Quantum phases of AB_2 fermionic chains

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Abstract

A fermionic chain is a one-dimensional system with fermions, which interact locally and can jump between sites in the lattice. In particular, an $\mathbf{AB_n}$ chain type, where **A** and **B** are sites that presents a difference energy level $\boldsymbol{\Delta}$, and the site **B** is repeated **n**-times, such that the unit cell has $\mathbf{n+1}$ sites. A limit case of this model called ionic Hubbard model (n=1) has been widely studied due to the interesting physics and applications. In this paper, we study the ground state of an $\mathbf{AB_2}$ chain, which describe the material $\mathbf{R_4[Pt_2(P_2O_5H_2)_4X]\cdot nH_2O}$, specifically we consider a filling with two electrons per unit cell, and using the density matrix renormalization group method, we found that system presents the phases: band insulator, Mott correlated insulator and an intermediate phase between them. For couplings $\boldsymbol{\Delta = 2, 10}$ and $\mathbf{20}$, we estimate the critical points which separate this phases through the structure factor and the energy gap in the sector of charge and spin, finding that the critical points position increase as a function of $\boldsymbol{\Delta}$.

Introduction

The ionic Hubbard model (IHM) is a modification of Hubbard model (HM), which consider that exist a change energy level $\boldsymbol{\Delta}$ between sites in the lattice. This model exhibits the phases: the band insulator, Mott insulator and ferroelectric phase between them. Some materials like tetrathiafulvalene-p-chloranil can be modelled with this model.
Thinking in generalize the ideas of the IHM, in 2006, Aligia *et al.* [1], raised an $\mathbf{AB_n}$ fermionic chains model, where **A** is a type of atom with an energy level and **B** is another type of atom in a different site that repeats **n**-times. They used different techniques like bosonization, perturbation theory and exact diagonalization method for small clusters. However, their phase diagram not indicate clearly the critical values where transitions occur and this is an open point in the literature yet. This motivates us to study the $\mathbf{AB_n}$ fermionic chains, in particular the $\mathbf{n=2}$ case, through density matrix renormalization group (DMRG) method for large lattice sizes.

Model

The Hamiltonian for the $\mathbf{AB_2}$ chain is defined by:

$$\mathcal{H} = -\mathbf{t}\sum_{\mathbf{i}\sigma}(\hat{\mathbf{c}}^{\dagger}_{\mathbf{i+1},\sigma}\hat{\mathbf{c}}_{\mathbf{i},\sigma} + \mathbf{h.c.}) + \mathbf{U}\sum_{\mathbf{i}}\hat{\mathbf{n}}_{\mathbf{i}\uparrow}\hat{\mathbf{n}}_{\mathbf{i}\downarrow} + \sum_{\mathbf{i}}\boldsymbol{\Delta}_{\mathbf{i}}\hat{\mathbf{n}}_{\mathbf{i}}, \qquad (1)$$

where $\hat{\mathbf{c}}^{\dagger}_{\mathbf{i},\sigma}$ creates an electron at site **i** with spin σ, $\mathbf{n_{i\sigma}} = \hat{\mathbf{c}}^{\dagger}_{\mathbf{i},\sigma}\hat{\mathbf{c}}_{\mathbf{i},\sigma}$, and $\mathbf{n_i} = \mathbf{n_{i\uparrow}} + \mathbf{n_{i\downarrow}}$. The parameter **t** is the nearest-neighbour hopping amplitude (we take $\mathbf{t=1}$), **U** is the on-site Hubbard interaction and $\boldsymbol{\Delta}_{\mathbf{i}}$ is the difference in on-site energies. When we talk about $\mathbf{AB_2}$ chain, we have an unit cell with three sites, so two sites have an energy difference $\boldsymbol{\Delta}_{\mathbf{i}} = \mathbf{0}$, the other one have $\boldsymbol{\Delta}_{\mathbf{i}} = -\boldsymbol{\Delta}$ and this structure is repeated periodically.
For a fill equal to two electrons per unit cell, we have some limit case for the $\mathbf{AB_2}$ chain: for $\mathbf{U} < \boldsymbol{\Delta}$, the site **A** is doubly occupied and the site **B** is empty, so the systems behaves like a band insulator (BI). And for $\mathbf{U} > \boldsymbol{\Delta}$ and for any value of **t**, in the Hubbard model we take a Mott insulator (MI) with $\mathbf{n=1}$. In the case of $\mathbf{n=1}$ and $\mathbf{U} - \boldsymbol{\Delta} \gg \mathbf{t}$, the system adopts a form of modified MI state, called "correlated insulator" (CI) [2].
To study the ground state energy of our system, we calculate the spin $\boldsymbol{\Delta}_{\mathbf{s}}$ and charge $\boldsymbol{\Delta}_{\mathbf{1}}$ gaps defined by,

