RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 50, NUMBER 9 1 SEPTEMBER 1994-I

Reduced-density-matrix analysis of superconducting correlation in two-dimensional and two-chain Hubbard models

Y. Asai
Fundamental Physics Section, Electrotechnical Laboratory, Umezono 1-1-4, Tsukuba, Ibaraki 305, Japan
(Received 12 May 1994; revised manuscript received 29 June 1994)

We have calculated the largest eigenvalues of the reduced density matrix of the singlet superconducting correlation function and pair-field susceptibility in two-dimensional and two-chain Hubbard models with quantum Monte Carlo methods. A singlet superconducting channel opens upon doping but is otherwise closed at half-filling when $U/t=4$. The interaction vertex contribution to the largest eigenvalue of the singlet pair-field susceptibility grows with a power law as temperature is decreased. With these two observations, we revise our previous understanding of the interaction vertex in the two-dimensional Hubbard model. We observe that some phases reside in the two-chain Hubbard model. An analysis of the $2k_F$ charge correlation up to 32×2 sites suggests that the $2k_F$ correlation is dominant over the superconducting correlation ($0.25\leq K_\rho \leq 1.00$) in the two-component Luttinger-liquid phase ($U/t=2$ and $t_v/t=1.4$). We conclude the reduced-density-matrix analysis discussed here is needed to unveil the nature of Hubbard and related models.

Superconducting correlation in strongly correlated electron systems such as described the Hubbard model and the t-J model has received much attention in the context of the mechanism of high-T_c superconductivity in cuprate superconductors. Numerical studies, such as quantum Monte Carlo[1] and Lanczos diagonalization, have been performed[2] but we have not yet reached a definitive conclusion of whether the superconducting phase is truly described by such a model.

It is partly because the numerical methods have technical difficulties in accessing when a system size is sufficiently large to perform finite-size scaling at low temperature. The notorious "negative sign problem" in quantum Monte Carlo methods and a very severe restriction of system size in Lanczos diagonalization are examples of such difficulties.

There are other difficulties, such as the lack of an *a priori* algorithm to locate possible superconducting pairing structures. In most cases, nearest-neighbor (NN) d-wave, NN extended s-wave, and on-site s-wave, etc., pairing functions were assumed.[3] Even when further neighbors are taken into account, only some of the possible forms of pairing functions in each symmetry were tested.[4] We need a systematic method to find the most likely candidate for a superconducting pairing structure in a given model with given physical parameters.

Here, we introduce a reduced-density-matrix (RD) analysis of the superconducting correlation function and pair-field susceptibility with quantum Monte Carlo methods for that purpose. The method was originally introduced by Lin *et al.* in studying the superconducting pair-field susceptibility of the Hubbard model on as few as eight sites by the Lanczos method.[5] We combine the RD analysis with the analysis of the full and the uncorrelated part of the correlation function and the susceptibility. This combination enables us to perform a general search for the superconducting channel.

We define the following singlet pairing operator: $O_j=1/\sqrt{N}\Sigma_{\bar{i}}\lambda_{\bar{i}}c_{j\downarrow}c_{j+\bar{i}\uparrow}$. The most general form of the singlet superconducting correlation function $C(0)$ is

$$C(0)=\sum_{\bar{i},\bar{i}'} \lambda_{\bar{i}}\lambda_{\bar{i}'}\gamma_{\bar{i}\,\bar{i}'}, \tag{1a}$$

$$\gamma_{\bar{i}\,\bar{i}'}=\frac{1}{N}\sum_{ij} \langle c_{\bar{i}\downarrow}c_{\bar{i}+\bar{i}\uparrow}c^\dagger_{\bar{j}+\bar{i}'\uparrow}c^\dagger_{\bar{j}\downarrow}\rangle. \tag{1b}$$

After a spectral decomposition, $C(0)$ can be expressed as a sum that includes every superconducting mode:

$$C(0)=\sum_m |\eta_m|^2\omega_m, \tag{2}$$

where ω_m and η_m are the mth eigenvalue and normal coordinate of $\{\gamma_{\bar{i}\,\bar{i}'}\}$. As Eq. (1) is a special form of Löwdin's reduced density matrix[6] for the singlet superconducting correlation, we call $\{\gamma_{\bar{i}\,\bar{i}'}\}$ the RD of the singlet superconducting correlation function. Similarly, we define the RD of the singlet pair-field susceptibility $\{\chi_{\bar{i}\,\bar{i}'}\}$ by

