Physics of the Hubbard model and high temperature superconductivity

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Abstract. The electronic state of high-temperature cuprates is investigated on the basis of the two-dimensional Hubbard model. We investigate the three-band Hubbard model (which is sometimes called the d-p model) as well as the single-band Hubbard model. In particular, the three-band Hubbard model with d and p orbitals in the CuO\textsubscript{2} plane probably captures the physics of high-temperature superconductivity. Numerical studies of the two-dimensional d-p and Hubbard models have shown that they exhibit antiferromagnetism, stripes, d-wave pairing, coexistent antiferromagnetism with superconductivity, and arc spectra. They are basic phenomena seen in the high-temperature cuprates.

1. Introduction
Since the discovery of cuprate high-\(T_c\) superconductors many authors tried to explain the occurrence of superconductivity (SC) in the cuprates in terms of the two-dimensional (2D) Hubbard model \cite{1,2}. It is believed that the three-band Hubbard model with d and p orbitals in the CuO\textsubscript{2} plane (called the d-p model) captures the physics of high temperature superconductivity. The d-p model may be a minimum model for high temperature cuprates. Thus it is important to clarify the electronic state of this model. Since the simple d-p model is still a complicated model for numerical studies, simplified single-band models such as the Hubbard and t-J models have also been studied as a basic model for high temperature superconductors. It is not clear whether we must take into account the electron-interaction into the minimum model.

Numerical studies have been carried out for these models using various numerical methods. We have studied the ground state of the two-dimensional Hubbard model as well as the d-p model on the basis of the numerical methods such as the variational Monte Carlo method \cite{3,4} and the Quantum Monte Carlo method\cite{5}. It has been clarified that these basic models can exhibit antiferromagnetism, stripes (incommensurate antiferromagnetism), d-wave pairing, coexistence of antiferromagnetism and superconductivity, arc spectra and pseudogap behavior.

The occurrence of superconductivity in the Hubbard model has been questioned for many years. It is extremely difficult to show the existence of superconducting phase for the two-dimensional Hubbard model in a reasonable way. For the present we cannot answer this long-standing question soon. This is also the case for the two-dimensional t-J model. Instead of examining the possibility of superconductivity, we can explore possible symmetries of Cooper pairs if we assume the paired wave function for the ground state.
The paper is organized as follows. The effective Hamiltonian for paired state is examined in Section 2. The phase diagram in the weak-coupling limit is presented for the 2D Hubbard model and d-p model. In Section 3 the incommensurate antiferromagnetic state (striped state) is studied away from half filling to show that the relationship δ-κ in lower doping region where δ is the incommensurability and κ is the doping rate. In Section 4 a discussion on the spectral function in the light-doping region is presented. In Section 5 we investigate the coexistence of superconductivity and incommensurate antiferromagnetism. A summary of the work presented in this paper is presented in the last section.

2. Effective Hamiltonian

First, let us consider the single-band Hubbard Hamiltonian given as

\[ H = \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \]  

where \( t_{ij} \) do not vanish only for the nearest-neighbor and next-nearest-neighbor pairs and \( U \) is the on-site Coulomb repulsion. The total number of sites and the number of electrons are denoted as \( N \) and \( N_e \), respectively. The effective Hamiltonian is derived using the perturbation theory for small \( U \) [6]. The canonical transformation \( H_{\text{eff}} = e^{-S} H e^S \) also maps the Hubbard model to an effective Hamiltonian with the attractive interaction where [7,8]

\[ S = \frac{U}{N} \sum_{kk',q\neq 0} \xi_{kk'q} + \frac{1}{N} \sum_{kk',q\neq 0} \xi_{kk'q} - \xi_{kk} - \xi_{kk'} + \xi_{kk'q} c_{k\sigma}^\dagger c_{k'\sigma}^\dagger c_{-k-q\sigma} c_{-k-q\sigma}. \]  

