Bogoliubov quasiparticle spectra of the effective $d$-wave model for cuprate superconductivity

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An exact-diagonalization technique on finite-size clusters is used to study the ground state and excitation spectra of the two-dimensional effective fermion model, a fictitious model of hole quasiparticles derived from numerical studies of the two-dimensional $t$–$J$ model at low doping. We show that there is actually a reasonable range of parameter values where the $d_{x^2-y^2}$-wave pairing of holes occurs and the low-lying excitation can be described by the picture of Bogoliubov quasiparticles in the BCS pairing theory. The gap parameter of a size $\Delta \approx 0.13|V|$ (where $V$ is the attractive interaction between holes) is estimated at low doping levels. The paired state gives way to the state of clustering of holes for some stronger attractions.

I. INTRODUCTION

High-temperature superconductors are characteristic of the very short coherence length and small carrier number, and may be in an intermediate regime between two limits, a BCS superconductor and a condensate of preformed bosons, and this observation may provide a possible way of explaining the so-called pseudo-gap (or spin-gap) anomaly commonly observed in the lightly doped regime of cuprate superconductors \[1\]. Analyses of the two-dimensional (2D) $t$–$J$ model at low doping have suggested a possible picture \[2,3\]: under strong antiferromagnetic spin correlations, low-energy properties may be described by the coherent drift-motion of the spin-bag–like quasiparticles \[4\] where the rapid incoherent oscillation of the ‘bare hole’ is eliminated as excitations inside the bag \[4\]. This picture immediately suggests an effective fermion model, i.e., a fictitious system of interacting fermions representing the hole quasiparticles \[4,5\]. Since the attractive interaction acting between hole quasiparticles (or binding energy) is fairly strong $\sim 0.8J$ in comparison with the quasiparticle bandwidth $\sim 2J$ \[5\], one may hope that the effective model simulating this situation would provide a possible explanation of some of the anomalous quasiparticle properties of cuprate superconductors.

The purpose of this paper is then to present an analysis of the ground states and some excitation spectra of finite-size clusters of the effective fermion model at $T=0$ K. We show that there is actually a reasonable range of parameter values where the $d$-wave pairing of holes occurs and the low-lying excitation can be described by the picture of Bogoliubov quasiparticles in the BCS pairing theory \[1\]. Also we show that the $d$-wave gap parameter is nearly in proportion to but much smaller than the strength of the attractive interaction between holes. However, clustering of holes occurs for some stronger attractions, unlike, e.g., in the negative-$U$ Hubbard model where the coherence length continuously decreases with the attraction strength and a condensate of tightly-bound real-space pairs becomes a good description \[1\].

The effective fermion model considered here may be defined by the Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + V \sum_{<ij>} n_{i\sigma} n_{j\sigma}$$ \tag{1}$$

with a negative value of the density interaction $V$ acting on holes in the nearest-neighbor sites \(<ij>\). $n_{i\sigma}$ is the number operator at site $i$, and $c_{\mathbf{k}\sigma}^{\dagger}$ creates a hole (‘spinless’ fermion) with momentum $\mathbf{k}$ in the sublattice $\sigma (=\uparrow, \downarrow)$ sublattice; we have the two-sublattice model where the holes with up-spin (down-spin) are always in the $\uparrow$-sublattice ($\downarrow$-sublattice) and the numbers of up-spin and down-spin holes are the same. The single-hole dispersion in the 2D antiferromagnet is taken as the noninteracting band structure

$$\varepsilon_{\mathbf{k}} = 4t_{11} \cos k_x \cos k_y + 2t_{20} (\cos 2k_x + \cos 2k_y)$$

where $t_{11}$ and $t_{20}$ are the second- and third-neighbor hopping integrals with positive sign. We employ the Lanczos
exact-diagonalization technique on finite-size clusters of up to 64 sites with periodic boundary condition; we can take clusters much larger in size than those feasible for the $t$–$J$ model. Hereafter we refer to the momentum defined with respect to the ‘nonmagnetic’ Brillouin zone (see Fig. 1).