$$\chi_{\bar{i}\,\bar{i}'}=\frac{1}{N}\sum_{ij}\int_0^\beta d\tau\langle T_\tau c_{\bar{i}\downarrow}(\tau)c_{\bar{i}+\bar{i}\uparrow}(\tau)c^\dagger_{\bar{j}+\bar{i}'\uparrow}(0)c^\dagger_{\bar{j}\downarrow}(0)\rangle, \tag{3}$$

where $\beta=1/T$ and T is the temperature. The uncorrelated part of the RD of the singlet superconducting correlation function $\{\bar{\gamma}_{\bar{i}\,\bar{i}'}\}$, and the RD of the singlet pair-field susceptibility $\{\bar{\chi}_{\bar{i}\,\bar{i}'}\}$ are defined, respectively, by

$$\bar{\gamma}_{\bar{i}\,\bar{i}'}=\frac{1}{N}\sum_{ij} \langle c_{\bar{i}\downarrow}c^\dagger_{\bar{j}\downarrow}\rangle\langle c_{\bar{i}+\bar{i}\uparrow}c^\dagger_{\bar{j}+\bar{i}'\uparrow}\rangle, \tag{4a}$$

$$\bar{\chi}_{\bar{i}\,\bar{i}'}=\frac{1}{N}\sum_{ij}\int_0^\beta d\tau\langle T_\tau c_{\bar{i}\downarrow}(\tau)c^\dagger_{\bar{j}\downarrow}(0)\rangle \times\langle T_\tau c_{\bar{i}+\bar{i}\uparrow}(\tau)c^\dagger_{\bar{j}+\bar{i}'\uparrow}(0)\rangle. \tag{4b}$$

It should be noted that the mode vectors of superconducting modes of the full and the uncorrelated RD are not identical in general. In our method, the pairing structure of the supercon-

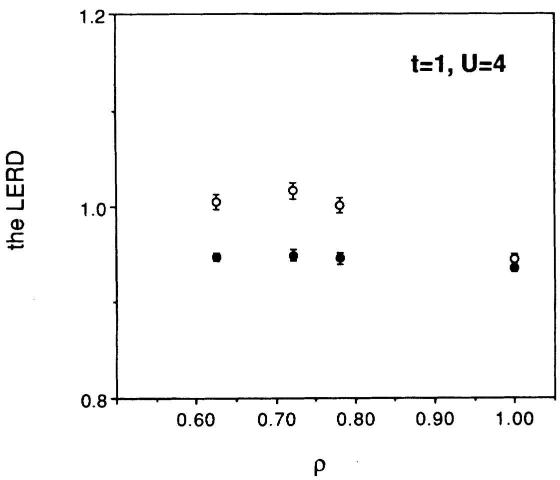

FIG. 1. Filling ($\rho \equiv N_e/N_s$) dependence of the LERD of the ground-state singlet superconducting correlation function of the two-dimensional Hubbard model with $t=1$ and $U=4$. The data at $\rho=0.625$, 0.72, 0.78, and 1.00 were calculated with 4×4, 6×6, 8×8, and 4×4 lattices with projecting time $\tau=15$, 7, 4, and 15 in units of t, respectively. We have also calculated the $\rho=1.00$ case with the 6×6 lattice, and we found no change in quantity. In all fillings, open circles and closed circles are the full and the uncorrelated LERD, respectively. We find an opening of the superconducting channel upon doping otherwise closed at $\rho=1.00$.

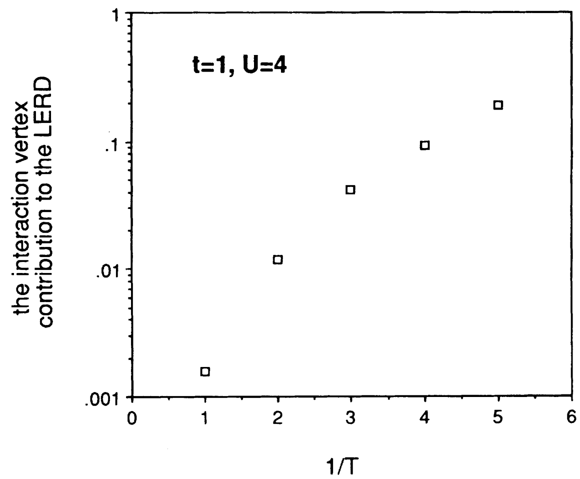

FIG. 2. Temperature dependence the interaction vertex contribution to the LERD of the singlet pair-field susceptibility defined by the difference between the full and the uncorrelated LERD of the two-dimensional 4×4 Hubbard model. The interaction vertex contribution to the LERD is plotted against the inverse temperature $1/T$ in log-linear scale. The physical parameters are the same as in Fig. 1. The filling is 0.89. The interaction vertex contribution to the pair-field susceptibility grows as $1.57\times10^{-3}(1/T)^{2.97}$ as temperature is decreased.

ducting mode has the freedom to be changed upon turning on the interaction vertex, as it should be.

