

## Bogoliubov Quasiparticle Excitations in the Two-Dimensional $t$ - $J$ Model

Y. Ohta, T. Shimozato, R. Eder, and S. Maekawa

*Department of Applied Physics, Nagoya University, Nagoya 464-01, Japan*

(Received 10 March 1994)

Using a proposed numerical technique for calculating anomalous Green's functions characteristic of superconductivity, we show that the low-lying excitations in a wide parameter and doping region of the two-dimensional  $t$ - $J$  model are well described by the picture of dressed Bogoliubov quasiparticles in the BCS pairing theory. The pairing occurs predominantly in the  $d_{x^2-y^2}$ -wave channel and the energy gap has a size  $\Delta_d \simeq 0.15J - 0.27J$  between quarter and half fillings. Opening of the superconducting gap in the photoemission and inverse-photoemission spectra is demonstrated.

PACS numbers: 74.20.Mn, 71.27.+a, 75.10.Jm, 75.40.Mg

Recent issues in the theory of high-temperature superconductivity include the fundamental question whether the two-dimensional (2D)  $t$ - $J$  model contains a superconducting phase relevant to cuprate materials, and if so, what types of superconductivity the model has. There are a number of mean-field based, variational Monte Carlo, and other approximate calculations, but a commonly agreeable phase diagram has still been out of our reach. Thus, at this stage, unbiased numerically exact calculations of the model certainly offer important information on this question. Among such exact calculations [1-3], Dagotto and Riera [1] have recently found indications of superconductivity near the region of phase separation [4] by examining equal-time pairing correlations in finite-size clusters; the existence of a  $d_{x^2-y^2}$ -wave condensate has thereby been conjectured.

In this Letter, we propose a new technique for examining the low-lying excitation spectrum, i.e., the exact calculation of anomalous Green's functions for Bogoliubov quasiparticles in finite-size clusters; we can thereby calculate the quasiparticle excitation spectrum directly to examine the superconducting pairing interactions in the 2D  $t$ - $J$  model. Then, we show that the low-energy excitations in a wide parameter ( $J/t$ ) and doping region of the model are well described by the picture of dressed Bogoliubov quasiparticles within the BCS (Bardeen-Cooper-Schrieffer) pairing theory: the singlet pairing of electrons with opposite momenta occurs near the Fermi energy unlike in the regime of Bose condensation of a gas of spin singlets in real space. The pairing occurs predominantly in the  $d_{x^2-y^2}$ -wave channel, and the gap energy scales with  $J$  and has a magnitude  $\Delta_d \simeq 0.15J - 0.27J$ . We also demonstrate the opening of a superconducting gap in the photoemission and inverse-photoemission spectra. This work provides the first demonstration of the validity of the BCS pairing theory for a strongly correlated electron model.

The  $t$ - $J$  model is defined by the Hamiltonian

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + J \sum_{\langle ij \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right),$$

where  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) is the projected electron creation (annihilation)

operator at site  $i$  and spin  $\sigma$  ( $=\uparrow, \downarrow$ ) allowing no doubly occupied sites,  $\mathbf{S}_i$  is the electronic spin operator, and  $n_i = n_{i\uparrow} + n_{i\downarrow}$  is the electron number operator. The summation is taken over all the nearest-neighbor pairs  $\langle i, j \rangle$  on the two-dimensional square lattice. The average number of electrons per site  $n$  is defined with the terms half filling ( $n=1$ ) and quarter filling ( $n=1/2$ ).

We adopt the working hypothesis that low-lying states of the clusters can be described by the microcanonical version of the BCS pairing theory [5]. Hence, we assume that a cluster ground state with an even electron number  $N$  can be written as  $|\psi_0^N\rangle = P_N |\text{BCS}\rangle$  where  $|\text{BCS}\rangle$  is a BCS wave function (formulated in terms of "quasiparticles" so that the effects of strong correlations are already included) and  $P_N$  projects on the  $N$ -electron subspace. Similarly, we assume that the low-lying states with an odd electron number  $N+1$  can be written as  $|\psi_\nu^{N+1}\rangle = P_{N+1} \gamma_{\mathbf{k}\sigma}^\dagger |\text{BCS}\rangle$  where  $\gamma_{\mathbf{k}\sigma}^\dagger$  creates a Bogoliubov quasiparticle with momentum  $\mathbf{k}$ . Then, if we define the following anomalous Green's functions, our working hypothesis predicts that they should describe the excitations of Bogoliubov quasiparticles in the clusters.