II. GROUND STATES

The ground states with zero total momentum are calculated as a function of the parameter values $t_{20}/t_{11}$ and $V/t_{11}$ for all the clusters with 32, 36, 50, and 64 sites. We find that, irrespective of the size of the clusters, the ground states have the point-group symmetries in the parameter space, as those shown in Fig. 2; there are some quantitative differences in the phase boundary among clusters but the basic features are the same.

First, we note that two holes in the empty lattice form a $d_{x^2-y^2}$-wave bound pair for $t_{20}/t_{11} \leq 0.6$–0.8; this is simply because the two holes can gain kinetic energy only by changing the spatial sign of the pair wave-function since a hole goes round the other with the positive hopping parameter $t_{11}$ .

For $t_{20}/t_{11} \geq 0.6$–0.8, this mechanism of $d$-wave pairing works less favorably, and also in the $k$-space, holes tend to accumulate around $k=(\pm \pi/2, \pm \pi/2)$ where there is a node of the $d$-wave pair wave-function, so that the $p$-wave pairing occurs.

There are two regions in the four-hole case: at $t_{20}/t_{11} \leq 0.6$ and $|V|/t_{11} \leq 4$ we have the region where there are two $d$-wave pairs (as will be shown in Sec. IV). In the six-hole case we again find a parameter region where three $d$-wave pairs present. Clustering of holes occurs however for larger attraction strength, suggesting the model to be phase separated. This is evident in the calculated density correlation function $\langle n_i n_j \rangle$ where $\langle \ldots \rangle$ denotes the ground-state expectation value: we find that with increasing $|V|/t_{11}$ the probability of finding a hole in the nearest and next-nearest neighbors of a site with a hole increases suddenly across the level-crossing line in Fig. 2 and saturates rapidly to a constant value, and it also increases very rapidly around $V/t_{11} \approx -2$ even for $t_{20}/t_{11} \geq 0.5$.

We should note here that in the effective model the hole can jump over the other because of the hopping term to the second and third neighbors. This process however is forbidden in the $t$–$J$ model. The stronger tendency to hole clustering in the effective model may therefore be suppressed by somehow implementing a ‘conditional hopping’ of the $t$–$J$ model so as to gain in kinetic energy of holes. Such a correction however will be discussed elsewhere. Hereafter, we present our analysis of the model Eq. (1) in the parameter region where the clustering of holes does not occur (i.e., smaller $|V|/t_{11}$ values) and two holes in the empty lattice form a $d$-wave bound state (i.e., $t_{20}/t_{11} \leq 0.5$). We thereby examine what are the low-energy excitations in this parameter region.

III. SINGLE-PARTICLE SPECTRA

We first calculate the single-particle spectral function defined as $A(k, \omega) = A^-(k, -\omega) + A^+(k, \omega)$ with

$$A^-(k, \omega) = \sum_{\nu \sigma} \left| \langle \psi_{\nu}^{N-1} | c_{k\sigma} | \psi_0^{N} \rangle \right|^2 \delta(\omega - E_{\nu}^{N-1} + E_{0}^{N})$$

$$A^+(k, \omega) = \sum_{\nu \sigma} \left| \langle \psi_0^{N} | c_{k\sigma}^{\dagger} | \psi_{\nu}^{N+1} \rangle \right|^2 \delta(\omega - E_{\nu}^{N+1} + E_{0}^{N})$$

which simulates the angle-resolved photoemission (PES) and inverse photoemission (IPES) spectroscopy. $E_{\nu}^{N}$ and $\psi_\nu^N$ are the $\nu$-th excited eigenenergy and eigenstate ($\nu=0$ denotes the ground state) of the $N$-hole system of the cluster, respectively. We add a small imaginary number $i\eta$ to $\omega$ and give a Lorentzian broadening to the spectra which otherwise consist of a set of $\delta$ functions; the value $\eta/t_{11}=0.05$ is used. This spectra can in principle be compared to recent experimental data.