The effective Hamiltonian reads [9,10]

\[ H_{\text{eff}} = \sum_{kk\sigma} \xi_{kk\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{kk'q} V_{kk'} c_{k\sigma}^\dagger c_{-k'\sigma} c_{-k'\sigma} c_{k\sigma}, \]  

where

\[ V_{kk'} = \frac{U^2}{N} - \frac{U^2}{N} \chi(k + q), \]  

and \( \xi_k \) is the dispersion relation. \( \chi(k+k') \) is the magnetic susceptibility for the non-interacting band. The gap equation for this Hamiltonian is solved as shown in Refs. [10,11] using the point symmetry group. The phase diagram thus obtained is shown in Fig. 1 and Fig. 2. There is a wide region of d-wave pairing near half-filled case.

The gap function has a sharp peak due to the van Hove singularity showing a logarithmic increase. The second neighbor transfer integral \( t' \) could not be so large so that the optimum doping rate should be in the range of \( 0.8 < n_e < 0.85 \). The result suggests higher \( T_c \) for small \( -t' \). The antiferromagnetism, however, may compete with superconductivity suppress it near half filling. This leads to a bell-shape critical temperature as a function of the carrier density. Thus we have an optimum doping rate for finite \( t' \) such as \( t' \sim 0.2 \).

This method is also applied to the d-p model (three-band Hubbard model) [12]; the Hamiltonian is written as

\[ H = t_{dp} \sum_{i\sigma} \left[ d_{i\sigma}^\dagger \left( p_{i+x/2\sigma} + p_{i+y/2\sigma} - p_{i-x/2\sigma} - p_{i-y/2\sigma} \right) + h.c. \right] \]

\[ + t_{pp} \sum_{i\sigma} \left[ p_{i+x/2\sigma}^\dagger p_{i+y/2\sigma} - p_{i-x/2\sigma}^\dagger p_{i-y/2\sigma} - p_{i+y/2\sigma}^\dagger p_{i-x/2\sigma} + p_{i-y/2\sigma}^\dagger p_{i+x/2\sigma} + h.c. \right] \]

\[ + \epsilon_d \sum_{i\sigma} d_{i\sigma}^\dagger d_{i\sigma} + \epsilon_p \sum_{i\sigma} \left[ p_{i+x/2\sigma}^\dagger p_{i+y/2\sigma} + p_{i+y/2\sigma}^\dagger p_{i+x/2\sigma} \right] + U_d \sum_i d_{i\uparrow}^\dagger d_{i\uparrow}^\dagger d_{i\downarrow}^\dagger d_{i\downarrow}, \]  

where \( p_{i+\mu/2\sigma} \) denotes the operator of the p electrons at the site \( R_\mu \mu/2 \) for the unit vector \( \mu \) in the x and y directions. The energy is measured in units of \( t_{dp} \).
Figure 1. Phase diagram in the $n_e-t'$ plane for the single-band Hubbard model with $t' < 0$ in the weak coupling limit. $s$ denotes the pairing state with extended-$s$ wave symmetry. In the $s$-wave region for small $|t'|$, the $s$-wave and $p$-wave states are sometimes nearly degenerate.

We examine the doped case using the hole picture where the lowest band is occupied up to the Fermi energy. The effective interaction for the d-p model is

$$V_{k'} = \frac{U_d}{N} + \frac{U_d}{N} \chi^{dd}(k + k'),$$

where the d-electron susceptibility is

$$\chi^{dd}(q) = \frac{1}{N} \sum_p \sum_{\alpha \beta} W^\alpha_k \frac{f^\alpha_{q+p} - f^\beta_p}{\epsilon^\beta_p - \epsilon^\alpha_{q+p}}.$$  

(7)

Here $\alpha, \beta$ and $\gamma$ are band indices of the mixed three bands. $\epsilon_k^\alpha$ is the dispersion relation of the $\alpha$-th band and $f_k^\alpha = f(\epsilon_k^\alpha)$ is the Fermi distribution function. The weighting factor $W^\alpha_k$ is

$$W^\alpha_k = \frac{\eta_k - \epsilon_k^\alpha}{\epsilon_k^\beta - \epsilon_k^\alpha}(\epsilon_k^\alpha - \epsilon_k^\gamma),$$  

