Phase diagram of the two-chain Hubbard model

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We have calculated the charge gap and spin gap for the two-chain Hubbard model as a function of the on-site Coulomb interaction and the interchain hopping amplitude. We used the density matrix renormalization group method and developed a method to calculate separately the gaps numerically for the symmetric and antisymmetric modes with respect to the exchange of the chain indices. We have found very different behaviors for the weak and strong interaction cases. Our calculated phase diagram is compared to the one obtained by Balents and Fisher using the weak coupling renormalization group technique. [S0163-1829(99)05404-1]

Although the Luttinger liquid behavior of the one-dimensional Hubbard model has been well understood, the two-dimensional Hubbard model, which is believed to be related to the understanding of the high T_c superconductivity,[1] is not yet clear. As a crossover between one and two dimensions, the two-chain Hubbard model is certainly a good theoretical basis for the ladder compounds.[2,3] It is important to understand how two Luttinger liquid systems evolve to the ladder system as the interchain coupling is introduced.

The Hamiltonian for the two-chain Hubbard model is

$$H=-t_{||}\sum_{l,\langle i,j\rangle,\sigma}(c^{\dagger}_{li\sigma}c_{lj\sigma}+\text{H.c.}) -t_{\perp}\sum_{i,\sigma}(c^{\dagger}_{1i\sigma}c_{2i\sigma}+\text{H.c.})+U\sum_{l,i}n_{li,\uparrow}n_{li,\downarrow}, \quad (1)$$

where l is the chain index $l=1,2$. We have the intrachain hopping $t_{||}$ term, the interchain hopping $t_{\perp}$ term, and the on-site Coulomb interaction U term. $t_{||}=1$ in this paper.

Several authors have studied the phase diagram of the two-chain Hubbard model using the weak coupling renormalization group method.[4–6] At half filling the system is an insulator with a spin gap. Upon light hole doping, for small $t_{\perp}$ the spin gap remains finite. For large $t_{\perp}$ the complete separation between the bonding band and the antibonding band leads the system to a Luttinger liquid phase. However, it remains unclear for large U case which is equivalent to the t-J ladder.[7–10] Balents and Fisher described the phase in terms of number of gapless charge and spin modes, which they denoted by CnSm, where n is the number of gapless charge modes and m is the number of gapless spin modes.[6] For our work we also use this notation. Their phase diagram is rather diverse in the hole-doped region. Interestingly, they found phases such as C2S2 and C2S1 between the C1S1 Luttinger liquid phase and the spin-gapped C1S0 phase. The phase diagram is qualitatively the same for different electron filling n, except for the cases of half filling, quarter filling, and a half-filled bonding band, where the umklapp process will be relevant.

Since most of the previous results done by the weak coupling renormalization group method may be reliable only in the $U\rightarrow 0^{+}$ limit, the questions are whether it will be similar for finite U and whether it will depend on U. Noack *et al.* have studied the correlation functions and the gaps for finite U using the density matrix renormalization group (DMRG) method.[11] They found the enhancement of the d-wave pairing correlation function for the spin-gapped phase at a rather anisotropic regime $t_{\perp}>t_{||}$, though they cannot distinguish the symmetric and antisymmetric modes. Hence it is difficult to determine which CnSm phase it is. To understand the phase diagram in detail and to make a comparison with the weak coupling result it is necessary to study the charge and spin excitations in different modes for finite U.

In this paper we study the phase diagram of the two-chain Hubbard model by calculations of the charge and spin gaps for the symmetric mode and antisymmetric mode, respectively, for finite values of U at a fixed electron filling $n=0.75$. Using this result, we can easily understand the result for other electron filling. For our study, we use the DMRG method[12,13] and develop a method to differentiate the modes.

