Cluster approach to the charge density plateaux in *t–J* ladders

2005 J. Phys.: Condens. Matter 17 S1299

(http://iopscience.iop.org/0953-8984/17/14/020)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **17** (2005) S1299–S1304 doi:10.1088/0953-8984/17/14/020

Cluster approach to the charge density plateaux in t–J ladders

A Fledderjohann[1], A Langari[2,3] and K-H Mütter[1]

[1] Physics Department, University of Wuppertal, 42097 Wuppertal, Germany
[2] Institute for Advanced Studies in Basic Sciences, Zanjan 45195-159, Iran

E-mail: langari@iasbs.ac.ir

Received 19 July 2004, in final form 8 October 2004
Published 24 March 2005
Online at stacks.iop.org/JPhysCM/17/S1299

Abstract

We study the ground state properties of the t–J model on two and three leg ladders. The phase diagram of the anisotropic couplings along the rungs and legs is investigated to find the opening of a charge transfer gap which appears as a charge density plateau. In a perturbative approach we start from isolated rungs at zero leg couplings. Then the stability of the charge density plateau is examined by first order perturbation theory in terms of an effective Hamiltonian using the numerical Lanczos method on finite size ladders. The results of this approach are compared with the exact diagonalization of finite systems. We have found that an improvement of our results depends on the initial clusters for zeroth order perturbation which cannot be recovered by higher order perturbation in rung clusters. For the two leg ladder case the application of 4-site (2×2) plaquettes helped us to overcome earlier flaws when the charge density is greater than one-half. We have also addressed the generalization of our method to trace phase separation in this model, where a linear dependence of ground state energy versus charge density gives evidence of a phase separated state.

1. Introduction

It is now reasonably well established that the doped antiferromagnets found in cuprate compounds have a superconducting ground state. Moreover, synthesizing quasi-one-dimensional ladder materials with mobile charge carriers has raised an increased interest in the theoretical understanding of their rich phase diagram [1, 2]. The t–J model has been considered as the simplest model including the low energy physics of doped ladder systems [3, 4]. Among many interesting features of doped antiferromagnets [5] is the metal–insulator transition investigated in [6]. This transition is accompanied by the opening of a gap, which appears as a plateau in the charge density $\rho(\mu)$ as a function of the chemical potential

[3] Author to whom any correspondence should be addressed.

(μ). The charge density plateaux in $\rho(\mu)$ look similar to the plateaux in the magnetization curve $M(h)$ found in spin systems [7]. A charge density plateau in $\rho(\mu)$ is signalled by discontinuous changes in the slope of the ground state energy per site as a function of ρ. It emerges immediately in the local rung approximation [8] or bond-operator theory [9]. The aim of this paper is to go beyond the local rung approximation by means of a systematic perturbation theory in leg couplings. Moreover, we are going to explain the effect of the initial cluster on perturbation theory. This on the other hand shows the formation of clusters in the ground state of t–J ladders. The extension of the cluster approach to a product ansatz of the ground state shows the evidence of phase separated states. This can be generalized to predict the boundary of phase separation [10].

2. The model

We have considered t–J models with ladder geometry (see figures 1 and 2 of [11]). The Hamiltonian for such models is the following:

$$\begin{aligned} H &= \sum_{\text{legs}} \sum_{i} h_{i,i+1}(t', \alpha') + \sum_{\text{rungs}} \sum_{j} h_{j,j+1}(t, \alpha), \\ h_{i,i+1}(t, \alpha) &= P\left\{ t\left[\sum_{\sigma} (c^{\dagger}_{i,\sigma} c_{i+1,\sigma} + \text{h.c.}) + \alpha(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{4} n_i n_{i+1}) \right] \right\} P, \end{aligned} \tag{1}$$

where $c_{i,\sigma}$ is the fermion annihilation operator with spin σ, $\mathbf{S}_i$ is the spin $1/2$ operator and P is the projection to the singly occupied subspaces. In our notation the exchange coupling J is defined to be $J = t\alpha$. The Hamiltonian between two sites (bond) of the system is $h_{i,j}$. We have considered open boundary conditions in both leg and rung directions.

