor types.

There are preceding analytical [3] and also Monte Carlo [4,5] studies on the present problem. However, our variational Monte Carlo calculation treats a larger system size of 16×16 which allows to get rid of the size effect [2c]. As well as t' the model takes account of t'' which also plays an important role in the stability of the metallic region. In the studied range of $U = 2$–12, where the energy unit is the nearest-neighbor transfer energy t, the normal metallic state is destroyed by the appearance of SDW; its boundary value $|t'_{cr}|$ for $|t'|$ increases almost linearly in the whole range of U. Jump-wise transition to the Mott insulator state was not observed.

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Using the boundary curve with a representative set of t' and t'' values, we get $U \cong 4.2$–5.8 as plausible values for non-doped T′-214-type compounds close to the metal-insulator transition. Finally preceding works will be commented.

2. Model and method

The 2D Hubbard model and calculation method are basically the same as in [2]. The model is defined by

$$H = -t\sum_{\langle jl\rangle,\sigma}\left(c^{\dagger}_{j\sigma}c_{l\sigma}+H.c.\right) - t'\sum_{\langle\langle jl\rangle\rangle,\sigma}\left(c^{\dagger}_{j\sigma}c_{l\sigma}+H.c.\right) - t''\sum_{\langle\langle\langle jl\rangle\rangle\rangle,\sigma}\left(c^{\dagger}_{j\sigma}c_{l\sigma}+H.c.\right) + U\sum_{j}c^{\dagger}_{j\uparrow}c_{j\uparrow}c^{\dagger}_{j\downarrow}c_{j\downarrow}, \quad (1)$$

where $c^{\dagger}_{j\sigma}$ ($c_{j\sigma}$) is the creation (annihilation) operator of an electron with spin σ at the jth site; electronic sites form a rectangular lattice; $\langle jl\rangle$ denotes the nearest-neighbor pairs; H.c. stands for Hermite conjugate; $\langle\langle jl\rangle\rangle$ and $\langle\langle\langle jl\rangle\rangle\rangle$ mean the second- and third-neighbor pairs, respectively; t, t', t'' and U are defined in Section 1.

Our trial wave function for the SDW state is a modified Gutzwiller-projected BCS-type wave function defined by

$$\Psi_{\rm SDW} = \Pi_{\langle jl\rangle}h^{n_jn_l}P_{N_e}\Pi_i(1-(1-g)n_{i\uparrow}n_{i\downarrow})\psi_{\rm SDW}, \quad (2)$$

where the last factor $\psi_{\rm SDW}$ is the mean-field SDW wave function; the third factor is the Gutzwiller projection operator with g being a variational parameter and i labels a site in the real space; $n_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$; P_{N_e} is a projection operator which extracts the components with a fixed total electron number N_e; h is another variational parameter which takes a value around unity and optimizes the electronic correlation between the nearest neighbor (*n.n.*) sites j and l [2b] but in this work we do not optimize the electron correlation between neither the second neighbor nor the third neighbor sites since the improvement is not so remarkable. We call this type of trial function as Jastrow type. $\psi_{\rm SDW}$ is given by

$$\psi_{\rm SDW} = \Pi_{k_4}\Pi_{k_3}\Pi_{k_2}\Pi_{k_1}\beta^{\dagger}_{k_4\downarrow}\beta^{\dagger}_{k_3\uparrow}\alpha^{\dagger}_{k_2\downarrow}\alpha^{\dagger}_{k_1\uparrow}|0\rangle, \quad (3)$$

where $\alpha^{\dagger}_{k\sigma}$ and $\beta^{\dagger}_{k\sigma}$ are creation operators of electrons having wave vector k and spin σ in the lower and upper bands

$$E^{(\pm)}_k = (\varepsilon_k+\varepsilon_{k+Q})\Big/2 \pm \sqrt{w_k^2+M^2}, \quad (4)$$

where

$$\varepsilon_k = -2t(\cos k_x+\cos k_y) - 4t'\cos k_x\cos k_y - 2t''(\cos 2k_x+\cos 2k_y) \quad (5)$$

$$W_k = \varepsilon_k - \varepsilon_{k+Q}, \quad (6)$$

respectively, on the both sides of the SDW gap with its parameter M; k is restricted in the reduced Brillouin zone and $Q = (\pi,\pi)$ is the fixed SDW wave vector; k_1, k_2, k_3 and k_4 represent the electrons occupying the respective bands from the band bottom to up to the Fermi energy. The creation operators are defined by

$$\alpha^{\dagger}_{k\sigma} = u_kc^{\dagger}_{k\sigma} + v_kc^{\dagger}_{k_Q\sigma} \quad \text{and} \quad \beta^{\dagger}_{k\sigma} = v_kc^{\dagger}_{k\sigma} - \sigma u_kc^{\dagger}_{k+Q\sigma}, \quad (7)$$

with

$$u_k = \left[\left(1-w_k\Big/\sqrt{w_k^2+M^2}\right)/2\right]^{1/2}, \qquad v_k = \left[\left(1+w_k\Big/\sqrt{w_k^2+M^2}\right)/2\right]^{1/2}. \quad (8)$$

Even when the Fermi energy lies at a degenerate level, allowing an arbitrariness of the mean-field wave function, the resulting total energy showed only little dependence on the choice of the orbital and spin states occupied at the Fermi level.