We take the transform of c operators in terms of bonding and antibonding forms

$$c_{\pm i\sigma}=\frac{1}{\sqrt{2}}(c_{1i\sigma}\pm c_{2i\sigma}). \quad (2)$$

Then the Hamiltonian becomes

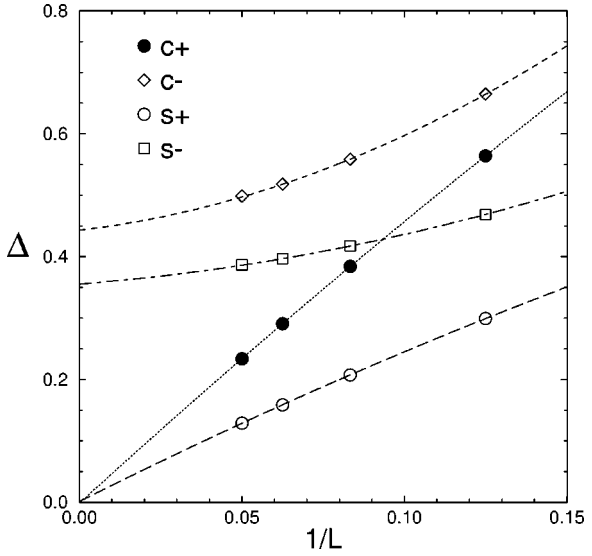

FIG. 1. Gaps versus $1/L$ to calculate the thermodynamic values of gaps for $U=8$ and $t_\perp=1.7$. We denote symmetric charge gaps with closed circles, antisymmetric charge gaps with diamonds, symmetric spin gaps with open circles, and antisymmetric spin gaps with squares.

$$
\begin{aligned}
H=&-t_{\|}\sum_{\langle i,j\rangle,\sigma}(c^{\dagger}_{+i\sigma}c_{+j\sigma}+c^{\dagger}_{-i\sigma}c_{-j\sigma}+\text{H.c.})\\
&-t_{\perp}\sum_{i,\sigma}(c^{\dagger}_{+i\sigma}c_{+i\sigma}-c^{\dagger}_{-i\sigma}c_{-i\sigma})\\
&+\frac{U}{2}\sum_{i}[(n_{+i\uparrow}+n_{-i\uparrow})(n_{+i\downarrow}+n_{-i\downarrow})\\
&+c^{\dagger}_{+i\uparrow}c^{\dagger}_{+i\downarrow}c_{-i\downarrow}c_{-i\uparrow}+c^{\dagger}_{-i\uparrow}c^{\dagger}_{-i\downarrow}c_{+i\downarrow}c_{+i\uparrow}\\
&+c^{\dagger}_{+i\uparrow}c^{\dagger}_{-i\downarrow}c_{+i\downarrow}c_{-i\uparrow}+c^{\dagger}_{-i\uparrow}c^{\dagger}_{+i\downarrow}c_{-i\downarrow}c_{+i\uparrow}]. \qquad (3)
\end{aligned}
$$

Besides the usual symmetry of the total spin S and S_z, the translational symmetry along the chain direction, the Hamiltonian also has the symmetry of the exchange of the chain indices. The symmetry of the total state under the exchange of two-chain indices depends on the symmetries of the wave function of each particle. It is decided by the number of particles on the odd chain of the newly transformed Hamiltonian since the evenness and oddness of the number of particles on the odd chain is not changed by the Hamiltonian. If the number of particles on the odd chain is odd, the total state is antisymmetric; if the number is even, the total state is symmetric. In the DMRG calculation, we define the symmetry under the chain exchange of each base or sector in terms of the number of particles on the odd chain and so we have the option to choose the symmetry and to be able to calculate the ground state energy of a given symmetry. We also use the open boundary condition here, hence there is no translational symmetry along the chain direction.

For a set of given values of U, $t_\perp$, and electron filling n, the charge gaps and spin gaps are defined as

$$
\begin{aligned}
\Delta_{c+}=&\frac{1}{2}[E_+(Q+2,S=S_z=0)\\
&+E_+(Q-2,S=S_z=0)-2E_+(Q,S=S_z=0)], \qquad (4)
\end{aligned}
$$