3. Cluster approach

3.1. Rung clusters

The cluster approach we have considered is a perturbation theory in terms of the cluster basis. At first glance the trivial cluster seems to be given by the rungs, i.e. a system of two sites in two leg ladders and three sites in three leg ladders. At the zeroth order perturbation theory ($t' = 0$) the ground state of the ladder ($|E_0\rangle$) at any charge density $\rho = Q/N$ (where Q is the total charge and N is the total number of sites) is a direct product of the rung ground states.

$$|E_0\rangle = \prod_{x} |q(x)\rangle = |q(1), q(2), \ldots, q(N_{\text{r}})\rangle \tag{2}$$

where $|q(x)\rangle$ refers to the ground state of rung x with charge q and N_{r} is the number of rungs. It is imposed that $Q = \sum_x q(x)$. A detailed calculation in [11] shows a discontinuity in the chemical potential ($\mu = \frac{\mathrm{d}E_0}{\mathrm{d}Q}$) at a specific charge density at zeroth order approximation. This is the first indication of a charge density plateau at $\rho = 1/2$ for the two leg ladder and $\rho = 1/3, 2/3$ for the three leg ladder.

We have then studied the stability of a charge density plateau in the presence of leg couplings in terms of first order perturbation [11]. In this approach the rung states with odd charges are considered as *quasi-electrons* and those with even charges as *quasi-holes*. The first order correction is obtained as an effective Hamiltonian on a chain which is a modified t–J model with renormalized couplings plus an extra diagonal term. Numerical computation using the Lanczos method gives us the area in the parameter space where the charge density plateau survives. This is actually an opening of an energy gap in the spectrum of charge degrees of freedom. The phase diagram for two leg ladder is plotted in figure 5 of [11]. We found that the

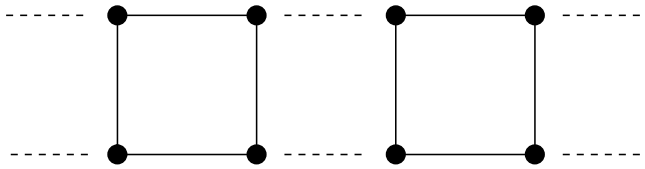

Figure 1. Decomposition of a two leg ladder into 4-site plaquettes.

formation of a charge density plateau is favoured for small values of α and large values of α'. The parameter space of the three leg ladder consists of four different phases where plateaux at $\rho = 1/3, 2/3$ can coexist, exclude each other or disappear completely. It is shown in figure 7 of [11].

3.2. Plaquettes

From now on we will restrict ourselves to two leg ladders to show the main features of our perturbative approach. By comparing the results of the rung cluster approach with an exact diagonalization on finite lattice sizes we arrive at the following arguments.

- Fairly good results for $\rho < 1/2$.
- Discrepancies for $\rho > 1/2$.

We have convinced ourselves that it is not a perturbative artefact to be improved by higher orders; instead the initial clusters for zeroth order bases have to be improved. In this respect we have considered the 4-site plaquettes to decompose our ladder at the zeroth order perturbation as in figure 1. In this case the bases of zero order perturbation also contain the information of leg couplings. To be more specific and able to obtain clean results, we will consider two different cases of the coupling constants, namely:

- (a) small α, large α',
- (b) large α, small α'.

To examine the improvement of results at the first stage, we have considered two special values of charge density, $\rho = 1/2, 1$. We have found that the ground state energy per site (E_0/N) of an $N = 16$ ladder can be very well reproduced by the ground state energy density ($\epsilon_0^{(p)}$) of a 4-site plaquette with a correction factor (f) close to unity.

$$\frac{E_0}{N}(\rho, t', \alpha, \alpha') = \epsilon_0^{(p)}(\rho, t', \alpha, \alpha') f(\rho, t', \alpha, \alpha'); \qquad \rho = 1/2, 1. \tag{3}$$

We have plotted the factor f in figure 2 for $\rho = 1/2$ and $0 \leqslant t' \leqslant 1$. The maximum deviation in the t'-regime (i.e. at $t' = 1$) turns out to be 20% for case (a) and is less than $\sim$6% for case (b). A similar conclusion is obtained for the results of $\rho = 1$ [12]. The interaction between plaquettes is responsible for the deviation from unity. We have chosen special parameters for the horizontal axis of figure 2 to show the scaling behaviour for different values of α and α'. To go beyond zero order approximation the product ansatz equation (2) with plaquettes is considered for the ground state and the following constraints are imposed.

$$Q = \sum_j Q_j, \qquad N = 4 \times N_{\mathrm{p}}. \tag{4}$$

Here Q_j is the charge of jth plaquette and N_{p} is the number of plaquettes. By comparing the ground state energy of plaquettes at different charge sectors [12] we found that only plaquettes