(8)

where $\alpha, \beta$ and $\gamma$ are different from each other and $\eta_k$ is the p-electron hybridization parameter

$$\eta_k = -4t_{pp} \sin(k_x/2) \sin(k_y/2).$$

The phase diagram for this model is shown in Fig.3 for $\epsilon_p - \epsilon_d = 2$. The $d$-wave pairing is predominant over the whole range in the parameter space. In particular, $d_{x^2-y^2}$-wave pairing is stabilized near half-filling. Although the extended-$s$ wave pairing state is more stable than $d$-wave pairing in the narrow region near half filling in the Gutzwiller variational Monte Carlo study [13], the $s$-wave pairing is never stabilized within the weak-coupling perturbation theory.
Figure 2. Phase diagram in the $n_e$-$t'$ plane for the single-band Hubbard model for $t'>0$ in the weak coupling limit. The $s$-, $g$- and $d$-wave pairing states are almost degenerate in the low-carrier region for large $t'$.

Figure 3. Phase diagram for the three-band Hubbard (d-p) model in the plane of the carrier density $n$ and $t_{pp}$ in the weak coupling limit. We set $\varepsilon_p - \varepsilon_d = 2$. $n = 0$ indicates the half-filling band, and the positive and negative $n$ are for hole doping and electron doping, respectively.
3. Incommensurate antiferromagnetism and stripes

The influence of doping holes on the antiferromagnetic state in the parent materials of cuprates is one of the most important problem in the study of high temperature superconductivity. In the elastic neutron scattering experiment on Nd-doped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) with the hole density of $x \approx 0.125$, incommensurate magnetic and charge peaks were observed at $(1/2,1/2 \pm \delta)$ or $(1/2 \pm \delta,1/2)$ and $(2 \pm 2\delta,0)$ or $(0,2 \pm 2\delta)$ in a reciprocal space, respectively\cite{14}. This result indicated the possibility of an incommensurate spin- and charge-density wave order stabilized at low temperatures. This state is called vertical stripe state. It was also experimentally found that the stripe order is stabilized in a wide under-doped region of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) at low temperatures. The elastic neutron scattering experiment of LSCO in the light-doping region of $0.03 < x < 0.07$ revealed that the position of incommensurate magnetic peaks changed from $(1/2,1/2 \pm \delta)$ to $(1/2 \pm \delta',1/2 \pm \delta')$ (the diagonal striped state) as $x$ becomes less than 0.06 \cite{15,16}. In the region both for the vertical and diagonal striped state the magnetic peaks were observed to keep a relationship $\delta \sim x$.

We have carried out the variational Monte Carlo computation on the ground state of the 2D Hubbard model to examine whether the relationship $\delta \sim x$ holds in the lower doping region or not \cite{17}. The results clearly have shown the linear relation $\delta \sim x$ showing the relevance of the 2D Hubbard model. The incommensurate antiferromagnetic state is also stable for the d-p model in the variational Monte Carlo computations \cite{18}.

4. Arc Spectra and Spin Density Wave

Recently a peak crossing the Fermi level in the nodal direction of the d-wave gap has been observed in the light-hole doping LSCO by angle-resolved photoemission spectroscopy (ARPES). The spectral weight exhibits a peak at $(\pi/2,\pi/2)$ for the light-doping case and it extends along the Fermi surface with increasing carrier density \cite{19,20}. Instead, in the lightly electron-doped case, the peaks at $(\pi,0)$ and $(0,\pi)$ were reported \cite{21}. These results suggest that the hole- or electron-doped spin-density wave is formed in the low carrier region. If the second neighbor transfer $t'$ is negative, the density of states has a peak at near $(\pi/2,\pi/2)$ for hole doping and has a peak at $(\pi,0)$ for electron doping. We have proposed a model of the d-density wave induced by the buckling of oxygen atoms in the CuO$_2$ plane \cite{22}. We can understand the arc spectra in the light-doping case on the basis of density wave. Similarly the spectra in the electron-doped case are consistently reproduced using the electron-doped spin-density wave as shown in Fig.4. We also show the spectral function for lightly hole-doped case in Fig.5 where we have a peak at $(\pi/2,\pi/2)$.