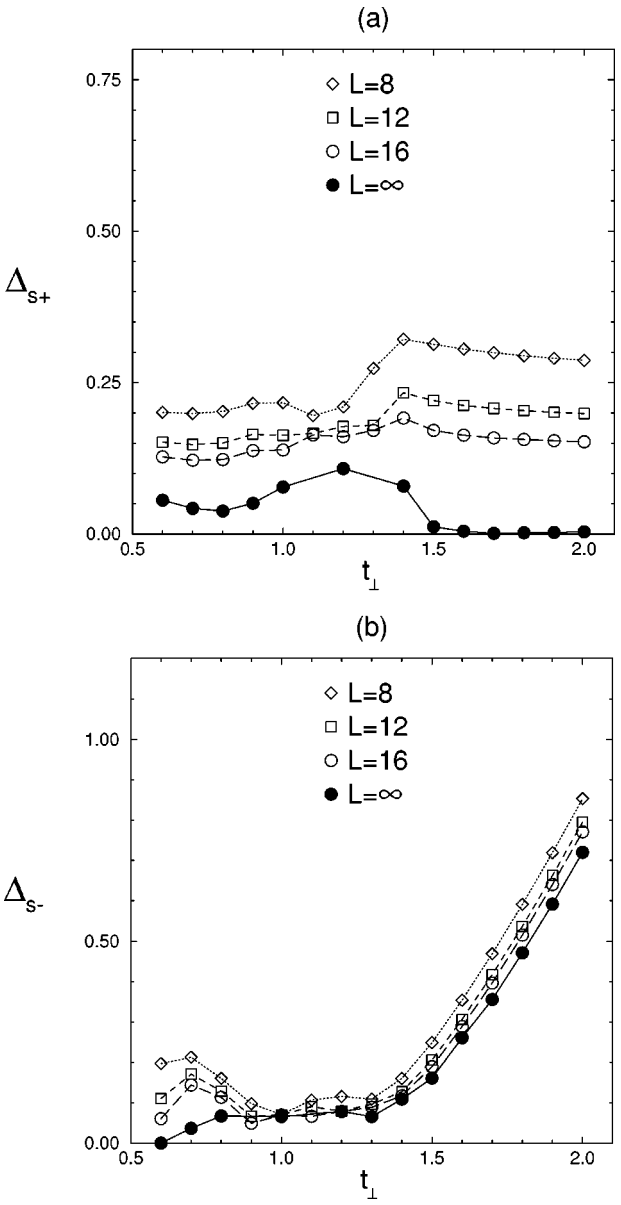

FIG. 2. Spin gaps versus $t_\perp$ for $U=8$ for (a) the symmetric mode and (b) the antisymmetric mode. We denote values for $L=8$ with diamonds, $L=12$ with squares, $L=16$ with open circles, and $L=\infty$ extrapolated values with closed circles.

$$\Delta_{c-}=E_-(Q,S=S_z=0)-E_+(Q,S=S_z=0), \qquad (5)$$

$$\Delta_{s+}=E_+(Q,S=S_z=1)-E_+(Q,S=S_z=0), \qquad (6)$$

$$\Delta_{s-}=E_-(Q,S=S_z=1)-E_+(Q,S=S_z=0), \qquad (7)$$

where $\pm$ is the symmetric or antisymmetric mode and all energies are the lowest energy for each set of quantum numbers. Here we assume the total number of the particles is even. In each iteration of the DMRG calculation, we typically keep $M=200$ states for the block. We calculated gaps for various size of lattices with length $L=8$, 12, 16, and 20 and extrapolated the thermodynamic values by $1/L$ polynomial expansions. In the DMRG calculation, we only utilize the conservation of S_z, not the total spin S. To identify the total spin S correctly it is necessary to check S values of the lowest energy state in each sector. For the $S_z=0$ sector with