The calculated results for $A(k, \omega)$ are given in Fig. 3. When $|V|/t_{11}$ value is small the spectra simply reflect the noninteracting band structure, but for larger values of $|V|/t_{11}$ we find that the spectra are sharp near the Fermi energy but become broad away from the Fermi energy and momentum, reminiscent of the ‘dressing’ of the particle of correlated Fermi-liquid systems: the Bloch electron added into the correlated Fermi sea may be scattered out of its single electron level, leaving the system in the manifold of excited states.

The calculated spectra also show how the attractive interaction affects the single-particle excitation spectrum. The gap-like structures can be seen in the spectra at (and around) $k_F$, and the size of the gap increases with increasing attraction strength. The spectral feature, i.e., spectral-weight transfer appearing in both PES and IPES sides near $k_F$ and vanishing far away from $k_F$, is noticed, which is consistent with the expectation of the BCS theory. This feature is absent along the diagonal ($k_x=k_y$) of the Brillouin zone and is consistent with the $d_{x^2-y^2}$-wave pairing. The spectral-weight transfer also indicates a tendency toward smearing of the jump at $k_F$ in the momentum distribution function.

IV. BOGOLIUBOV QUASIPARTICLES

Now let us examine the validity of the Bogoliubov quasiparticle picture for the low-lying states of the effective model. We use the technique proposed in Ref. [12], i.e., an exact calculation of Bogoliubov quasiparticle spectrum on small clusters, and see if this picture works in this model. We define the one-particle anomalous Green’s function as

$$G(k, z) = \langle \psi_0^{N+1} | c_{k}^{\dagger} z - H + E_{0} c_{k}^{\dagger} | \psi_0^{N} \rangle$$

(3)
with the spectral function
\[ F(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} G(\mathbf{k}, \omega + i\eta) \]
and its frequency integral
\[ F_k = \langle \psi^N_0 | c_{\mathbf{k}\downarrow}^{\dagger} c_{\mathbf{k}\uparrow} | \psi^N_0 \rangle, \]
where \( E_0 \) is chosen as the average of \( E_0^N \) and \( E_0^{N+2} \).

The hypothesis (see Ref. [12] for details) that low-lying states of the clusters can be described by the microcanonical version of the BCS pairing theory then predicts that
\[ F(\mathbf{k}, \omega) = F_k \delta(\omega - E_k) \]
with \( F_k = \Delta_k / 2E_k \), where \( E_k \) and \( \Delta_k \) are the quasiparticle energy and gap function, respectively. Similarly, we define the two-particle anomalous Green’s function as
\[ G(\mathbf{k}, \mathbf{k}', z) = \langle \psi^N_0 | c_{\mathbf{k}\sigma} c_{-\mathbf{k}\downarrow} | \psi^N_0 \rangle \frac{1}{z - H + E_0^N \delta_{\mathbf{k}, \mathbf{k}'}, \omega \rangle \delta_{\mathbf{k}, \mathbf{k}'} \] (4)
with \( n_{\mathbf{k}, \sigma} = \langle \psi^N_0 | c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} | \psi^N_0 \rangle \). Only the \( N \)-particle subspace is involved here unlike in Eq. (3). We define the spectral function \( F(\mathbf{k}, \mathbf{k}', \omega) \) and its frequency integral \( F_{\mathbf{k}k'} \) as above. The hypothesis then predicts
\[ F(\mathbf{k}, \mathbf{k}', \omega) = F_k F_{k'} \delta(\omega - E_k - E_{k'}) \]
by examining these two anomalous Green’s functions, we can see if the low-energy excitations of the model are described by the BCS pairing theory.

The spectral function \( F(\mathbf{k}, \omega) \) is calculated for a 64-site cluster of the effective model and is shown in Fig. 4 for a number of the attraction strength. Noticing that the calculation is made by the subtraction of two single-particle excitation spectra [12], we should first of all stress that nearly all incoherent spectral features in \( A(\mathbf{k}, \omega) \) are subtracted out, leaving only the low-energy features (stemming from weakly-interacting Bogoliubov quasiparticles as shown below).