![Figure 4](image-url)

**Figure 4.** Spectral function for the light-doping single-band Hubbard model with commensurate spin density wave where the electron density $n$ is 1.049. We set $t'=-0.2$ and $\Delta_{AF}=0.1$ in units of the nearest-neighbor transfer $t$. 

5. Coexistence of superconductivity and antiferromagnetism

As was shown in section 2, the $d$-wave pairing is stable near half filling for the 2D Hubbard model in the weak coupling limit. In fact, in the variational Monte Carlo computation, the SC condensation energy $E_{\text{cond}}$ is indeed finite and is estimated as $E_{\text{cond}} \approx 0.00117t = 0.59\text{meV}$ in the optimally doped case for the single-band Hubbard model in the bulk limit [23,24]. The 2D $d$-p model also gives the finite condensation energy $E_{\text{cond}}$ [13].

The interplay between superconductivity and antiferromagnetism is important in the underdoped region. Recently the phase diagram including the coexistent state of antiferromagnetism and superconductivity was reported for layered cuprate materials [25]. In order to investigate the ground state phase diagram of high-$T_c$ cuprates, we have carried out the variational Monte Carlo computations for the 2D $d$-p model. The ground-state wave function is the Gutzwiller ansatz:

$$\psi = P_G \psi_0$$  \hspace{1cm} (9)

$P_G$ is the Gutzwiller operator for the $d$ electrons. The trial wave function $\psi_0$ is made from the solution of the Bogoliubov-de Gennes equation which are given by

$$\sum_j \left( H_{ij} u_j^\lambda + F_{ij} v_j^\lambda \right) = E^\lambda u_i^\lambda$$  \hspace{1cm} (10)

$$\sum_j \left( F_{ji} u_j^\lambda + H_{ji} v_j^\lambda \right) = E^\lambda v_i^\lambda$$  \hspace{1cm} (11)

where $(H_{ij\sigma})$ and $(F_{ij})$ are $3N\times3N$ matrices for $d$, $p_x$ and $p_y$ orbitals. The antiferromagnetic order parameters are in $(H_{ij\sigma})$ and the SC order parameters $\Delta_{ij}$ are included in $(F_{ij})$. We assume the $d$-wave symmetry for SC order parameters of $d$ electrons. For the incommensurate antiferromagnetic state, the SC order parameters are assumed to have spatial dependence so that the amplitude has a maximum in the hole-rich region and has a minimum in the hole-poor region. The Bogoliubov operators are written in the form

$$\alpha_i = \sum_j \left( u_i^\lambda a_j^\lambda + v_i^\lambda a_j^\dagger \right), \quad \alpha_{\bar{i}} = \sum_j \left( u_i^\lambda a_j^\lambda + v_i^\lambda a_j^\dagger \right),$$  \hspace{1cm} (12)

for $E^\lambda > 0$ and $E^{\bar{\lambda}} < 0$, respectively. Here $a_{i\sigma}$ denotes $d_{i\sigma}$, $p_{i+x/2\sigma}$ or $p_{i+y/2\sigma}$ corresponding to the components of $u$ and $v$. Then the variational wave function is
\[ \psi = P_G P_N \prod \alpha \lambda \propto P_G \left[ \sum_y \left( U^{-1}V \right)_y a_{ij}^+ a_{j,k}^+ \right]^{N_v/2} |0\rangle . \]  

\( U \) and \( V \) are matrices defined by \( V_{\lambda j} = v_{\lambda j} \) and \( U_{\lambda j} = u_{\lambda j} \).