The one-particle anomalous Green's function is defined as

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

where  $c_{\mathbf{k}\sigma}^\dagger$  is the Fourier transform of  $c_{i\sigma}^\dagger$  and  $E_0$  is the ground-state energy. We 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  $F_{\mathbf{k}} = \langle \psi_0^{N+2} | c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger | \psi_0^N \rangle$ . The hypothesis then predicts  $F(\mathbf{k}, \omega) = F_{\mathbf{k}} \delta(\omega - E_{\mathbf{k}})$  with  $F_{\mathbf{k}} = z_{\mathbf{k}} \Delta_{\mathbf{k}} / 2E_{\mathbf{k}}$  via the Bogoliubov-Valatin transformation of operators [6], where  $z_{\mathbf{k}}$ ,  $E_{\mathbf{k}}$ , and  $\Delta_{\mathbf{k}}$  are the wave-function renormalization constant, renormalized quasiparticle energy, and gap function, respectively. Thus, this Green's function describes the excitation of one Bogoliubov quasiparticle in the cluster. Similarly, we define the two-particle anomalous Green's function as

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

with  $n_{\mathbf{k}\sigma} = \langle \psi_0^N | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | \psi_0^N \rangle$  and the ground-state energy  $E_0^N$ . Only the  $N$ -particle subspace is involved, unlike in Eq. (1). We define the spectral function  $F(\mathbf{k}, \mathbf{k}', \omega)$  and its frequency integral  $F_{\mathbf{k}\mathbf{k}'}$  as above. The hypothesis then predicts  $F(\mathbf{k}, \mathbf{k}', \omega) = F_{\mathbf{k}} F_{\mathbf{k}'}^* \delta(\omega - E_{\mathbf{k}} - E_{\mathbf{k}'})$ : the Green's function describes the excitation of two Bogoliubov quasiparticles. Note that Eq. (2) may also be defined with  $c_{\mathbf{k}'\sigma}^\dagger$  and  $c_{\mathbf{k}\sigma}$  interchanged and with  $n_{\mathbf{k}\sigma}$  replaced by  $\bar{n}_{\mathbf{k}\sigma} = \langle \psi_0^N | c_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger | \psi_0^N \rangle$ ; whereas no change occurs in the BCS theory, some difference appears in the calculated spectra because of the violation of the anti-commutation relation of the constrained operators; however, we find the difference to be insignificant. Thus, by examining these two anomalous Green's functions, we can see if the low-energy excitations of the 2D  $t$ - $J$  model are described by the BCS pairing theory.

The off-diagonal Green's functions Eqs. (1) and (2) may be evaluated by subtraction of diagonal ones, which in turn are computed in the standard Lanczos algorithm [7]: e.g., for the one-particle anomalous Green's function, we prepare the state  $c_{\mathbf{k}\uparrow} |\psi_0^{N+2}\rangle + c_{-\mathbf{k}\downarrow}^\dagger |\psi_0^N\rangle$  and calculate the spectral function, from which the usual single-particle spectral functions for  $c_{\mathbf{k}\uparrow} |\psi_0^{N+2}\rangle$  and  $c_{-\mathbf{k}\downarrow}^\dagger |\psi_0^N\rangle$  are subtracted; thereby  $F(\mathbf{k}, \omega) + \text{c.c.}$  is obtained. The majority of the spectral weight is canceled out; only the anomalous part remains (compare the spectra shown below). The imaginary part of  $F(\mathbf{k}, \omega)$  is also calculated by using the state  $c_{\mathbf{k}\uparrow} |\psi_0^{N+2}\rangle + i c_{-\mathbf{k}\downarrow}^\dagger |\psi_0^N\rangle$  and is always found to van-