We then find the following, all of which are consistent with expectations of the BCS pairing theory: A pronounced low-energy peak appears at \( \mathbf{k}_p \) and smaller peaks appear at higher energies for other momenta; the weights of the peaks are consistent with the BCS form of the condensation amplitude \( F_k \) with a maximum at \( \mathbf{k}_p \) (see Fig. 5). The momentum dependence of \( F(\mathbf{k}, \omega) \), i.e., the change in sign under rotation by \( \pi/2 \) and vanishing weight along the \( k_x = k_y \) line, is a clear indication of \( d_{x^2-y^2} \)-wave pairing. The size of the energy gap, which may be estimated directly from the positions of the peaks, increases with increasing \( |V|/t_{11} \) value. With decreasing gap size, the peaks at momenta other than \( \mathbf{k}_p \) lose their weight as expected from the BCS theory. We note that, when the attraction strength \( V/t_{11} \) exceeds some critical value, these features are collapsed and the spectra completely lose the significance of Bogoliubov quasiparticles, indicating that the clustering of holes takes place and the system seems to phase separate. The coherence length \( \xi \) estimated from the momentum dependence of \( F_k \) decreases with the attraction strength but still is more than twice as large as the nearest-neighbor lattice spacing even near the critical \( V/t_{11} \) value.

We further compare the calculated spectra \( F(\mathbf{k}, \omega) \) with the BCS predictions where we assume the quasiparticle energy \( E_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta_k^2} \) with the gap function \( \Delta_k = \Delta_0 \cos(k_x - k_y) \) and choose the chemical potential \( \mu \) to guarantee vanishing \( \varepsilon_k - \mu \) at \( \mathbf{k}_p \). The value of \( \Delta_0 \) is then evaluated by fitting the positions of the low-energy peaks in \( F(\mathbf{k}, \omega) \). We find that the fitted quasi-particle spectra are in a fair agreement with the exact spectra, which demonstrates the validity of the BCS pairing theory for low-lying excitations in the effective model. The estimated values of the gap parameter \( \Delta_0 \) are shown in Fig. 6. We find that \( \Delta_0 \) is insensitive to the doping levels examined and has the value \( \Delta_0 \approx 0.13|V| \) until reaching the region of phase separation, which is much smaller than the bandwidth for \( \varepsilon_k \). This value also corresponds to \( \Delta_0 \approx 130 \text{K} \) if we assume \( |V| \sim 0.8J \) and \( J \sim 1300 \text{K} \).

A consequence of \( d_{x^2-y^2} \)-wave pairing may be seen in the point-group symmetry of the ground states, i.e., an alternation of the symmetry between \( B_1 \) and \( A_1 \) for the two-, four-, and six-hole states in a parameter region (see Fig. 2). This alternation, present also in the \( l-J \) clusters [12], suggests the picture that holes are added in pairs with \( d_{x^2-y^2} \)-wave symmetry. \( G(\mathbf{k}, z) \) in Eq. (3) (and thus \( F(\mathbf{k}, \omega) \)) reflects the pairing symmetry via the point-group symmetries of \( \psi_0^N \) and \( \psi_0^{N+2} \). Note that \( F(\mathbf{k}, \mathbf{k}', \omega) \) is defined entirely within the \( N \)-particle subspace and thus is not affected by this alternation; nevertheless it shows the same indication of \( d_{x^2-y^2} \)-wave pairing as \( F(\mathbf{k}, \omega) \). The calculated results for \( F(\mathbf{k}, \mathbf{k}', \omega) \) are shown in Fig. 6. We again find that the size of the excitation gap increases with increasing \( |V|/t_{11} \), and the \( \mathbf{k} \)-dependence of the spectra clearly indicates \( d_{x^2-y^2} \)-wave pairing. There are sharp peaks at low energies and broadened features at higher energies. As is the case for \( F(\mathbf{k}, \omega) \), these high-energy features lose their weight rapidly with decreasing \( |V|/t_{11} \) value, whereas the peaks at \( \mathbf{k}_p \) become sharp but remain finite with decreasing \( |V|/t_{11} \) value. These results are consistent with the notion of weakly-interacting Bogoliubov quasiparticles for low-lying excitations in the BCS superconductors. When the attraction strength \( V/t_{11} \) exceeds some critical value, the spectra \( F(\mathbf{k}, \mathbf{k}', \omega) \) again completely loose the significance of Bogoliubov quasiparticles, indicating that the clustering of holes takes place.

