Quantum Monte Carlo study of the pairing correlation in the Hubbard ladder

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(Received 20 September 1996)

An extensive quantum Monte Carlo calculation is performed for the two-leg Hubbard ladder model to clarify whether the singlet pairing correlation decays slowly, which is predicted from the weak-coupling theory but controversial from numerical studies. Our result suggests that the discreteness of energy levels in finite systems affects the correlation enormously, where the enhanced pairing correlation is indeed detected if we make the energy levels of the bonding and antibonding bands lie close to each other at the Fermi level to mimic the thermodynamic limit. [S0163-1829(96)51846-1]

Over the past several years, strongly correlated electrons on ladders have received much attention both theoretically and experimentally.[1] Interest stems from theoretical studies suggesting a formation of a spin gap and the possible occurrence of superconductivity in such systems.[2,3] Weak-coupling theory with bosonization and renormalization-group techniques[4–9] has indeed shown that the Hubbard model on a two-leg ladder has a spin gap, and if the system is free from umklapp processes, the singlet pairing correlation function decays as $\sim 1/r^{\alpha}$ with $\alpha = 1/2$ (where r is the real-space distance) in the weak-coupling limit.

Since spin-density wave and $2k_F$ charge-density wave (CDW) correlations have to decay exponentially in the presence of a spin gap in a two-leg ladder, the only phase competing with superconductivity will be $4k_F$ CDW, whose correlation should decay as $1/r^{1/\alpha}$. Hence the pairing correlation dominates over all the others if $\alpha < 1$.

As for the opening of the spin gap, the density-matrix renormalization-group (DMRG) studies in the strong-coupling regime also indicate its presence in both t-J and Hubbard ladder models.[10–12] If we further focus on the t-J ladder, DMRG[12] detects a pairing correlation decaying slightly slower than $\sim 1/r$ and a CDW correlation decaying faster than $\sim 1/r$ for an electron density of $n = 0.8$ with $J/t = 1$.[13]

However, the dominance of the pairing correlation in the *Hubbard* ladder model seems to be a subtle problem in numerical calculations. Namely, a DMRG study by Noack *et al.* for the doped Hubbard ladder with $n = 0.875$, $U/t = 8$, and $t_\perp = t$ (where t and $t_\perp$ are intra- and interchain hoppings, respectively) shows no enhancement of the pairing correlation over the $U = 0$ result,[10] while they do find an enhancement at $t_\perp = 1.5t$.[11] Asai performed a quantum Monte Carlo (QMC) calculation for a 36-rung ladder with $n = 0.833$, $U/t = 2$, and $t_\perp = 1.5t$,[14] in which no enhancement of the pairing correlation was found. On the other hand, Yamaji *et al.* have found an enhancement for the values of the parameters where the lowest antibonding band levels for $U = 0$ approaches the highest occupied bonding band levels, although their results have not been conclusive due to small system sizes ($\leqslant 6$ rungs).[15]

Thus, existing analytical and numerical results appear to be controversial. This is disturbing since the superconductivity in the Hubbard ladder, especially with $t_\perp \sim t$, is of great interest as a model for cuprate ladderlike materials, for which an occurrence of superconductivity has indeed been reported very recently.[16] In the present work, we have performed an extensive QMC calculation for the Hubbard ladder with $t_\perp \sim t$ in order to clarify the origin of the discrepancies among existing results. We conclude that the discreteness of energy levels in finite systems affects the pairing correlation enormously, where the enhanced pairing correlation is indeed detected if we tune the parameters so as to align the discrete energy levels of bonding and antibonding bands at the Fermi level in order to mimic the thermodynamic limit.

The Hamiltonian of the two-leg Hubbard ladder is given in standard notations as

$$\mathcal{H} = -t \sum_{\alpha i \sigma} (c^\dagger_{\alpha i \sigma} c_{\alpha i+1 \sigma} + \text{H.c.}) - t_\perp \sum_{i\sigma} (c^\dagger_{1,i\sigma} c_{2,i\sigma} + \text{H.c.}) + U \sum_{\alpha i} n_{\alpha i \uparrow} n_{\alpha i \downarrow}, \tag{1}$$

where $\alpha (= 1,2)$ specifies the chains.