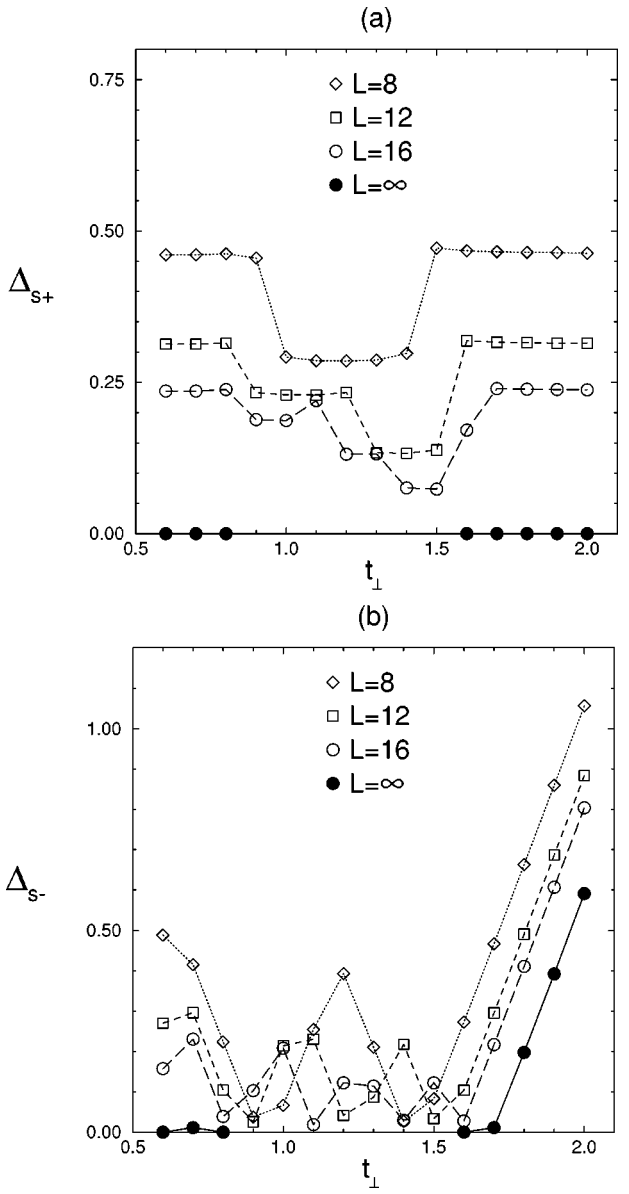

FIG. 3. Same as Fig. 2 but for $U=1$.

a symmetric mode, the ground state is the $S=0$ state. For the $S_z=1$ sector with a symmetric mode, the ground state is $S=1$ state and the same is true for the $S_z=1$ sector with an antisymmetric mode. However, for the $S_z=0$ sector with an antisymmetric mode, the ground state is the $S=1$ state rather than $S=0$, which implies that $\Delta_{c-} \geqslant \Delta_{s-}$ for finite size lattices. Therefore, to calculate the antisymmetric charge gap we need to find the $S=0$ state, which is an excited state. We find this state by calculating the expectation values of S for a few excited states.

Figure 1 shows the finite size extrapolation used to obtain the thermodynamic values of the gaps for $U=8$ and $t_\perp=1.7$. The symmetric charge gap Δ_{c+} and the symmetric spin gap Δ_{s+} vanish. In particular, for the entire range of U and $t_\perp$, Δ_{c+} always vanishes at $n=0.75$. The antisymmetric charge gap Δ_{c-} and the antisymmetric spin gap Δ_{s-} are finite. Δ_{c-} is larger than Δ_{s-} for all sizes of lattices but for the longer lattice the difference between them is smaller. Since we take the ground state as the target state for the calculations of the density matrix in the DMRG method, the

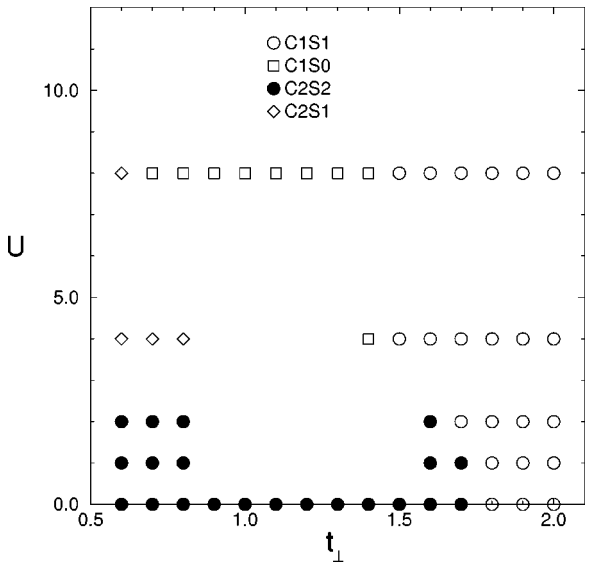

FIG. 4. Phase diagram at $n=0.75$. We denote the C1S1 phase with open circles, C1S0 with squares, C2S2 with closed circles, and C2S1 with diamonds. We also show the phases for the noninteracting case.

accuracy of the excited states is not as high as that of the ground state and this is even more serious for longer lattices and for small $t_\perp$.

