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Intra- and Inter-Chain Excitations near a Quantum Phase Transition in Quasi-One-Dimensional Conductors

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We study intra- and inter-chain excitation spectra near a quantum phase transition in a spinless fermion model on a two-leg ladder at half filling by the finite-temperature density-matrix renormalization-group method. Above a critical strength of intrachain nearest-neighbor repulsion, a gap appears, accompanied with a long-range order of density modulation in the checkerboard pattern at zero temperature. The *intra*chain excitation spectra do not change so much in the gapless phase below the critical strength, while the *inter*chain excitation spectra are considerably altered by the *intra*chain repulsion even in the gapless phase. Relevance to the optical conductivity in quasi-one-dimensional electron systems is suggested.

Keywords: excitation spectrum; quantum phase transition; quasi-one-dimensional system; spinless fermion

INTRODUCTION

Various broken-symmetry ground states are realized by controlling the dimensionality of electronic conduction in molecular systems such as $(TMTCF)_2X$[1] and $(Et_nMe_{4-n}Z)[Pd(dmit)_2]_2$[2]. Above the phase transition temperatures, dimensional crossovers are observed in normal states. Charge is localized on the low-dimensional side, while the electronic conduction becomes

metallic in one to three directions with increasing dimensionality by applying pressure, substituting the donor, or changing the counter ion[3]. In the optical conductivity for the electric field perpendicular to the chains, a plasma edge is absent on the low-dimensional side, while it is present on the high-dimensional side[4], suggesting that electrons confined in the chains become delocalized over the chains with increasing dimensionality. We have pointed out the importance of the umklapp process at a commensurate filling, which suppresses a one-particle dimensional crossover and enhances a two-particle one[5], and studied how static and spatial correlation functions of coupled dimerized-extended-Hubbard chains change with the interchain transfer integral t_b and other model parameters[6]. Here, we study *dynamic* and *local* correlation functions to clarify different behavior between intra- and inter-chain charge-transfer excitation spectra near a quantum phase transition in a much simpler model. The density-matrix renormalization-group (DMRG) technique[7] is applied to the quantum transfer matrix[8,9,10].

SPINLESS FERMION MODEL ON A TWO-LEG LADDER

As a first step to quasi-one-dimensional systems, we use a spinless fermion model on a two-leg ladder at half filling,

$$H = -t\sum_i\sum_{j=1}^{2}\left(c^+_{i,j}c_{i+1,j} + \text{h.c.}\right) - t_b\sum_i (c^+_{i,1}c_{i,2} + \text{h.c.}) + V\sum_i\sum_{j=1}^{2} n_{i,j}n_{i+1,j} ,$$

where $n_{i,j}=c^+_{i,j}c_{i,j}$, and $c^+_{i,j}(c_{i,j})$ creates (annihilates) a spinless fermion on the ith site of the jth leg. The intra- and inter-chain transfer integrals are denoted by t and t_b, respectively, and the intrachain nearest-neighbor repulsion strength by V.

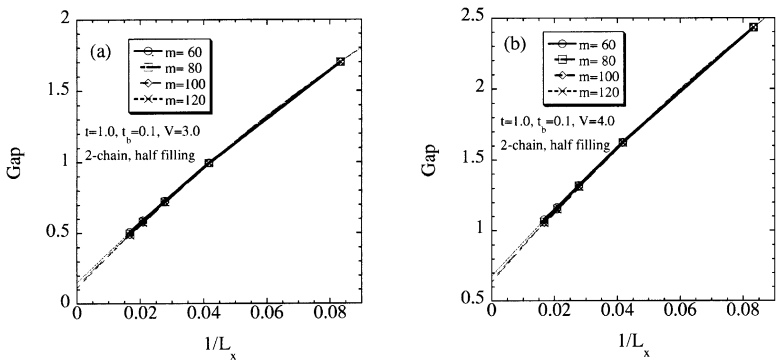

FIGURE 1 Gap for t=1, t_b=0.1, (a) V=3, and (b) V=4, with m=60, 80, 100, and 120, each with extrapolation by parabolic functions.

First, the gap, defined as $\Delta = E(L_x/2-1) + E(L_x/2+1) - 2E(L_x/2)$ with $E(n)$ being the ground state energy for n fermions, is calculated by the zero-temperature DMRG technique for ladders with finite length L_x (Fig.1). For the number of states kept in the DMRG technique m, we take different values up to 120. From the extrapolation to the thermodynamic limit, we estimate the gap for t=1 and t_b=0.1 to be about 0.1 for V=3 and about 0.6 for V=4.