We apply the method to the two-dimensional square lattice and the two-chain Hubbard models. The Hamiltonian of the two-dimensional Hubbard model is given by

$$H=-t\sum_{\langle i,j\rangle\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}, \qquad (5)$$

where $\langle ij\rangle$ represents sum over the nearest neighbors.

The square lattice Hubbard model is the most promising model that has explained many experimental observations of cuprates such as the gap formation at $Q=(\pi,\ \pi)$ in the spin excitation spectrum[7] observed in neutron scattering experiments and it is still the most likely candidate for a model for the cuprate.

We have used the determinantal quantum Monte Carlo and projector Monte Carlo methods in calculating finite-temperature and ground-state physical properties, respectively.[1] We have developed the codes previously.[8] We have adopted the matrix-stabilization techniques proposed by Loh and Gubernatis in calculating both equal-time and imaginary-time-dependent Green functions.[9] These theoretical techniques should be consulted in Refs. 1 and 9.

We have calculated the largest eigenvalue of the RD (LERD) of the ground-state superconducting correlation functions in the two-dimensional square lattice Hubbard model. We have also calculated the uncorrelated part of the LERD of the ground-state correlation function. The results are summarized in Fig. 1. We used 10 electron 4×4 site, 26 electron 6×6 site, and 50 electron 8×8 site systems with the periodic boundary condition, respectively. These system forms closed-shell in the noninteracting case that reduces "negative sign" ratio in the projector Monte Carlo sampling.[10,11] The ratio strongly depends on filling but also depends on U and the projecting time τ. In any case the ratio in the closed-shell system is much smaller than that in the open-shell condition provided that the other parameters are the same. The reason for this observation is still unknown. The notorious "negative sign" problem in the open-shell condition of the projector Monte Carlo calculation does not allow us to do meaningful finite-size scaling analysis with sufficiently large projecting time. This prevents us from making a definitive conclusion on superconductivity through the analysis of the correlation function. The physical parameters are $t=1.0$ and $U=4$. While the full LERD of the correlation function is almost identical to the uncorrelated LERD of the correlation function at half-filling, the full LERD surpasses the uncorrelated LERD in the less than half-filling case. The enhancement has a broad peak at $\rho\equiv N_e/N_s=0.70$. This indicates that while the interaction vertex opens a superconducting channel in the less than half-filling cases the channel is closed at half-filling. This is quite different from the previous observation with NN d-wave pairing.[3,12] The enhancement with the interaction vertex of the NN d-wave pairing is largest at half-filling.

We have calculated the LERD of the singlet pair-field susceptibility and its uncorrelated part of the two-dimensional 4×4 Hubbard model with the same physical parameters. The filling is $\langle n\rangle=0.89$. We plotted the interaction vertex contribution, i.e., the difference of the full and the uncorrelated part, against the inverse of the temperature, $1/T$ in Fig. 2. The unit of the temperature T is t. As temperature is decreased, the interaction vertex contribution grows as $1.57\times10^{-3}(1/T)^{2.97}$. While a low enough temperature ($T\approx0.01t$) cannot be reached for us to make a definitive conclusion on a possible superconducting transition in this model due to the "negative sign" problem and bad statistical independence, the data we obtained down to $T=0.2$ may be an indication of the possibility. The pairing symmetry that gives the LERD of the singlet pair-field susceptibility is d-wave-like. The real-space singlet pairing structure factor includes a large contribution from distanced pairs as well as the NN d-wave pair. The d-wave-like superconducting channel is one of the most plausible superconducting channels in the two-dimensional Hubbard model. The eigenvalue of the RD of the ground-state singlet superconducting correlation function with an extended s-wave-like pairing structure factor accompanied with a contribution from distanced pairs with nodes in radial directions is a bit larger than that of a d-wave-like structure factor. We cannot exclude the possibility of an extended s-wave-like pairing channel, before we find a way to overcome the "negative sign" problem to make it possible to do a finite-size scaling analysis in the two-dimensional Hubbard model.

It should be mentioned that we have made the same analysis on the 4×2 Hubbard model, which Lin *et al.* studied. We have used the same parameters as in Fig. 1 of their paper.[5] We do not observe enhancements due to the interaction vertex at low temperature.