The total energy is computed by means of the variational technique on the square lattice of the size $L\times L$ with electrons of the number $N_e = L\times L$. The SDW condensation energy is obtained as the decrease per site of the total energy from the normal state total energy. The latter is also variationally computed using a trial wave function of the type $\Psi_{\rm SDW}$ in which, however, $\psi_{\rm SDW}$ is replaced by the wave function for the Fermi sea.

3. Results with the SDW condensation energy

First, the size dependence of the SDW condensation energy $E_{\rm cond}$ is shown in Fig. 1, in which $E_{\rm cond}$ for the $L\times L$ lattices are plotted as a function of t' (t'' is assumed to be $-t'/2$, as suggested in [6]). This was computed for a different purpose and electron density ρ is approximately fixed around 0.84 close to the optimal density, but it clearly shows that the size dependence of $E_{\rm cond}$ is very strong when L is less than 16. When L becomes as large as 16 the size dependence becomes mild so that the results with this lattice can be regarded close to the bulk limit in the case of SDW problem [2c]. This tendency was checked to be correct in the present case with $\rho = 1$ by computations up to $L = 20$. Therefore, $L = 16$ is employed in this work. The boundary conditions for the two directions are periodic and anti-periodic, respectively. Fig. 2 shows the dependence of $E_{\rm cond}$ on $t' = -2t''$ in the case of $U = 7$ with $\rho = 1$. One can clearly recognize the boundary t'_{cr} where SDW disappears; t'_{cr} is negative and when $t'_{cr} > t'$ the condensation energy $E_{\rm cond}$ of the SDW state is negative and the SDW disappears. The final result for $|t'_{cr}|$ is plotted as a function of U in Fig. 3. At all values of U shown in the figure the transition is of the first order since the SDW amplitude M has a jump there. When U is large and t' is close to t'_{cr} there appeared many local minima as a function of M in the neighborhood of t'_{cr}; we took care to get the largest $|t'_{cr}|$ by manually searching the relevant minimum. As is seen, the value of $|t'_{cr}|$ increases monotonously from the weak-coupling to strong-coupling region.

There are suggestions that in the strong-coupling region the system becomes a Mott insulator when U exceeds a critical value nearly independent of t' [5]. In order to check this possibility, the expectation value $\langle n_k\rangle$ of n_k was computed as a function of $(\pi\nu/L, \pi(\nu+1)/L)$ with $\nu = 0, 1, \ldots, L$ for $t' = -2t''$ fixed at -0.26. As is seen in Fig. 4, $\langle n_k\rangle$ as a function of ν has a Fermi-edge-like sharp change when U is small and gradually it becomes smoothened but does not show a phase-change-like sudden transition as a function of

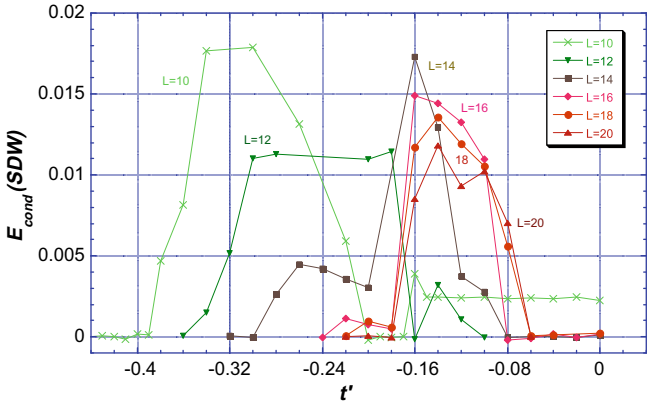

Fig. 1. Dependence of the SDW condensation energy versus t' curve on the model lattice size $L\times L$ for $L = 10$–20. $t'' = -t'/2$ Is assumed. Electron density is chosen at about 0.84. Periodic boundary conditions are taken on the two directions. Employed variational Monte Carlo method is the same as in the text except for parameter h which is fixed at unity in this figure.