For a strong interaction $U=8$, Δ_{s+} and Δ_{s-} are plotted in Fig. 2 as functions of $t_\perp$ for various sizes of lattices including $L=\infty$ extrapolated values. For most values of $t_\perp$ we get very good extrapolations for both Δ_{s+} and Δ_{s-} with three L values: 8, 12, and 16. There are some points near $t_\perp=1.0$ for which we are not able to get a good extrapolation. As $t_\perp$ decreases from $t_\perp=2.0$, Δ_{s-} decreases, but does not vanish until $t_\perp=0.6$, and Δ_{s+} opens up around $t_\perp=1.5$. Since we always have one gapless symmetric charge mode, that is, $\Delta_{c+}=0$ and $\Delta_{c-} \geqslant \Delta_{s-}$, the phase changes from the C1S1 phase to the C1S0 phase around $t_\perp=1.5$. Between these two phase we do not have phases such as C2S2 and C2S1, which are found in the results for $U \rightarrow 0^+$ limit by Balents and Fisher.[6] We stop our calculations at $t_\perp=0.6$ because the DMRG calculation has poor accuracy for small $t_\perp$.

The vanishing of Δ_{s-} at $t_\perp=0.6$ can be understood from the $t_\perp=0$ limit. In this limit, two chains will be completely decoupled to two one-dimensional chains, which is the Luttinger phase, and we will have the C2S2 phase with all gapless modes. So, as $t_\perp$ decreases all gaps will vanish one by one and eventually we will have the C2S2 phase in the $t_\perp=0$ limit. The linear behavior of Δ_{s-} in the C1S1 phase region for $t_\perp>1.5$ can be understood in the limit of infinitely large $t_\perp$. In this limit, Δ_{s-} measures the separation between the bonding band and the empty antibonding band. In the physically interesting isotropic region $t_\perp=1.0$, both spin gaps are similar in magnitude but are finite, which is consistent with previous results.[11] Also, they increase slowly as $t_\perp$ increases. This is compatible with the results for the t-J ladder, which is the linear behavior of the spin gap in $J_\perp$ ($\Delta_s \sim J_\perp \sim t_\perp^2/U$).[7,9] The increasing behavior of Δ_{s+} for $t_\perp<0.7$ is an artifact from the poor convergence of the DMRG method for small $t_\perp$.

Figure 3 shows the same figures as in Fig. 2 but for the

weak interaction $U=1$. Unlike the $U=8$ case, Δ_{s+} does not open up and Δ_{s-} vanishes around $t_\perp=1.7$, where Δ_{c-} also vanishes so that we have a transition from the C1S1 phase to the C2S2 phase. As $t_\perp$ decreases further, we have finite size fluctuations so that we cannot calculate $L=\infty$ gaps until $t_\perp=0.8$. Surprisingly, in a small region of $t_\perp$, $0.6\leqslant t_\perp\leqslant 0.8$, there is little finite size fluctuation. We find that both Δ_{s+} and Δ_{s-} vanish. On the other hand, Δ_{c-} is finite, but considering the overestimation of Δ_{c-} because of the inaccuracy of the excited states and the system being two decoupled Luttinger liquid systems for small $t_\perp$, presumably it also vanishes and we have the C2S2 phase. If we smoothly connect this region to the region with $t_\perp\simeq 1.7$, it is plausible to assume that the phase remains gapless. Therefore, in this weak interaction case, there will be only one transition from the C1S1 phase at large $t_\perp$ to the C2S2 phase at small $t_\perp$ and this is rather consistent with the noninteracting limit. In the C1S1 phase, we also have the linear behavior of Δ_{s-} with smaller Δ_{s-} than $U=8$ case but with larger slope.

With calculations for other values of U, we plot the phase diagram in the space of $t_\perp$ and U at $n=0.75$ in Fig. 4. It is clear that the strong interaction case ($U=8$) and the weak interaction case ($U=1$) are clearly different. $U=2$ case is the same as the $U=1$ case and $U=4$ seems to be similar to the $U=8$ case regardless of the existence of the finite size fluctuations. The transition point of $t_\perp$ between two different phases decreases from $t_\perp\simeq 1.7$ for the noninteracting case as U increases. When we have different n, the transition point of $t_\perp$ will be changed because it is around the value of the noninteracting limit $t_\perp=1-\cos\pi n$, just as in the weak coupling case.[6] Therefore, for different n the whole phase diagram will be shifted in the $t_\perp$ direction.

In conclusion, we have derived the phase diagram of the two-chain Hubbard model in terms of charge and spin excitations for both symmetric and antisymmetric modes at fixed electron filling. We have found very different behaviors for the weak and strong interaction cases. The transition from the noninteracting limit to the interaction case seems to be rather gradual, and beyond a finite value of U we have the spin-gapped phase at the isotropic region $t_\perp=1.0$, which is consistent with the previous results for the strong interaction case and the t-J model.

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