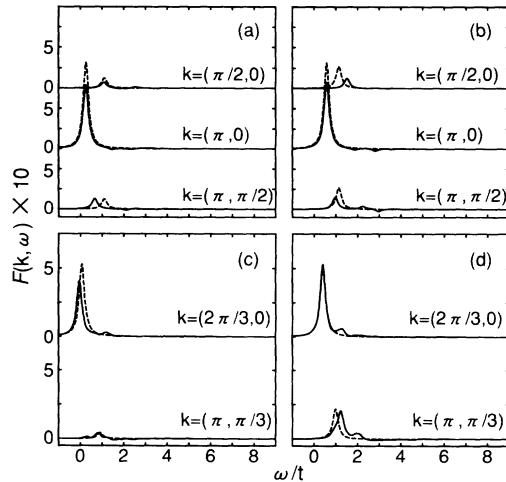


FIG. 1. Bogoliubov quasiparticle spectrum  $F(\mathbf{k}, \omega)$  for the 16-site cluster with doping between 4 and 6 holes at (a)  $J/t=0.8$  and (b) 1.5, and for the 18-site cluster with doping between 4 and 6 holes at (c)  $J/t=0.4$  and (d) 1.5. The spectra at other momenta  $\mathbf{k}$  are identical with those shown here except the sign that follows the  $d_{x^2-y^2}$ -wave symmetry; the spectra along the line  $k_x=k_y$  vanish exactly.  $\mathbf{k}_F$  is located at  $(\pi, 0)$  in (a) and (b), and at  $(2\pi/3, 0)$  in (c) and (d). The dotted curves show the BCS spectral function obtained for parameter values  $\Delta_d/t=0.13$  in (a) and 0.29 in (b) with  $t_{\text{eff}}/t=0.55$  and  $z_B=1.0$ , and  $\Delta_d/t=0.05$  in (c) and 0.27 in (d) with  $t_{\text{eff}}/t=0.45$  and  $z_B=0.5$ . We use the value  $\eta/t=0.15$ .

ish. We use clusters of the size  $4 \times 4$  and  $\sqrt{18} \times \sqrt{18}$  with periodic boundary condition; the Green's functions are evaluated for zero-momentum ground states to simulate the excitations in the thermodynamic limit. The Fermi momentum  $\mathbf{k}_F$  is located at the  $k$  points where  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$  show the lowest-energy peak.

The calculated results for  $F(\mathbf{k}, \omega)$  are shown in Fig. 1. We choose the average value of  $E_0^N$  and  $E_0^{N+2}$  as the value of  $E_0$  used in Eq. (1). We find the following, all of which are consistent with expectations of the BCS pairing theory: a pronounced low-energy peak appears at  $\mathbf{k}_F$  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  $F_{\mathbf{k}}$  with a maximum at  $\mathbf{k}_F$ . 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, scales well with  $J/t$  value. With decreasing gap size, the peaks at momenta other than  $\mathbf{k}_F$  lose their weight as expected from the BCS theory. An important 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  $A_1$  and  $B_1$  in, e.g., the 18-site cluster for fillings of 10, 12, 14, and 16 electrons in a fairly wide  $J/t$  region. This alternation, absent in, e.g., attractive- $U$  Hubbard clusters, suggests the picture that electrons are added in pairs with  $d_{x^2-y^2}$ -wave symmetry.  $G(\mathbf{k}, z)$  in Eq. (1) [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  $F(\mathbf{k}, \omega)$ .