In the weak-coupling theory, the amplitude of the pair hopping process between the bonding and antibonding bands in momentum space flows into the strong-coupling regime upon renormalization, resulting in a formation of gaps in both of the two spin modes and a gap in one of the charge modes when the umklapp processes are irrelevant. This leaves one charge mode massless, where the mode is characterized by a critical exponent K_ρ, which should be close to unity in the weak-coupling regime. Then the correlation function of an interchain singlet pairing, $O_i = (c_{1i\uparrow} c_{2i\downarrow} - c_{1i\downarrow} c_{2i\uparrow})/\sqrt{2}$, decays like $1/r^{1/(2K_\rho)}$.

Here, we have applied the projector Monte Carlo method[17] to look into the ground state correlation function $P(r) \equiv \langle O^\dagger_{i+r} O_i \rangle$ of this pairing. We assume periodic boundary conditions along the chain direction, $c_{N+1} \equiv c_1$, where N is the number of rungs.

The details of the QMC calculation are the following. We took the noninteracting Fermi sea as the trial state. The projection imaginary time τ was taken to be $\sim 60/t$. We need such a large τ to ensure the convergence of especially the long-range part of the pairing correlation. This sharply contrasts with the situation for single chains, where $\tau \sim 20/t$ suf-

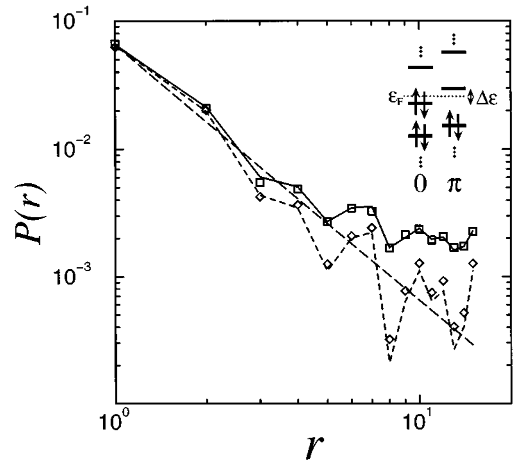

FIG. 1. The pairing correlation function, $P(r)$, plotted against the real space distance r in a 30-rung Hubbard ladder having 52 electrons for $U=1$ with $t_\perp=0.98$ (□) and $t_\perp=1.03$ (◇). The dashed line is the noninteracting result for the same system size, while the straight dashed line represents $1/r^2$. The solid line is a fit to the $U=1$ result with $t_\perp=0.98$ (see text). The inset shows a schematic image of the discrete energy levels of bonding (0) and antibonding (π) bands for $U=0$.

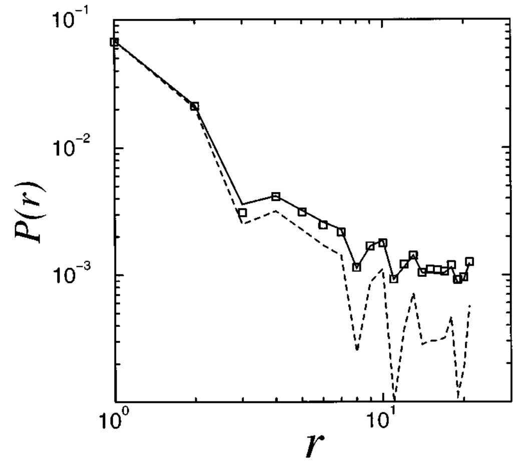

FIG. 2. A similar plot as in Fig. 1 for a 42-rung system having 76 electrons with $t_\perp=0.99$.

fices for the same sample length considered here. The large value of τ, along with a large on-site repulsion U, makes the negative-sign problem serious, so that the calculation is feasible for $U/t\leqslant 2$. In the Trotter decomposition, the imaginary time increment [τ/(number of Trotter slices)] is taken to be $\leqslant 0.1$. We have concentrated on band fillings for which the closed-shell condition (no degeneracy in the noninteracting Fermi sea) is met. We set $t=1$ hereafter.