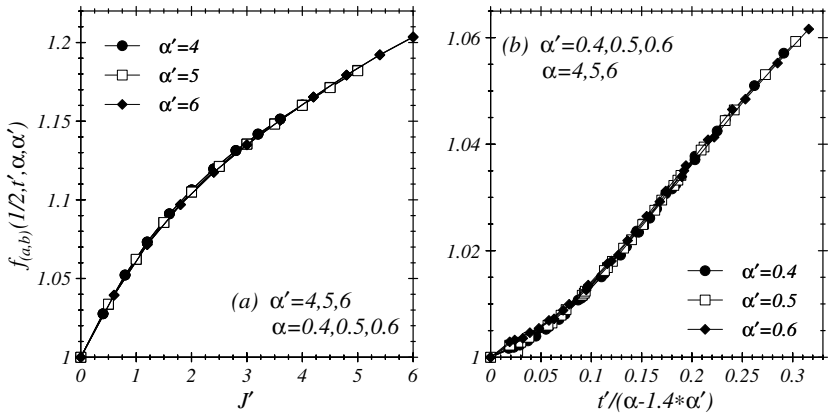

Figure 2. Correction factor $f(1/2, t', \alpha, \alpha')$ of equation (3) for a 2×8 t–J ladder with parameters (a), (b) and $\rho = 1/2$.

with charges $Q = 0, 2, 4$ contribute to the ground state in both (a) and (b) regimes. The reason is simply formulated in the following equations.

$$\epsilon_0^{(p)}(Q=0) + \epsilon_0^{(p)}(Q=2) < 2\epsilon_0^{(p)}(Q=1), \tag{5}$$

$$\epsilon_0^{(p)}(Q=2) + \epsilon_0^{(p)}(Q=4) < 2\epsilon_0^{(p)}(Q=3). \tag{6}$$

Equation (5) means that the creation of two $Q = 1$ plaquettes from a $Q = 0$ and a $Q = 2$ one is not favoured energetically. A similar argument is drawn for equation (6). In the next step we have calculated the interaction between different plaquettes by using the product ansatz [12]. Let us define $W(Q_i, Q_j)$ as the interaction energy between two neighbouring plaquettes of charge Q_i and Q_j. Since only $Q = 0, 2, 4$ plaquettes contribute to the ground state ansatz then $W(Q_i, Q_j)$ will be diagonal, because a charge exchange of more than one (electron) is forbidden in first order perturbation. Finally we arrive at

$$W(Q_i, Q_j) = -t'\alpha' \frac{Q_i Q_j}{32}. \tag{7}$$

Summing up the zeroth and first order perturbation theory we arrive at the following results for the two leg ladder ground state energies for $\rho \geqslant 1/2$ additionally shown in figure 3. There is a big improvement for $\rho > 1/2$ of case (a) compared to the results of rung clusters (see figure 4 of [11]). Moreover, we can now explain the reason why at a specific t' value for $\rho > 1/2$ the chemical potential is zero. In first order perturbation theory the ground state energy per site is

$$\frac{E_0(\rho)}{N} = \frac{1}{4}[\epsilon_0^{(p)}(Q=2) + W(2,2) - 2\epsilon_0^{(p)}(Q=4) - 2W(4,4)] + \frac{\rho}{2}[\epsilon_0^{(p)}(Q=4) + W(4,4) - \epsilon_0^{(p)}(Q=2) - W(2,2)]. \tag{8}$$

The chemical potential goes to zero when the ground state energy does not depend on ρ. In our approach this happens when the second term in equation (8) is about to vanish. This gives a point (t_0') where the energy of all charge sectors cross each other. The plaquette approach gives $t_0' = 0.329$ and the corresponding energy density $E_0/N = -0.650\,99t$, compared with the numerical Lanczos results which are $t_0' = 0.323$ and $E_0/N = -0.663t$. This shows a very good agreement. Thus the plaquette approach improves the results very much—in particular for $\rho > 1/2$. Moreover, it still shows a discontinuity in the slope of energy density versus ρ, indicating the presence of a charge density plateau at $\rho = 1/2$.