V. SUMMARY

By using an exact-diagonalization technique on finite-size clusters, we have studied the ground states and excitation spectra of the 2D effective fermion model, i.e., a system of spin-bag–like quasiparticles corresponding to
doping holes, which is derived from numerical studies of the 2D $t-J$ model at low doping. We have examined the point-group symmetries and density correlations of the ground states of various size clusters with two, four, and six holes over a wide range of parameter values, and have found that the results are insensitive to the size of the clusters and can be summarized as the schematic phase diagram reflecting the pairing symmetry of holes. We then have calculated the single-particle spectra of the model in a parameter region and have detected some indications of the $d_{x^2-y^2}$-wave hole pairing in the obtained spectral features. We have further calculated the one-particle and two-particle anomalous Green’s functions and found that there is actually a reasonable range of parameter values where the $d_{x^2-y^2}$-wave pairing of holes occurs and the low-lying excitation can be described by the picture of Bogoliubov quasiparticles in the BCS pairing theory. The gap parameter is estimated to be $\Delta \simeq 0.13|V|$ at low doping levels. It seems however that with increasing the attraction strength the state of clustering of holes overwhelms this $d_{x^2-y^2}$-wave pairing state before the picture of a condensate of tightly-bound pairs with the $d_{x^2-y^2}$-wave internal structure becomes appropriate.

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FIG. 1. Available $k$-points in the Brillouin zone for (a) 32-, (b) 36-, (c) 50-, and (d) 64-site clusters with periodic boundary condition. The dotted lines indicate the Brillouin zone defined for the two-sublattice model.

FIG. 2. Schematic representation of the point-group symmetry of the ground state at $k=(0,0)$ obtained for the 32-, 36-, 50-, and 64-site clusters with (a) two holes, (b) four holes, and (c) six holes; $B_1$ ($d_{x^2-y^2}$), $E$ ($p_x$ and $p_y$), and $A_1$ ($s$) symmetries appear in the parameter space.

FIG. 3. Single-particle spectra $A(k,\omega)$ calculated for various attraction strengths ($V/t=-1$, $-2$, and $-3$ for left, center, and right columns, respectively) and hole numbers (two, four, and six holes). $\omega$ is the energy of the hole. The spectra for the 64-site cluster are arranged from top to bottom in each panel as $k=(\pi/2,\pi/2)$, $(\pi/4,\pi/4)$, $(0,0)$, $(\pi/4,0)$, $(\pi/2)$, $(3\pi/4,0)$, $(\pi,0)$, $(3\pi/4,\pi/4)$, and $(\pi/2,\pi/4)$. Those for the 32-site cluster are as $k=(\pi/2,\pi/2)$, $(\pi/4,\pi/4)$, $(0,0)$, $(\pi/2,0)$, $(\pi,0)$, and $(3\pi/4,\pi/4)$.

FIG. 4. Bogoliubov quasiparticle spectra $F(k,\omega)$ for a number of attraction strengths. The upper four panels show the results from the anomalous Green’s function between two- and four-hole ground states for the 64-site cluster with $t_{20}/t_{11}=0.3$, and the lower four panels show the results between four- and six-hole ground states for the 32-site cluster with $t_{20}/t_{11}=0.3$. The arrangements of the spectra in each panel follow those in Fig. 3.

FIG. 5. Attraction strength dependence of the condensation amplitude $F_k$ calculated for the 64-site cluster with the filling between two and four holes (left column) and for the 32-site cluster between four and six holes (right column).

FIG. 6. Gap parameter $\Delta_d/t_{11}$ as a function of the attraction strength $|V|/t_{11}$ estimated from the calculated $F(k,\omega)$ for two-, four-, and six-hole systems.

FIG. 7. Bogoliubov quasiparticle spectra $F(k,k',\omega)$ calculated for the 32-site cluster with six holes. The spectra for various $k$ points with $k'=(3\pi/4,-\pi/4)$ are shown. $t_{20}/t_{11}=0.3$ and $V/t_{11}=-2.0$ are used.