We have carried out the Monte Carlo calculations up to 16×16 sites (768 atoms in total). We have found that in the underdoped region of the doping rate \( x<0.18 \) the coexistent state of incommensurate antiferromagnetism and superconductivity is the ground state (where \( x \) denotes the hole-doping rate). In the overdoped region in the range of 0.18<\( x \)<0.28 we obtain the purely d-wave pairing state as the ground state. In Fig.6 the phase diagram is shown for \( t_{pp} = 0.4 \) and \( \epsilon_p - \epsilon_d = 2 \) in units of \( t_{dp} \) where the order parameter \( \Delta_{AF} \) and \( \Delta_{SC} \) were evaluated from the formula \( E_{cond} = (1/2)N(0)\Delta^2 \) where \( N(0) \) is the density of states. Here we set \( N(0) \sim 5/t_{dp} \). The phase diagram is consistent with the recently reported phase diagram for layered cuprates.

6. Possibility of superconductivity

The quest for the possibility of superconductivity in the 2D d-p model and simplified single-band Hubbard and t-J models is a long-standing question concerning high temperature superconductivity. Although the perturbation theory, fluctuation-exchange theory [26] and variational theory (as presented above) give the stable d-wave pairing away from half filling, quantum Monte Carlo simulations performed so far do not give support of superconductivity for the 2D Hubbard model [27,28]. We must remind that the band structure is important for stability of superconducting and antiferromagnetic state. In fact, recent variational Monte Carlo studies suggest that the condensation energy \( E_{cond} \) in the bulk limit is extremely small for the simple square lattice with \( t'=0 \) [29]. Quantum Monte Carlo simulations are now in progress with taking into account the band structure parameters such as \( t' \) and \( t'' \).

Figure 6. Phase diagram for the three-band Hubbard (d-p) model in the plane of the carrier density \( x \) and the order parameter \( \Delta \) in units of \( t_{dp} \). We set \( U_d = 8, \epsilon_p - \epsilon_d = 2 \) and \( t_{pp} = 0.4 \). \( x = 0 \) corresponds to the half-filling band. ‘AFM+SC’ indicates the coexistent phase.
7. Summary
We have examined the phase diagram with respect to pairing symmetry on the basis of the two-dimensional single-band and three-band Hubbard models. The weak coupling formulation is convenient to investigate the phase diagram in detail. The results are almost consistent with the strong-coupling perturbation theory. The d-wave pairing is stable near half filling for the square lattice and the anisotropic square lattice.

In the weak coupling evaluations, the gap function has a maximum at the van Hove singularity. As the second-neighbor transfer $t'$ increases, the energy of the van Hove singularity decreases. For large $t'=-0.3$ to $-0.4$, the optimal doping is more than 25 percent doping, i.e. $n_e<0.75$. For small third neighbor transfer $t''$, the situation remains the same. The large $-t'$ is assigned to several high-temperature cuprates to fit the angle resolved photoemission spectroscopy (ARPES) data or the Fermi surface obtained by the band structure calculations. Most of them, however, have optimum critical temperature in the range of $0.8<n_e<0.85$. Thus we must consider other electronic or lattice interactions, or reexamine the band parameters $t'$ and $t''$. Recent ARPES studies have reported the band structure which is well fitted using rather smaller $t'$ such as $t'\sim -0.2$ [30].

We have carried out the variational Monte Carlo calculations for the 2D Hubbard and d-p models to investigate the ground state for large Coulomb repulsion. The incommensurate antiferromagnetic state is stable in the light-doping region and the incommensurability shows the relationship $\delta\sim x$ up to $x=0.125$. We have determined the phase diagram within the Gutzwiller ansatz. Our phase diagram is consistent with the recent experimental work for layered cuprates [25] where the coexistent state of antiferromagnetism and superconductivity has been explored. There is a possibility that the real phase structure is hidden from us due to disorder in the well-known phase diagram for La$_{2-x}$Sr$_x$CuO$_4$.

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