We first show in Fig. 1 the result for $P(r)$ for $t_\perp=0.98$ and $t_\perp=1.03$ with $U=1$ and the band filling $n=0.867=52$ electrons/(30 rungs $\times$ 2 sites). The $U=0$ result (dashed line) for these two values of $t_\perp$ are identical because the Fermi sea remains unchanged. However, if we turn on U, the 5% change in $t_\perp=0.98\rightarrow 1.03$ is enough to cause a dramatic change in the pairing correlation: the $t_\perp=0.98$ result has a large enhancement over the $U=0$ result at large distances, while the enhancement is not seen for $t_\perp=1.03$.

In fact we have deliberately chosen these values to control the alignment of the discrete energy levels at $U=0$ in finite, two-band systems. Namely, when $t_\perp=0.98$, the one-electron energy levels of the bonding and antibonding bands for $U=0$ lie close to each other around the Fermi level with the level offset ($\Delta\varepsilon$ in the inset of Fig. 1) being as small as 0.004, while they are staggered for $t_\perp=1.03$ with the level offset of 0.1. On the other hand, the size of the spin gap is known to be around $0.05t$ for $U=8$,[11] and is expected to be of the same order of magnitude or smaller for smaller values of U. The present result then suggests that if the level offset $\Delta\varepsilon$ is too large compared to the spin gap, the enhancement of the pairing correlation cannot be seen. By contrast, for a small enough $\Delta\varepsilon$, by which an infinite system is mimicked, the enhancement is indeed detected as expected from the weak coupling theory, in which the spin gap is assumed to be infinitely large at the fixed point of the renormalization flow.

Our result is reminiscent of those obtained by Yamaji *et al.*,[15] who found an enhancement of the pairing correlation in a restricted parameter regime where the lowest antibonding levels approaches the highest occupied bonding levels. They conclude that superconductivity occurs when the antibonding band ''slightly touches'' the Fermi level. However, our result in Fig.1 is obtained for the band filling for which no less than seven out of 30 antibonding levels are occupied at $U=0$. Hence the enhancement of the pairing correlation is not restricted to the situation where the antibonding band edge touches the Fermi level.

Now, let us more closely look into the form of $P(r)$ for $t_\perp=0.98$. It is difficult to determine the decay exponent of $P(r)$, but here we attempt to fit the data by assuming a trial function expected from the weak-coupling theory. Namely, we have fitted the data with the form $P(r)=(1/4\pi^2)\sum_{d=\pm}\{c r_d^{-1/2}+(2-c)\,r_d^{-2}-[\cos(2k_F^0 r_d)+\cos(2k_F^\pi r_d)]\,r_d^{-2}\}$ with the least-square fit (by taking logarithm of the data) $c=0.11$. Because of the periodic boundary condition, we have to consider contributions from both ways around, so there are two distances between the 0th and the rth rung, i.e, $r_+=r$ and $r_-=N-r$. The period of the cosine terms is assumed to be the noninteracting Fermi wave numbers of the bonding and the antibonding bands in analogy with the single-chain case. The overall decay should be $1/r^2$ as in the pure one-dimensional (1D) case. We have assumed the form $c/r^{1/2}$ as the dominant part of the correlation at large distances because this is what is expected in the weak-coupling theory. A finite $U\sim 1$ may give some correction, but the result (solid line in Fig. 1) fits to the numerical result surprisingly accurately. If we least-square fit the exponent itself as $1/r^\alpha$, we have $0.2<\alpha<0.7$ with a similar accuracy. Thus a finite U may change α, but $\alpha>1$ may be excluded. To fit the short-range part of the data, we require nonoscillating $(2-c)/r^2$ term, which is not present in the weak-coupling theory. We believe that this is because the weak-coupling theory only concerns with the asymptotic form of the correlation functions.