EXCITATION SPECTRA

The excitation spectra of one- and two-body correlation functions are obtained through Fourier transformation and analytic continuation of the corresponding imaginary-time-dependent correlation functions. For a one-body correlation function, we calculated the density of one-particle states (DOS) $\rho(\omega) = -(1/\pi)\,\mathrm{Im}G(\omega+i\delta)$, where $G(\tau) = -\langle c_{i,j}(\tau)c^{+}_{i,j}(0)\rangle$ for $0 < \tau < \beta$ with the inverse temperature β=1/T. As V increases, the DOS is shifted to the $\omega > 0$ and $\omega < 0$

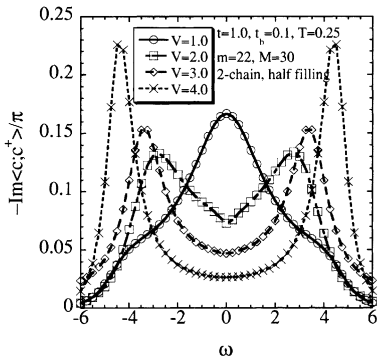

FIGURE 2 Density of one-particle states for t=1, t_b=0.1 with V= 1, 2, 3, and 4 at temperature T=0.25. The number of states kept in the DMRG technique is m=22. The Trotter number is M=30.

parts, with peaks becoming narrower and appearing around $+V$ and $-V$ for large V (Fig.2). Because the magnitude of the gap is comparable with the temperature at most, the gap structure is not clearly seen. From an experience with the easily converging single-chain case, we suspect that the absence of a gap structure for V = 4 is due to the insufficient number of states kept m. However, the overall structure is not much altered by taking different m values and the Trotter numbers M. In any case, it is certain that the DOS at zero energy decreases steadily with increasing V.

For two-body correlation functions, we calculated the corresponding dynamical structure factors[10], $S_{AA}(\omega) = -(1/\pi)\ \mathrm{Im}\chi_{AA}(\omega+i\delta)/(1-e^{-\beta\omega})$, where $\chi_{AA}(\tau) = -\langle A_{i,j}(\tau)A^{+}_{i,j}(0)\rangle$ for $0 < \tau < \beta$. We adopt $A_{i,j} = j_{x,i,j} = i(c^{+}_{i,j}\, c_{i+1,j} - c^{+}_{i+1,j}\, c_{i,j})$ for the charge transfer along the chain, and $A_{i,j} = j_{y,i,j} = i(c^{+}_{i,1}\, c_{i,2} - c^{+}_{i,2}\, c_{i,1})$ for that perpendicular to the chains. For large V, the main structure appears at ω=V for

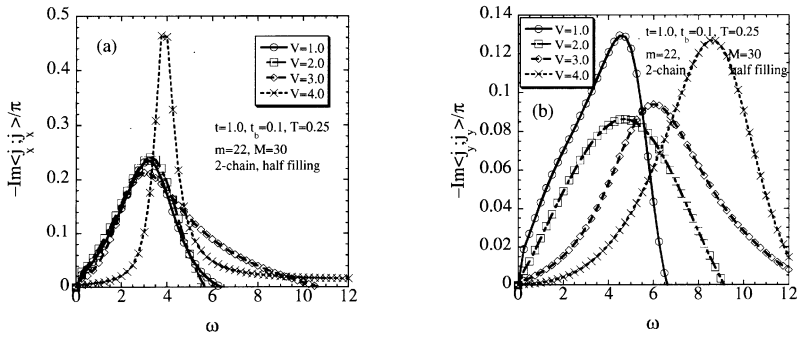

FIGURE 3 Imaginary part of the local charge-transfer correlation function (a) in the leg direction, and (b) in the rung direction, for the parameters used in Fig. 2.

$S_{j_xj_x}(\omega)$ and at $\omega=2V$ for $S_{j_yj_y}(\omega)$ (Fig.3). It is due to the process, where the number of nearest-neighbor pairs is increased by one for the intrachain charge transfer, while it is increased by two for the interchain charge transfer. The physically important, low-energy part of $S_{j_xj_x}(\omega)$ shows a small change in the gapless phase ($V < V_c$) and rapid shift to higher energies in the phase with a gap ($V > V_c$), where the critical strength V_c lies between 2 and 3 for the parameters used in the figures. Meanwhile, the low-energy part of $S_{j_yj_y}(\omega)$ is much more sensitively altered by V. Even for $V < V_c$, much of the spectral weight is transferred to higher energies. Kinks and anti-kinks separate the degenerate density-alternating phases, collectively propagating along the chains. They "fill" the low-energy part of $S_{j_xj_x}(\omega)$ only. That is why $S_{j_yj_y}(\omega)$ for the *inter*chain excitations is sensitive to the strength V of the *intra*chain repulsion.

Though the present results are limited to local correlations and do not

contain spin fluctuations, the sensitivity of *inter*chain excitation spectra to *intra*chain electron correlation is a general consequence in quasi-one-dimensional conductors, which we believe is relevant to $(TMTCF)_2X$[4].

Acknowledgments

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