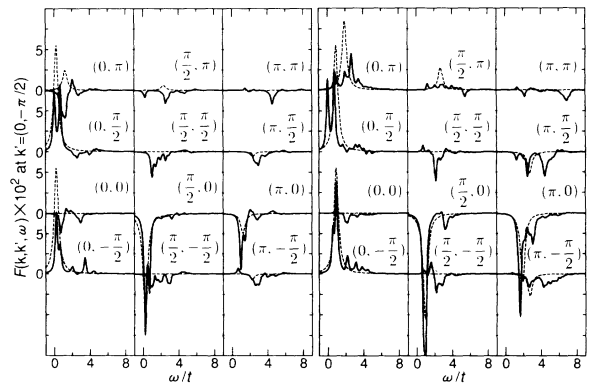


FIG. 2. Bogoliubov quasiparticle spectrum  $F(\mathbf{k}, \mathbf{k}', \omega)$  for the 16-site cluster with 8 holes at  $J/t=0.4$  (left panel) and 2.5 (right panel). The momentum  $\mathbf{k}$  dependence is shown with  $\mathbf{k}'$  fixed at  $(0, -\pi/2)$ ,  $(0, \pi/2)$ , and  $(\pi, \pi/2)$ .  $\mathbf{k}_F$  is located at  $(\pi/2, 0)$  and its equivalent points. The value  $\eta/t=0.15$  is used. The dotted curves show the BCS spectral function obtained for parameter values  $\Delta_d/t=0.105$  (left panel) and 0.47 (right panel) with  $t_{\text{eff}}/t=0.55$  and  $z_B=0.7$ .

The calculated results for  $F(\mathbf{k}, \mathbf{k}', \omega)$  are shown in Figs. 2 and 3. We again find that the size of the excitation gap scales well with  $J/t$ , 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  $J/t$ , whereas the peaks at  $\mathbf{k}_F$  become sharp but remain finite with decreasing  $J/t$ . These results are consistent with the notion of weakly interacting Bogoliubov quasiparticles for low-lying excitations in the BCS superconductors.

To be more quantitative, let us compare the calculated spectra  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$  with the BCS predictions for the spectral functions: the quasiparticle energy  $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$  with one-electron energy  $\xi_{\mathbf{k}} = -2t_{\text{eff}}(\cos k_x + \cos k_y) - \mu$  and gap function  $\Delta_{\mathbf{k}} = \Delta_d(\cos k_x - \cos k_y)$  is assumed. We use the effective hopping parameter  $t_{\text{eff}}$  to take into account the quasiparticle band narrowing. The chemical potential  $\mu$  is chosen to guarantee vanishing  $\xi_{\mathbf{k}}$  at  $\mathbf{k}_F$ . The value of  $\Delta_d$  is then evaluated by fitting the positions of the low-energy peaks in  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$ . The renormalization factor  $z_B$  (defined by assuming  $z_{\mathbf{k}}$  to be  $\mathbf{k}$  independent) is estimated from weights of the low-energy peaks in  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$ . The parameters  $t_{\text{eff}}$  and  $z_B$  reflect the effects of strong correlation and imply the use of a *dressed* Bogoliubov quasiparticle description. The fitted quasiparticle spectra are shown by dotted curves in Figs. 1–3. We find a fair agreement with the exact spectra, which demonstrates the validity of the BCS pairing theory for

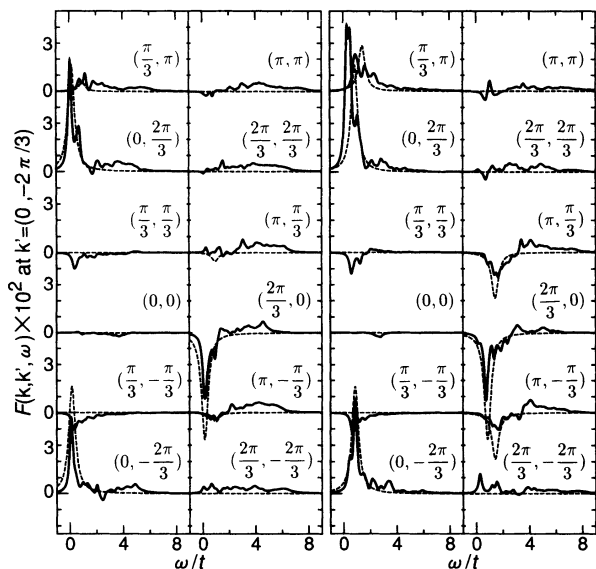


FIG. 3. As in Fig. 2 but for the 18-site cluster with 6 holes at  $J/t=0.4$  (left panel) and  $1.5$  (right panel). The momentum  $\mathbf{k}'$  is fixed at  $(0, -2\pi/3)$ , and  $\mathbf{k}_F$  is located at  $(2\pi/3, 0)$  and its equivalent points. The value  $\eta/t=0.15$  is used. The BCS spectra are for the parameter values  $\Delta_d/t=0.05$  (left panel) and  $0.285$  (right panel) with  $t_{\text{eff}}/t=0.45$  and  $z_B=0.5$ .