Following the experimental observation of a line defect in $SrCuO_2$,[13] some groups studied the two-chain t-J model[14] and/or the two-chain Hubbard model.[15–18] The Hamiltonian of the two-chain Hubbard model is given by

$$H=-t\sum_{\langle i,j\rangle\sigma}(c^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.})+U\sum_{i} n^{c}_{i\uparrow}n^{c}_{i\downarrow}$$

$$-t\sum_{\langle i,j\rangle\sigma}(d^{\dagger}_{i\sigma}d_{j\sigma}+\text{H.c.})+U\sum_{i} n^{d}_{i\uparrow}n^{d}_{i\downarrow}$$

$$-t_v\sum_{i\sigma}(c^{\dagger}_{i\sigma}d_{i\sigma}+\text{H.c.}), \qquad (6)$$

where t_v is a transfer integral in the direction vertical to the chains. In this anisotropic system, we need a RD analysis to make the arguments more clear. We have made a RD analysis of the ground-state superconducting correlation function. We have also tried a finite-size scaling analysis of the $2k_F$ charge correlation to estimate the upper and the lower bounds of K_ρ.

We have calculated the LERD of the ground-state correlation function and its uncorrelated part of the 16×2 Hubbard model at 0.75 filling. We used $t=1.0$ and $U=2.0$. We changed t_v and traced the changes of the full and uncorrelated LERD. We plotted the results in Fig. 3. The interval $(0.0<t_v\leqslant 2.0)$ can be classified into four regions, some of which are characterized by bumps of the LERD. We have labeled the four regions with Roman numerals in Fig. 3. In region IV, we observe little enhancements of the LERD by the interaction vertex and hence attractions. We found stronger attraction in the other regions. On the basis of a calculated momentum-dependent spin correlation function along with the help of a weak-coupling renormalization-group (RG) result,[18] we tentatively assign regions I and II, region III, and region IV a strong-coupling phase (SC2), a two-component Luttinger-liquid phase, and a Luttinger-liquid phase, respectively. The presence of a Luttinger-liquid phase

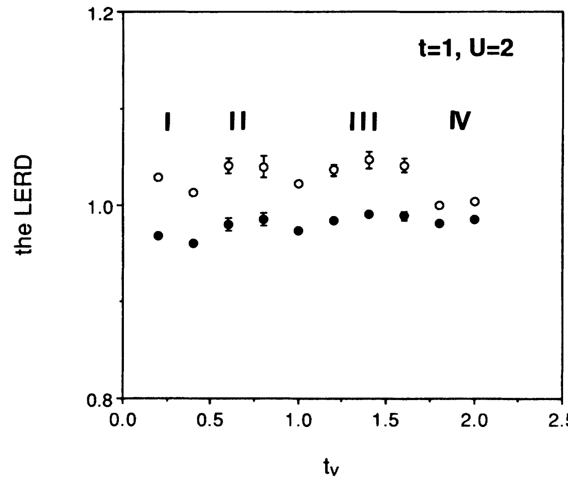

FIG. 3. The vertical transfer integral t_v dependence of the LERD of the ground-state singlet superconducting correlation function of the 16×2 two-chain Hubbard model with $t=1$, $U=2$, and $\rho=0.75$. We used projecting time $\tau=10$ except at $t_v=1$, where we used $\tau=7.5$. The open and closed circles are the full and the uncorrelated LERD, respectively. We found four regions in this model. We labeled each of them with Roman numbers. We found attraction except in phase IV.

at $t_v=0$ is trivial. Besides the possibility of two distinct strong-coupling phases in $0.0<t_v\leqslant 1.0$, our projector Monte Carlo result does not contradict the weak-coupling RG result predicting the SC2, the two-component Luttinger-liquid phase, and the Luttinger-liquid phase in the interval.

We have tried finite-size scaling analysis of the $2k_F$ charge correlation with the same physical parameters and fillings as before but with a fixed value of $t_v=1.4$ (the two-component Luttinger-liquid phase) by use of 8×2 site, 12×2 site, 16×2 site, 28×2 site, and 32×2 site systems. We used a periodic boundary condition and used systems that give a closed-shell for the lower band in the noninteracting case. The upper band touches the Fermi level in the noninteracting case. We define the following quantity for the finite-size scaling analysis:[19] $b(k,L/2)=2C(k)-C(k+2\pi/L)-C(k-2\pi/L)$ and $C(k)=1/N\Sigma_{ij}\exp\{ik(r_i-r_j)\}\langle n^c_i n^c_j\rangle$, where L is the length of the double chains. We notice that $\langle n^c_0 n^c_{L/2}\rangle = 1/(4L)\Sigma_k \exp\{ikL/2\}b(k,L/2)$. If the following relation holds:

