

Excitation spectra of the negative- U Hubbard model: A small-cluster study

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An exact-diagonalization technique on small clusters is used to study low-lying excitations and superconductivity in the two-dimensional negative- U Hubbard model. We first calculate the Bogoliubov-quasiparticle spectrum, condensation amplitude, and coherence length as functions of the coupling strength U/t , thereby working out how the picture of Bogoliubov quasiparticles in the BCS superconductors is affected by increasing the attraction. We then define the Cooper-pair operator as a spatially extended composite boson and make a variational evaluation of its internal structure. We thereby calculate the single-particle spectral function of the Cooper pair and obtain the dispersion relation for its translational motion. The dynamical density correlation function of the pairs is also calculated. We thus demonstrate the applicability of our numerical method for gaining insight into low-lying excitations of models for the intermediate coupling superconductivity relevant to cuprate materials.

I. INTRODUCTION

High-temperature superconductors typically show very short coherence length and small carrier numbers, and may be in an intermediate regime between two well-understood regimes, i.e., the BCS weak-coupling superconductivity and Bose-condensation of preformed bosons. Although much theoretical effort has been devoted to examining this cross-over regime, not very much is known, in particular, of the low-lying excitations.^{1,2} To consider this problem, we have studied the negative- U Hubbard model because of its controllable strength of attraction. This model, much discussed recently,³⁻¹⁰ may be a good reference system to more relevant models, such as the t - J model, for cuprate superconductivity.

The negative- U Hubbard Hamiltonian is written

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_{\mathbf{i}} n_{i\uparrow} n_{i\downarrow} \quad (1)$$

with a negative value of U , where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) is the electron creation (annihilation) operator at site \mathbf{i} and spin σ ($=\uparrow, \downarrow$), and $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$. The summation $\langle \mathbf{ij} \rangle$ is taken over all the nearest-neighbor pairs on the two-dimensional square lattice. We employ an exact-diagonalization technique on small clusters; a 4×4 cluster with periodic boundary condition is used throughout the work, and ground states and dynamical correlation functions are calculated by the Lanczos algorithm.

As an approach from weak-attraction limit we first calculate the Bogoliubov quasiparticle spectra in the BCS pairing theory as a function of U/t , and demonstrate how the picture of Bogoliubov quasiparticles is affected by increase of the strength of attraction.¹¹ Condensation amplitude and coherence length are also estimated. We then make a variational calculation of the Cooper-pair wave function and examine U/t dependence of the internal structure of the pair. Next we calculate the wave functions of pairs with nonzero momenta and examine the single-particle excitation spectra of the pair to see its translational motion. Finally we calculate the dynamical pair-density correlation, and examine a density fluctuation

of the pairs. We thus demonstrate the applicability of our numerical method for gaining insight into low-lying excitations of models for the intermediate coupling superconductivity.

II. BOGOLIUBOV QUASIPARTICLE

Let us first examine the validity of the Bogoliubov-quasiparticle picture in the negative- U Hubbard model as a function of attraction U/t . We use a recently proposed technique,¹² i.e., an exact calculation of Bogoliubov quasiparticle spectrum on small clusters. We thereby see whether low-lying states of the negative- U Hubbard cluster of a given attraction U/t can be described by this picture.

We define the one-particle anomalous Green's function as

$$G(\mathbf{k}, z) = \left\langle \psi_0^{N+2} \left| c_{\mathbf{k}\uparrow}^\dagger \frac{1}{z - H + E_0} c_{-\mathbf{k}\downarrow}^\dagger \right| \psi_0^N \right\rangle, \quad (2)$$

where $|\psi_0^N\rangle$ is the cluster ground state with N (even) electrons, E_0 is the ground-state energy (averaged over energies of the N and $N+2$ electron states), and $c_{\mathbf{k}\sigma}^\dagger$ is the Fourier transform of $c_{i\sigma}^\dagger$. We then define the spectral function $F(\mathbf{k}, \omega) = -(1/\pi) \text{Im} G(\mathbf{k}, \omega + i\eta)$ with $\eta = +0$ and its frequency integral

$$F_{\mathbf{k}} = \langle \psi_0^{N+2} | c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | \psi_0^N \rangle. \quad (3)$$

This Green's function should describe the excitation of a Bogoliubov quasiparticle in the cluster, i.e., $F(\mathbf{k}, \omega) = F_{\mathbf{k}} \delta(\omega - E_{\mathbf{k}})$ with $F_{\mathbf{k}} = \Delta_{\mathbf{k}}/2E_{\mathbf{k}}$ for the quasiparticle energy $E_{\mathbf{k}}$ and gap function $\Delta_{\mathbf{k}}$, provided that the low-lying states of the cluster can be described by the microcanonical version of the BCS pairing theory.¹³