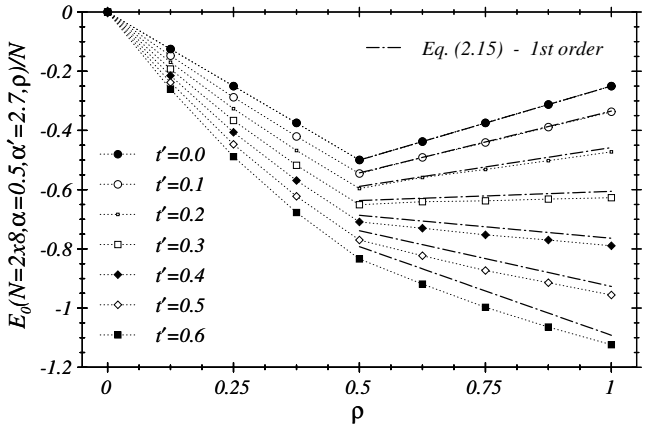

Figure 3. Ground state energy density versus charge density (ρ) for case (a) where $\alpha = 0.5$, $\alpha' = 2.7$. Additionally shown are first order perturbation results for $\rho \geqslant 1/2$.

4. Discussion and extensions

A generalization of our cluster approach to clusters with half of the lattice size provides a way to trace the interesting phenomenon of phase separation. Suppose that in a phase separated ground state the system is divided into two clusters. The first cluster with $N_1(\rho_1)$ sites has charge density ρ_1 and the other cluster covers the remaining sites, namely $N_2(\rho_2)$ with charge density ρ_2. The Hamiltonian of the whole ladder can be written as $H = H_1(N_1)+H_2(N_2)+H_{1,2}$, where $H_1(N_1)$ ($H_2(N_2)$) is the Hamiltonian of an N_1 (N_2)-site cluster respectively and $H_{1,2}$ represents the interaction between the two clusters. We then use the following product ansatz for the ground state:

$$|\psi_0(N, \rho)\rangle = |\psi_0(N_1, \rho_1)\rangle|\psi_0(N_2, \rho_2)\rangle, \tag{9}$$

where $|\psi_0(N_i, \rho_i)\rangle$ is the ground state of the Hamiltonian of the first ($i = 1$) and second ($i = 2$) cluster with the corresponding energy $E_0^p(\rho_i)$, imposing that $N = N_1 + N_2$ and $\rho = (N_1\rho_1 + N_2\rho_2)/N$. Since the value of $\langle H_{1,2}\rangle/N$ is zero in the thermodynamic limit, the ground state energy per site ($\langle\psi_0(N, \rho)|H|\psi_0(N, \rho)\rangle/N$) is a linear function of charge density for $\rho_1 < \rho < \rho_2$ [12]:

$$\frac{E_0(\rho)}{N} = \frac{1}{\rho_2 - \rho_1}[E_0^p(\rho_1)(\rho_2 - \rho) + E_0^p(\rho_2)(\rho - \rho_1)]. \tag{10}$$

Thus we argue that a linear dependence of the ground state energy versus charge density is a signature of phase separation.

In summary, the plaquette approach is able to reproduce very well the ground state properties of the two leg ladder. It asserts that a charge density plateau appears at $\rho = 1/2$. Moreover, a phase separation appears for $1/2 < \rho < 1$. The generalization of this approach to the two dimensional t–J model for tracing the phenomenon of phase separation is under consideration. The latter topic has received much interest since the early experimental [13] and theoretical [14] studies of the phenomenon.

References

[1] Uehara M *et al* 1996 *J. Phys. Soc. Japan* **65** 2764
[2] Mayaffre H *et al* 1998 *Science* **279** 5349

[3] Dagotto E and Rice T M 1996 *Science* **271** 618
[4] Rice T M 1997 *Z. Phys.* B **103** 165
[5] Sachdev S 2000 *Science* **288** 475
[6] Riera J *et al* 1999 *Eur. Phys. J.* B **7** 53
[7] Oshikawa M *et al* 1997 *Phys. Rev. Lett.* **78** 1984
[8] Kagan M Y *et al* 1999 *Physica* C **317/318** 185
[9] Park K *et al* 2001 *Phys. Rev.* B **64** 184510
[10] Rommer S *et al* 2000 *Phys. Rev.* B **61** 13424
[11] Fledderjohann A, Langari A and Mütter K-H 2003 *Eur. Phys. J.* B **36** 193
[12] Fledderjohann A, Langari A and Mütter K-H 2004 *J. Phys.: Condens. Matter* at press
[13] Jorgensen J D *et al* 1988 *Phys. Rev.* B **38** 11337
[14] Emery V J, Kivelson S A and Lin H Q 1990 *Phys. Rev. Lett.* **64** 475