$$b(2k_F,L/2)\propto (L/2)^{-K_\rho}, \qquad (7)$$

then the long-range behavior of the $2k_F$ charge correlation is

$$\langle n^c_0 n^c_r\rangle \propto \cos(2k_F r) r^{K_\rho+1}. \qquad (8)$$

We plotted $\ln b(k,L/2)$ versus $\ln L$ in Fig. 4. While the curvature is large in the smaller-L region, the curvature gets smaller in the larger-L region. As the system size becomes larger over 32×2 sites, $b(2k_F,L/2)$ becomes smaller even than statistical error. The finite-size scaling analysis by use of $b(2k_F,L/2)$ becomes more difficult in that situation. We are still able to estimate the upper and the lower bounds of K_ρ from the information involved in Fig. 4. Our estimate of K_ρ in this system is $0.25\leqslant K_\rho \leqslant 1.00$. We have used the 16×2, 28×2, and 32×2 lattices for the estimates of the

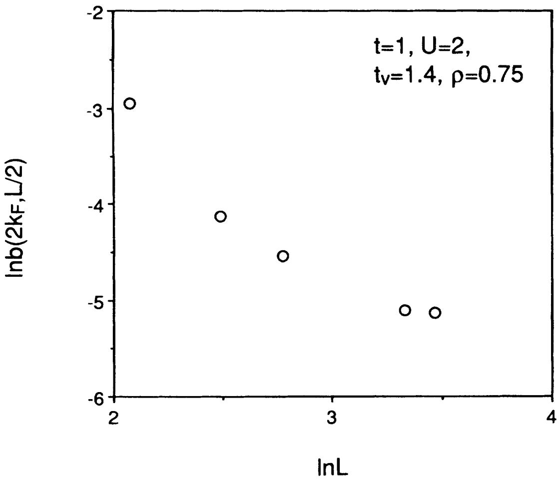

FIG. 4. Finite-size scaling analysis of the $2k_F$ charge correlation in the two-chain Hubbard model with $t=1$, $U=2$ and $t_v=1.4$, $\rho=0.75$. $\ln b(k,L/2)$ is plotted against $\ln L$. We have used 8×2, 12×2, 16×2, 28×2, and 32×2 lattices. Projecting time τ is 10 in all cases. By use of the 16×2, 28×2, and 32×2 lattices we estimate $0.25\leqslant K_\rho\leqslant1.0$.

bounds. We do not support the result obtained by diagonalization study of very small clusters.[17] The $2k_F$ correlation is dominant over superconducting correlation, if we assume the Luttinger universality relations hold.[20] The weak-coupling RG study does not contradict our result.

To summarize, we have introduced the reduced-density-matrix analysis to the quantum Monte Carlo and the projector Monte Carlo methods. We have applied our method to the two-dimensional and the two-chain Hubbard models. We observe opening of a superconducting channel upon doping otherwise closed at the half-filling in the two-dimensional Hubbard model. The interaction vertex contribution to the largest eigenvalue of the reduced density matrix of the singlet pair-field susceptibility grows with a power law as temperature is decreased in that model. These may indicate a superconductivity parameter phase in the two-dimensional Hubbard model. We revise the previous understanding of the interaction vertex in the two-dimensional Hubbard model. We have made the reduced-density-matrix analysis of the ground-state superconducting correlation function and finite-size scaling analysis of the $2k_F$ part of the charge correlation function of the two-chain Hubbard model. We found some phases present in the two-chain Hubbard model with $t=1$, $U=2$, $0.0<t_v\leqslant2.0$ and $\rho=0.75$. The analysis of the $2k_F$ charge correlation up to 32×2 sites suggests that the $2k_F$ correlation is dominant over superconducting correlation ($0.25\leqslant K_\rho\leqslant1.00$) in the two-component Luttinger-liquid phase ($U/t=2$ and $t_v/t=1.4$). Except for the possibility of two distinct phases in the strong-coupling region, our result does not contradict a weak-coupling renormalization-group result on the two-chain Hubbard model.

Applications of the RD analysis were found to be very successful in the two-dimensional and the two-chain Hubbard models. We conclude the analysis is needed to unveil the nature of Hubbard and related models.

The author would like to thank to Dr. Richard L. Martin and Dr. J. E. Gubernatis of Los Alamos National Laboratory for stimulating conversations on the quantum-chemical reduced-density-matrix concepts. He is also thankful to the computer center of Institute of Molecular Science for allocating CPU time to the author.

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