The calculated results for $F(\mathbf{k}, \omega)$ at $N=8$ and 10 are shown in Figs. 1(a) and 1(b), respectively. Fermi momentum \mathbf{k}_F is at $(\pi/2, 0)$ for $N=8$ and at $(\pi/2, \pi/2)$ and $(\pi, 0)$ for $N=10$. We find that, at $U/t = -2$, the spectrum fits fairly well with the BCS spectrum (dotted curves) with s -wave gap function $\Delta_{\mathbf{k}} = \Delta_0$: pronounced low-energy peaks appear at

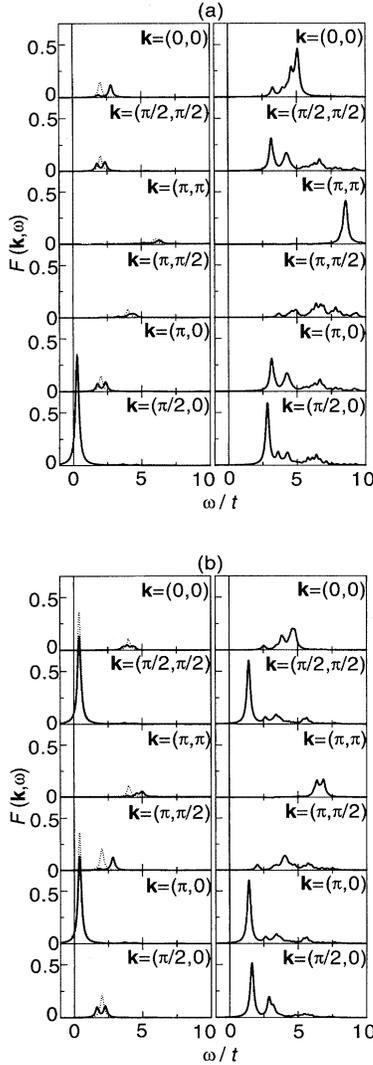


FIG. 1. Bogoliubov quasiparticle spectra $F(\mathbf{k}, \omega)$ for the 4×4 cluster with filling of (a) $N=8$ at $U/t = -2$ (left panel) and -6 (right panel), and (b) $N=10$ at $U/t = -2$ (left panel) and -6 (right panel). Dotted curves in the left panels show the BCS spectral function obtained for (a) $\Delta_0/t = 0.28$ and (b) 0.4 . We use the value $\eta/t = 0.15$ for Lorentzian broadening of the spectra.

\mathbf{k}_F , smaller peaks appear at higher energies for other momenta. The observed gap is isotropic, and the spectral weights are consistent with the BCS form of the condensation amplitude $F_{\mathbf{k}}$ with a maximum at \mathbf{k}_F (see Fig. 2). However, at $U/t = -6$, the peaks already extend to higher-energy regions and the dispersion becomes rather deformed, indicating that the Bogoliubov quasiparticle is becoming a less well defined excitation although the lowest-energy peaks at \mathbf{k}_F are still sharp and well defined. For much larger values of $|U|/t$ the spectra are totally incoherent and the notion of Bogoliubov quasiparticles loses its significance.

We also calculate the coherence length ξ defined as

$$\xi^2 = \sum_{\mathbf{k}} |\nabla_{\mathbf{k}} F_{\mathbf{k}}|^2 / \sum_{\mathbf{k}} |F_{\mathbf{k}}|^2. \quad (4)$$

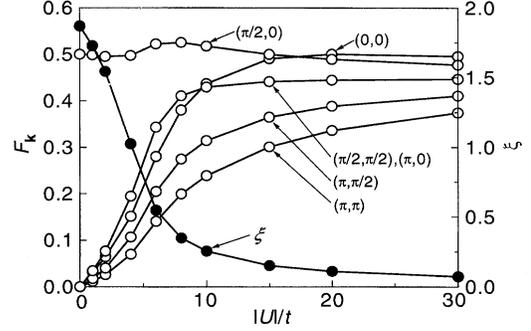


FIG. 2. Condensation amplitude $F_{\mathbf{k}}$ and coherence length ξ as a function of the attraction U/t calculated for the 4×4 cluster with filling of $N=8$.