$$\boldsymbol{\Delta}_{\mathbf{s}} = \mathbf{E_0(N,1) - E_0(N,0)}, \qquad (2)$$

$$\boldsymbol{\Delta}_{\mathbf{1}} = \mathbf{E_0(N+1,1/2) + E_0(N-1,1/2) - 2E_0(N,0)}, \qquad (3)$$

where $\mathbf{E_0(N,S_z)}$ is the ground state energy for a lattice of size **L** with **N** particles in a spin sector $\mathbf{S_z}$, being $\mathbf{S_z}$ the **z** component of the total spin [2]. Also, we decide to calculate the spin $\mathbf{S(k)}$ and charge $\mathbf{N(k)}$ structure factors, which indicates how is ordering the spin and charge in the real space. For the ground state, the spin and charge structure factor can be defined by $\mathbf{S(k)} = \frac{1}{\mathbf{L}}\sum_{\mathbf{j,l}} \mathbf{e^{ik(j-l)}}\langle \mathbf{S_j \cdot S_l}\rangle$ and $\mathbf{N(k)} = \frac{1}{\mathbf{L}}\sum_{\mathbf{j,l}} \mathbf{e^{ik(j-l)}}\langle \hat{\mathbf{n}}_{\mathbf{j}} \cdot \hat{\mathbf{n}}_{\mathbf{l}}\rangle$ respectively, where **S** is the electron spin in the **j** and **l** sites, and $\hat{\mathbf{n}}$ is the charge density per sites **j** and **l**.

Results

To study numerically the ground-state of the $\mathbf{AB_2}$ chain, for two electrons per unit cell, we used the DMRG method with 7 sweets and 300 states per block, and we obtain an error of the order of $\mathbf{10^{-9}}$ or less, for system sizes $\mathbf{L = 18, 36, 54, 72, 90}$ and $\mathbf{108}$.
In Fig. (1), for all $\boldsymbol{\Delta}$ values, we observe that exists a first left region in which the gap difference is equal to zero.

Results

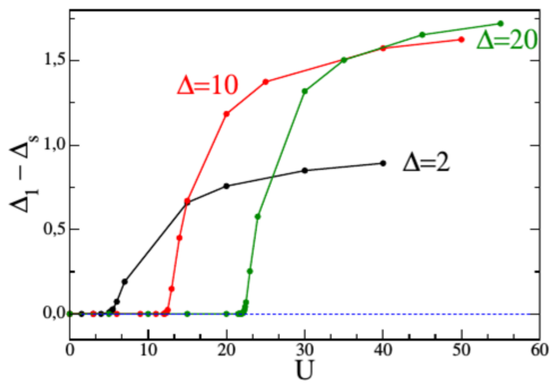

Figure 1. Gap difference $\Delta_1 - \Delta_s$ as a function of U for $L = 72$.

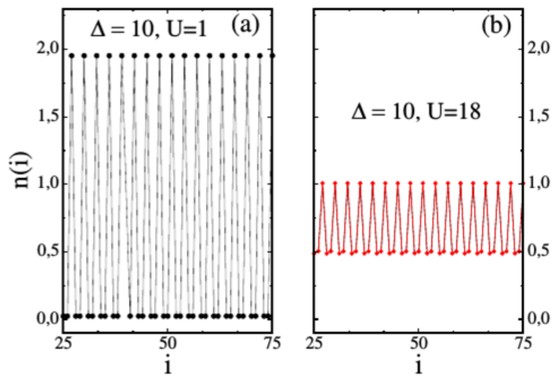

Figure 2. Charge Density for: (a) BI and (b) MI.

So the system is in a region type BI (as was noted by Aligia [1]). Also, we see that the gap difference increase rapidly in a short interval of values of **U** and after that, there is a small increase in the gap difference tending to a constant value, which indicates that we are in a zone which gaps are different and there is a particular ordering in the system.
For $\boldsymbol{\Delta} = \mathbf{10}$ and $\mathbf{U = 1}$, in Fig. (2a) we are inside of BI region. In Fig. (2b), we can see that the probability density of an electron is between A and B sites, which we are in the MI region (with $\mathbf{U = 18}$).