low-lying excitations in the 2D  $t$ - $J$  model. This is also the case at low doping levels: both  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$  exhibit well-defined low-energy peaks with  $d_{x^2-y^2}$ -wave symmetry which can be fitted to the BCS spectra with rather small  $t_{\text{eff}}$  and  $z_B$  values.

The estimated values of the gap parameter  $\Delta_d$  are shown in Fig. 4. We find that  $\Delta_d$  scales well with  $J$  and has the value  $\Delta_d \simeq 0.15J - 0.27J$  until reaching the region of phase separation. The gap value is large ( $\lesssim 0.27J$ ) near half filling and small ( $\sim 0.15J$ ) around quarter filling. The renormalization factor varies over  $z_B \simeq 0.2 - 1$  with smaller values at low doping levels. Note that the maximum gap energy  $2\Delta_d/t \simeq 0.9$  ( $0.5$ ) around quarter filling at  $J/t=2.5$  ( $1.5$ ) (see Fig. 4) is significantly smaller than the effective half-bandwidth  $4t_{\text{eff}}/t \simeq 2.2$  estimated from the fitting of  $F(\mathbf{k}, \omega)$  and  $F(\mathbf{k}, \mathbf{k}', \omega)$ . Also, at low doping levels, we note that the estimated value  $2\Delta_d \simeq 0.5J - 0.6J$  is smaller than the effective bandwidth of  $\sim 2J - 4J$ . Thus, even near phase separation or at low doping levels, the superconductivity in the 2D  $t$ - $J$  model seems not in a limiting regime of a Bose condensate of a gas of preformed bosons but rather in an intermediate regime between weak and strong couplings.

The single-particle spectral function  $A(\mathbf{k}, \omega)$  (see Ref. [8] for the definition) simulates angle-resolved photoemission (PES) and inverse-photoemission (IPES) spectroscopy. The calculated spectra are shown in Fig. 5, which shows how the superconductivity affects the single-particle excitations. We find that with increasing  $J/t$  a gaplike feature appears at  $\mathbf{k}=(2\pi/3, 0)$ , which may be interpreted as a superconducting gap as the BCS dispersion  $\pm E_{\mathbf{k}}$  suggests. An associated spectral-weight transfer also indicates a tendency toward smearing of the jump at  $\mathbf{k}_F$  in the momentum distribution function. We have also calculated the spin-excitation spectrum  $S(\mathbf{q}, \omega)$  (not shown) and compared it with the bare susceptibility in the BCS mean-field theory. We find overall agreement in

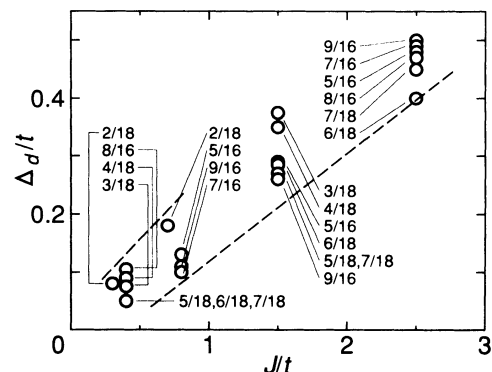


FIG. 4. Gap parameter  $\Delta_d$  for various  $J/t$  values and doping rates. The panel gives the number of holes (in the 16- or 18-site clusters) in the final state of the anomalous Green's functions: odd (even) numbers imply that the results are from the one-particle (two-particle) anomalous Green's function. The dashed lines are a guide to the eye.