The result (see Fig. 2) shows a rapid but smooth crossover from a Cooper-paired state to a Bose condensed state of tightly bound pairs. At $|U|/t \approx 3-4$, ξ is of the size of the nearest-neighbor to next-nearest-neighbor distance. Note that $F_{\mathbf{k}}$ goes to zero when $|U|/t \rightarrow 0$ for $\mathbf{k} \neq \mathbf{k}_F$ in agreement with the BCS pairing theory; nondivergence of ξ at $|U|/t \rightarrow 0$ is an obvious finite-size effect.

III. COOPER PAIR

As an approach from strong-attraction regime we introduce a spatially extended “composite-boson” operator defined as $b_{\mathbf{i}}^{\dagger} = \sum_{\mathbf{r}} \alpha(\mathbf{r}) c_{\mathbf{i}+\mathbf{r}\uparrow}^{\dagger} c_{\mathbf{i}\downarrow}$ (Ref. 14) and its Fourier transform $b_{\mathbf{q}}^{\dagger}$ with $\alpha(\mathbf{k}) = \sum_{\mathbf{r}} \alpha(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}$. We then define a variational wave function by adding a zero-momentum pair of up and down electrons to the N -electron ground state:

$$\begin{aligned} |\tilde{\psi}_0^{N+2}\rangle &= \text{const} \times b_{\mathbf{q}=0}^{\dagger} |\psi_0^N\rangle \\ &= \text{const} \times \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} \alpha(\mathbf{k}) c_{-\mathbf{k}\uparrow}^{\dagger} c_{\mathbf{k}\downarrow}^{\dagger} |\psi_0^N\rangle, \end{aligned} \quad (5)$$

where N_s is the number of lattice sites. We determine variational coefficients $\alpha(\mathbf{k})$ so as to maximize the overlap with the exact wave function $|\langle \psi_0^{N+2} | \tilde{\psi}_0^{N+2} \rangle|^2$ under the condition that $|\tilde{\psi}_0^{N+2}\rangle$ be normalized to unity, which leads to a generalized eigenvalue problem

$$\sum_{\mathbf{k}'} [F_{\mathbf{k}}^* F_{\mathbf{k}'} - \lambda N_{\mathbf{k}\mathbf{k}'}] \alpha(\mathbf{k}') = 0, \quad (6)$$

with $F_{\mathbf{k}}$ of Eq. (3) and

$$N_{\mathbf{k}\mathbf{k}'} = \langle \psi_0^N | c_{\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}'\uparrow}^{\dagger} c_{\mathbf{k}'\downarrow} | \psi_0^N \rangle$$

(see Ref. 15). We find for the cluster that an overlap of $\lambda \approx 0.95$ is generally achieved. Defining $\tilde{F}_{\mathbf{k}}$ by replacing ψ_0^{N+2} with $\tilde{\psi}_0^{N+2}$ in Eq. (3), we have $\tilde{F}_{\mathbf{k}} = \sum_{\mathbf{k}'} \alpha^*(\mathbf{k}') N_{\mathbf{k}\mathbf{k}'}$ and $\sum_{\mathbf{k}} \tilde{F}_{\mathbf{k}} \alpha(\mathbf{k}) = 1$. One may use these relations with the exact $F_{\mathbf{k}}$ to check the validity of the variational wave function; actually we find values of $\sum_{\mathbf{k}} F_{\mathbf{k}} \alpha(\mathbf{k})$ ($= \lambda^{1/2}$) to be close to 1 within a few percent.

Figure 3 shows the Cooper-pair wave function thus determined; the pair is added to the state with $N=8$ and

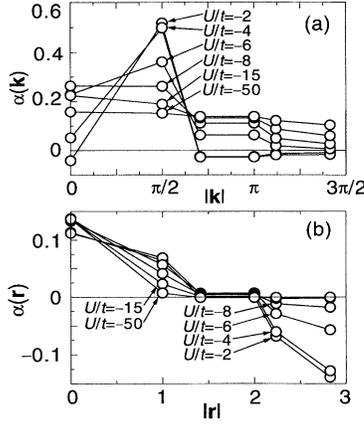


FIG. 3. (a) Cooper-pair wave function $\alpha(\mathbf{k})$ and (b) its Fourier transform $\alpha(\mathbf{r})$ calculated for the 4×4 cluster with filling of $N=8$.

$\mathbf{k}_F = (\pi/2, 0)$. We find in Fig. 3(a) that when $|U/t| \leq 6$ $\alpha(\mathbf{k})$ has a peak at \mathbf{k}_F , and with increasing $|U/t|$, it broadens over the entire Brillouin zone; the Pauli principle acting between the added electrons and Fermi sea plays an essential role in the structure of the Cooper-pair wave function. In real space, as is expected from the BCS pairing wave theory, $\alpha(\mathbf{r})$ [see Fig. 3(b)] shows an oscillation of wavelength $2\pi/k_F$ corresponding to the peak in $\alpha(\mathbf{k})$, and the oscillation decays with the length scale of ξ as one may see via U/t dependence of $\alpha(\mathbf{r})$.