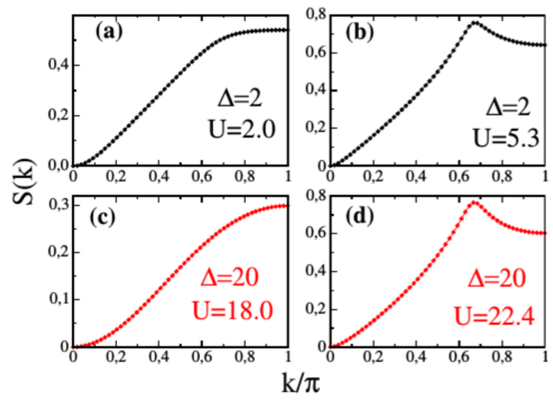

Figure 3. The spin structure factor $S(k)$ of the spin-spin correlation function for system size $L = 108$.

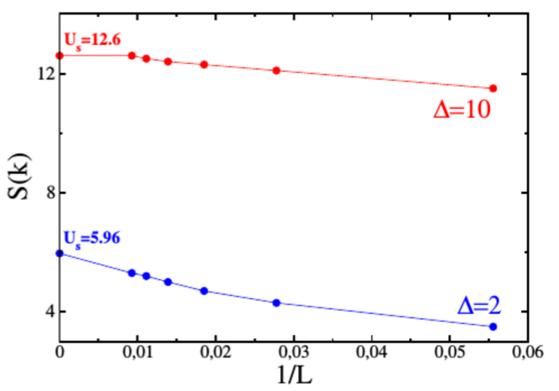

Figure 4. The spin structure factor $S(k)$ as a function of $1/L$ for $L = 18, 36, 54, 72, 90$.

In Fig. (3a), we can see that the structure factor shows an increasing and continuous behaviour, indicating that not exists particular ordering in the system. If we increase the value of **U** (for instance $\mathbf{U = 5.3}$ in Fig. 3b), we see that spin structure factor exhibits a maximum at $\mathbf{k = 2\pi/3}$. If we consider $\boldsymbol{\Delta} = \mathbf{20}$ for $\mathbf{U = 18}$, we are in the intermediate phase where the spin structure factor $\mathbf{S(k)}$ doesn't show a maximum value (Fig. 3c) so we don't have correlated phase. However, if we increase the value of **U** at $\mathbf{22.4}$ or larger than this, the behaviour changes indicating we have a maximum value for $\mathbf{S(k)}$ as we see in Fig. (3d).
We observe that the point where we have a maximum in the spin structure factor $\mathbf{S(k)}$ depends the size of the lattice, in order to find the transition point, we have to extrapolate to the thermodynamic limit, as in Fig. (4). And we found for $\boldsymbol{\Delta} = \mathbf{2}$, the critical point is $\mathbf{U_s = 5.96}$. However, the found value for Aligia *et al.* was $\mathbf{U_s \approx 8.2}$ for $\boldsymbol{\Delta} = \mathbf{2}$. Also, the values for $\boldsymbol{\Delta} = \mathbf{10}$ behaves in a similar way to $\boldsymbol{\Delta} = \mathbf{2}$, we found the transition point at $\mathbf{U_s = 12.6}$, so we can say that in thermodynamic limit, the critical points will have a crescent behaviour as function of $\boldsymbol{\Delta}$.

Conclusion

We could identify clearly two phases for $\mathbf{AB_2}$ chain model using DMRG: band insulator, which the gap difference is zero, and Mott correlated insulator. Also we show that the spin structure factor allow us calculating the transition point where Mott correlated phase begins. The transition points of the thermodynamic limit are determinated and, we see that the position of the points increases as a function of $\boldsymbol{\Delta}$.

References

[1] Torio M E, Aligia A A, *et al.* 2006 *Phys. Rev. Lett. B* **73** 115109
[2] Manmana S R, Meden V, *et al.* 2004 *Phys. Rev. Lett. B* **70** 155115
[3] Messer M, *et al.* 2015 arxiv:1503.05549 **1**
[4] Esslinger T 2010 arxiv:1007.0012

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