In Fig. 2, we show a result for a larger system size (42 rungs) for a slightly different electron density, $n=0.905$ with 76 electrons and $t_\perp=0.99$. We have again an excellent fit with $c=0.07$ this time.

In Fig. 3, we display the result for a larger $U=2$. We

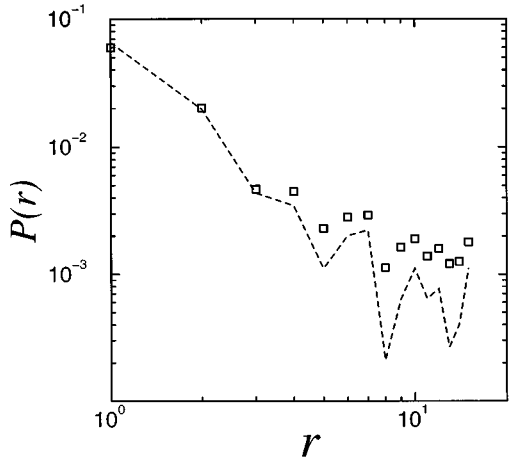

FIG. 3. A similar plot as □ in Fig. 1 except $U=2$ here.

again have a long-ranged $P(r)$ at large distances, although $P(r)$ is slightly reduced from the result for $U=1$. This is consistent with the weak-coupling theory, in which K_ρ is a *decreasing* function of U so that once the spin gap opens for $U>0$, the pairing correlation decays faster for larger values of U.

To explore the effect of umklapp processes, we now turn to the filling dependence for a fixed interaction $U=2$. We have tuned the value of $t_\perp$ to ensure that the level offset $(\Delta\varepsilon)$ at the Fermi level is as small as $O(0.01t)$ for $U=0$. In this way, we can single out the effect of umklapp processes from those due to large values of $\Delta\varepsilon$. If we first look at the half-filling [Fig. 4(a)], the decaying form is essentially similar to the $U=0$ result. At the half-filling interband umklapp processes emerge and, according to the weak-coupling theory, open a charge gap, which results in an exponential decay of the pairing correlation. It is difficult to tell from our data whether $P(r)$ decays exponentially. This is probably due to the smallness of the charge gap. In fact, Noack *et al.*[10] have obtained with DMRG an exponential decay for larger values of U, for which a larger charge gap is expected.

When n is decreased down to 0.667 [Fig. 4(b)], we again observe an absence of enhancement in $P(r)$. This is again consistent with the weak-coupling theory:[8] for this band filling, the number of electrons in the bonding band coincides with $N(=30)$ at $U=0$, i.e., the bonding band is half-filled. This will then give rise to intraband umklapp processes within the bonding band resulting in the ''C1S2'' phase discussed in Ref. 8, in which the spin gap is destroyed so that the pairing correlation will no longer decay slowly.[18]

In summary, we have seen that there are three possible causes that reduce the pairing correlation function in the Hubbard ladder: (i) the discreteness of the energy levels, (ii) reduction of K_ρ for large values of U/t, and (iii) effect of intra- and interband umklapp processes around specific band fillings. The first one is a finite-size effect, while the latter two are present in infinite systems as well. We can make a possible interpretation to the existing results in terms of these effects. For 60 electrons on 36 rungs with $t_\perp=1.5t$ in Ref. 14, for instance, the noninteracting energy levels have a significant offset $\sim 0.15t$ between bonding and antibonding levels at the Fermi level, which may be the reason why the