IV. EXCITATIONS OF COMPOSITE BOSONS

Let us next examine excitation spectra for translational motion of the Cooper pair. We first introduce a creation operator of the finite-momentum (\mathbf{q}) pair which is defined as

$$b_{\mathbf{q}}^{\dagger} = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{k}} \alpha_{\mathbf{q}}(\mathbf{k}) c_{-\mathbf{k}+\mathbf{q}}^{\dagger} c_{\mathbf{k}}^{\dagger}, \quad (7)$$

with \mathbf{q} -dependent internal structure $\alpha_{\mathbf{q}}(\mathbf{k})$ (which reduces to $b_{\mathbf{q}}^{\dagger}$ defined in Sec. III at $\mathbf{q}=0$), and again perform the variational evaluation of $\alpha_{\mathbf{q}}(\mathbf{k})$ by a generalization of the above procedure where $F_{\mathbf{k}}$ and $N_{\mathbf{k}\mathbf{k}'}$ also depend on \mathbf{q} . The operator thus obtained is compared below with the on-site pair-field operator $b_{\mathbf{q}}^{\dagger} = (1/\sqrt{N_s}) \sum_{i,j} c_{i+1}^{\dagger} c_{i,j}^{\dagger} e^{-i\mathbf{q} \cdot \mathbf{i}}$, i.e., Eq. (7) with $\alpha_{\mathbf{q}}(\mathbf{k}) = 1$. We find for the cluster with $N=8$ that the overlap $\lambda \geq 0.7$ (mostly around ~ 0.8) is achieved by the optimization; the presence of the Fermi sea is again found to play an important role in the \mathbf{k} and \mathbf{q} dependence of $\alpha_{\mathbf{q}}(\mathbf{k})$.

We then define the pair-addition spectrum as

$$P(\mathbf{q}, \omega) = -\frac{1}{\pi} \Im \left\langle \psi_0^N \left| b_{\mathbf{q}} \frac{1}{\omega + i\eta - H + E_0^N} b_{\mathbf{q}}^{\dagger} \right| \psi_0^N \right\rangle, \quad (8)$$

whereby examining the single-particle excitation of the Cooper pair. The chemical potential for the Cooper pair is defined as $\mu_p = \partial E / \partial N_p = E_0^{N+2} - E_0^N$ where $N_p (= N/2)$ is the number of pairs. Figure 4 shows the calculated result for $P(\mathbf{q}, \omega)$ with optimized values of $\alpha_{\mathbf{q}}(\mathbf{k})$; we compare this with the result obtained for the on-site pair-field operator. We

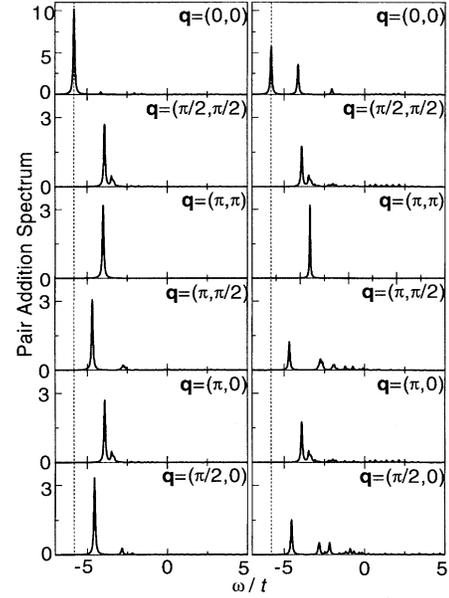


FIG. 4. Pair-addition spectra $P(\mathbf{q}, \omega)$ calculated for the 4×4 cluster with filling of $N=8$ at $U/t = -4$. Vertical dotted lines indicate μ_p . Left panel: the spectra for $b_{\mathbf{q}}^{\dagger}$ with optimized $\alpha_{\mathbf{q}}(\mathbf{k})$ values. Right panel: the spectra for the on-site pair-field operator. Lorentzian broadening of $\eta/t = 0.05$ is used.