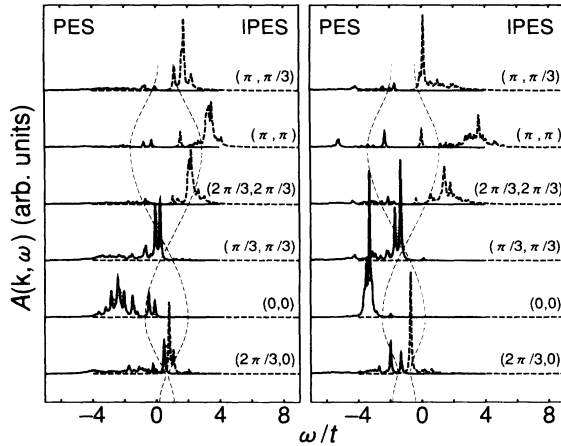


FIG. 5. Single-particle spectral function  $A(\mathbf{k}, \omega)$  for the 18-site cluster with 6 holes at  $J/t=0.4$  (left panel) and  $1.5$  (right panel).  $\omega$  is measured from the 6-hole ground-state energy,  $\mathbf{k}$ 's are shown in the panels, and the value  $\eta=0.05$  is used. The thin-dashed curves show the BCS dispersion  $\pm E_{\mathbf{k}}$  obtained for the parameter values used in Fig. 3: good agreement is seen near the Fermi energy while at higher energies meaningful comparison cannot be made because of the absence of damping effects.

cluding spectral-weight distributions and opening of the superconducting gap: the features are well interpreted in terms of the particle-hole excitations across the noninteracting Fermi surface, although at  $\mathbf{q}=(\pi, \pi)$  the effect of nearest-neighbor antiferromagnetic spin correlations becomes appreciable in the large  $J/t$  region or at low doping levels. Details will be discussed elsewhere.

Summarizing, we have studied the superconductivity in the 2D  $t$ - $J$  model with the use of a newly proposed technique for examining the low-lying excitation spectrum, i.e., the exact calculation of anomalous Green's

functions for Bogoliubov quasiparticle excitations characteristic of the superconducting state. The validity of the BCS pairing theory for a strongly correlated electron model has thereby been demonstrated for the first time. We have shown that the pairing occurs predominantly in the  $d_{x^2-y^2}$ -wave channel and the energy gap has a size  $\Delta_d \simeq 0.15J - 0.27J$  in a wide region between quarter and half fillings.

This work was supported by Priority-Areas Grants from the Ministry of Education, Science, and Culture of Japan. R. E. acknowledges financial support by the Japan Society for Promotion of Science. Computations were partly carried out in the Computer Center of the Institute for Molecular Science, Okazaki National Research Institutes.

- [1] E. Dagotto and J. Riera, Phys. Rev. Lett. **70**, 682 (1993); Phys. Rev. B **46**, 12 084 (1992).
- [2] E. Dagotto, J. Riera, Y. C. Chen, A. Moreo, A. Nazarenko, F. Alcaraz, and F. Ortolani, Phys. Rev. B **49**, 3548 (1994), and references therein.
- [3] J. A. Riera and A. P. Young, Phys. Rev. B **39**, 9697 (1989); E. Dagotto, J. Riera, and A. P. Young, *ibid.* **42**, 2347 (1990); P. Prelovšek and X. Zotos, *ibid.* **47**, 5984 (1993); D. Poilblanc, *ibid.* **48**, 3368 (1993).
- [4] V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990); W. O. Putikka, M. U. Luchini, and T. M. Rice, *ibid.* **68**, 538 (1992).
- [5] J. R. Schrieffer, *Theory of Superconductivity* (Benjamin, New York, 1964).
- [6] N. N. Bogoliubov, Nuovo Cimento **7**, 794 (1958); J. Valatin, *ibid.* **7**, 843 (1958).
- [7] See, e.g., review articles in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York, 1980), Vol. 35.
- [8] Y. Ohta, K. Tsutsui, W. Koshibae, T. Shimozato, and S. Maekawa, Phys. Rev. B **46**, 14 022 (1992).