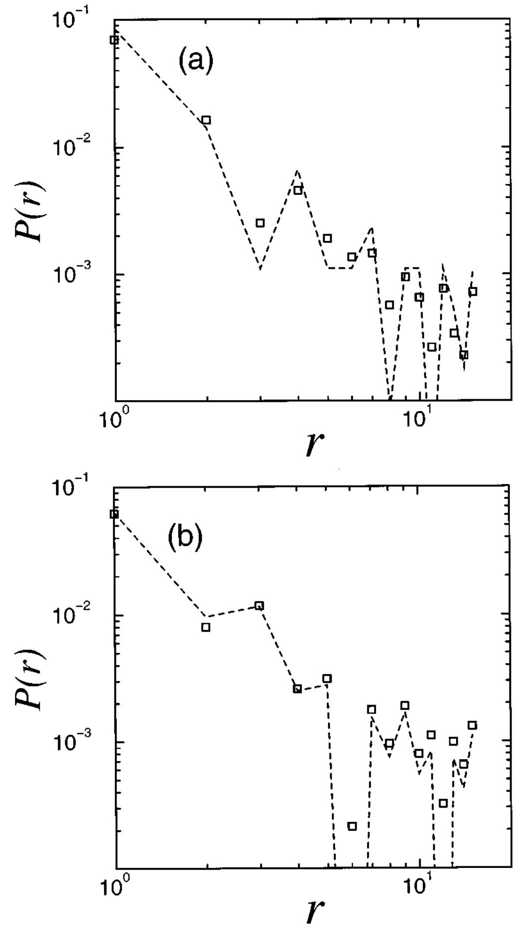

FIG. 4. The pairing correlation $P(r)$ (□) against r for a 30-rung system for $U=2$ with (a) $t_\perp=0.99$ and 60 electrons (half-filled), and (b) $t_\perp=1.01$ and 40 electrons (half-filled bonding band). The dashed line represents the noninteracting result.

pairing correlation is not enhanced for $U/t=2$. For a large $U/t(=8)$ in Refs. 10 and 11, (ii) and/or (iii) in the above may possibly be important in making the pairing correlation for $t_\perp=t$ not enhanced. The effect (iii) should be more serious for $t_\perp=t$ than for $t_\perp=1.5t$ because the bonding band is closer to the half-filling in the former. On the other hand, the discreteness of the energy levels might exert some effect as well, since the noninteracting energy levels for a 32-rung ladder with 56 electrons ($n=0.875$) in an open boundary condition have an offset of $0.15t$ at the Fermi level for $t_\perp=t$ while the offset is $0.03t$ for $t_\perp=1.5t$.

Finally, let us comment on a possible relevance of the present result to the superconductivity reported recently for a cuprate ladder,[16] especially for the pressure dependence. The material is $Sr_{0.4}Ca_{13.6}Cu_{24}O_{41.84}$, which contains layers consisting of two-leg ladders and those consisting of 1D chains. Superconductivity is not observed in the ambient pressure, while it appears with $T_C\sim 10$ K under the pressure of 3 GPa or 4.5 GPa, and finally disappears at a higher pressure of 6 GPa. This material is doped with holes with the total doping level of $\delta=0.25$, where δ is defined as the deviation of the density of electrons from the half-filling. It has been proposed that at ambient pressure the holes are mostly in the chains, while high pressures cause the carrier to transfer into the ladders.[19] If this is the case, and if most of the holes are transferred to the ladders at 6 GPa, the experimental result is consistent with the present picture, since there is no enhancement of the pairing correlation for $\delta=0$ and $\delta\sim0.3$ due to the umklapp processes as we have seen. Evidently, further investigation especially in the large-U regime is needed to justify this speculation.

Numerical calculations were done on HITAC S3800/280 at the Computer Center of the University of Tokyo, and FACOM VPP 500/40 at the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. For the former facility we thank Professor Y. Kanada for support in ''Project for Vectorized Supercomputing.'' This work was also supported in part by Grant-in-Aid for Scientific Research from the Ministry of Education, Science, Sports and Culture of Japan. One of the authors (T.K.) acknowledges the Japan Society for the Promotion of Science for financial support.

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