first of all find that with the optimization higher-energy peaks are suppressed strongly and the lowest-energy peak is enhanced at each momentum \mathbf{q} , indicating that the spatially extended “composite boson” describes the low-energy excitation of the system fairly well;¹⁶ its effective mass, e.g., is noted to become heavier with increasing $|U/t|$. An indication of the off-diagonal long-range order is also seen in the calculated momentum distribution $\langle b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \rangle$, i.e., its enhancement at $\mathbf{q} = (0,0)$, although in the thermodynamic limit a macroscopic number of bosons are condensed into $\mathbf{q}=0$ state. One may then check how the Bogoliubov theory for interacting bosons¹⁷ works for these composite operators; we directly calculate the density correlation function defined as

$$B(\mathbf{q}, \omega) = -\frac{1}{\pi} \Im \left\langle \psi_0^N \left| d_{-\mathbf{q}} \frac{1}{\omega + i\eta - H + E_0^N} d_{\mathbf{q}} \right| \psi_0^N \right\rangle, \quad (9)$$

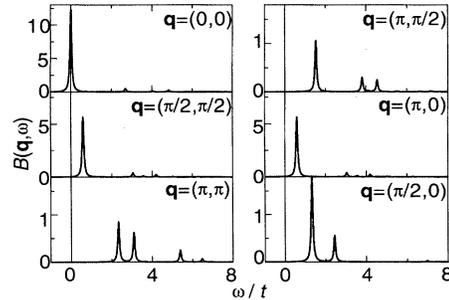


FIG. 5. Density correlation function $B(\mathbf{q}, \omega)$ of composite bosons calculated for the 4×4 cluster with $N=4$ and $U/t = -4$. Lorentzian broadening of $\eta/t = 0.05$ is used.

with the density operator $d_{\mathbf{q}} = (1/\sqrt{N_s}) \sum_{\mathbf{k}} b_{\mathbf{k}+\mathbf{q}}^\dagger b_{\mathbf{k}}$. The calculated result for $B(\mathbf{q}, \omega)$ at $U/t = -4$ is shown in Fig. 5; the spectrum is approximated well by a single peak around $\mathbf{q} = (0, 0)$, which is consistent with the expected picture of the collective sound mode. For larger momenta this mode decays into pair-breaking excitations observed in $F(\mathbf{k}, \omega)$.

V. SUMMARY

We have proposed numerical techniques for examining the low-lying excitation spectra of the two-dimensional negative- U Hubbard model and studied the (i) Bogoliubov-quasiparticle excitation, (ii) condensation amplitude and coherence length, (iii) internal structure of the Cooper pairs, and (iv) single-particle and density excitations of the pairs, as functions of the attractive interaction. We have demonstrated how the picture of Bogoliubov-quasiparticle excita-

tions in the BCS superconductors loses its significance as the coupling strength increases and how the picture of spatially extended composite bosons works as the coupling strength decreases. Application of the present numerical technique to strongly correlated electron models will help us gain insight into the intermediate-coupling superconductivity relevant to cuprate materials.

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¹⁴Bosonic commutation relations are not exactly satisfied reflecting fermionic nature of the operator although we use the term ‘‘composite boson’’ by convention; see Ref. 3. Also, the singlet pairing operator

$$b_{\mathbf{l}} = \alpha(0) c_{\uparrow\mathbf{l}} c_{\downarrow\mathbf{l}} + \frac{1}{\sqrt{2}} \sum_{\mathbf{r} \neq 0} \alpha(\mathbf{r}) (c_{\uparrow\mathbf{l}} c_{\downarrow\mathbf{l}+\mathbf{r}} - c_{\downarrow\mathbf{l}} c_{\uparrow\mathbf{l}+\mathbf{r}})$$

may be used but the results are not different because only the singlet s -wave pairing is relevant in the present model.

¹⁵Minimization of the total energy leads to a generalized eigenvalue equation $\sum_{\mathbf{k}'} [H_{\mathbf{k}\mathbf{k}'} - EN_{\mathbf{k}\mathbf{k}'}] \alpha(\mathbf{k}') = 0$ with $H_{\mathbf{k}\mathbf{k}'} = \langle \psi_0^N | c_{\mathbf{k}\downarrow} c_{-\mathbf{k}\uparrow} H c_{-\mathbf{k}'\uparrow}^\dagger c_{\mathbf{k}'\downarrow}^\dagger | \psi_0^N \rangle$, which may also be used to find values of $\alpha(\mathbf{k})$, although we find the results are very similar.

¹⁶A single peak is found at $\mathbf{q} = (\pi, \pi)$. This is because the state $b_{\mathbf{q}}^\dagger | \psi_0^N \rangle$ is an eigenstate of the Hamiltonian, i.e., $[H, b_{\mathbf{q}}^\dagger] = -U b_{\mathbf{q}}^\dagger$ with $\mathbf{q} = (\pi, \pi)$. See S. Zhang, *Phys. Rev. Lett.* **65**, 120 (1990).

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