Quantum phases of $AB_2$ fermionic chains

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Abstract. A fermionic chain is a one-dimensional system with fermions that interact locally and can jump between sites in the lattice, in particular an $AB_n$ chain type, where $A$ and $B$ are sites that exhibit a difference in energy level of $\Delta$ and site $B$ is repeated $n$-times, such that the unit cell has $n+1$ sites. A limit case of this model, called the ionic Hubbard model ($n = 1$), has been widely studied due to its interesting physics and applications. In this paper, we study the ground state of an $AB_2$ chain, which describes the material $R_4[Pt_2(P_2O_5H_2)_{4}X]\cdot nH_2O$. Specifically, we consider a filling with two electrons per unit cell, and using the density matrix renormalization group method we found that the system exhibits the band insulator and Mott correlated insulator phases, as well as an intermediate phase between them. For couplings of $\Delta = 2, 10$ and 20, we estimate the critical points that separate these phases through the structure factor and the energy gap in the sector of charge and spin, finding that the position of the critical point rises as a function of $\Delta$.

1. Introduction

The effect of the interactions of many particles in quantum systems and superconductivity applications has been shown to be one of the most fascinating problems in physics, because it has allowed understanding the behavior of the electrons in solids, using some models such as the Hubbard model (HM). This model, in general, includes a Coulomb interaction term at short range and another term to quantify the kinetic energy. An example of a material that could be described by this model is vanadium oxide [1]. The Hubbard model has an exact solution in one dimension [2], through the Bethe Anzatz method, but it has also been studied using several analytic and numerical methods. Recently, this model has been emulated in optical lattices, allowing precise control of the hopping and interaction parameters, and filling in the Hamiltonian [3].

Other materials, such as tetrathiafulvalene-p-chloranil, can be modelled with a modification of the Hubbard model that considers that there exists a change in energy level of $\Delta$ between sites in the lattice. This model is called the ionic Hubbard model, which exhibits the phases: band insulator and Mott insulator, with a ferroelectric phase between them [4].

Trying to generalize the ideas of the ionic Hubbard model, in 2006 Torio et al. proposed a $AB_n$ fermionic chain model, where $A$ is a type of atom with a certain energy level and $B$ is another type of atom at a different site that repeats $n$ times [5]. This type of chain describes systems like halogen-bridged binuclear metal $R_4[Pt_2(P_2O_5H_2)_{4}X]\cdot nH_2O$ [6]. They used different techniques, such as bosonization, perturbation theory, and the exact diagonalization method for small clusters, and determined the phase diagram for $AB_2$ and $AB_3$ chains (which exhibits a band insulator phase, a correlated insulator phase, and a ferroelectric insulator phase) for a system of $L$ sites by following the crossing of appropriate excited energy levels, which turns out
to be equivalent to the method of jumps in Berry phases. However, their phase diagram does not clearly indicate the critical values where transitions occur, and this is an open question in the literature yet.

Given that experimentalists in the area of cold atoms can construct real one-dimensional lattices and that the ionic Hubbard model in an optical honeycomb lattice has been studied measuring the double occupation [7], this motivates us to study $AB_n$ fermionic chains, in particular the $n = 2$ case, using the density matrix renormalization group (DMRG) method for large lattice sizes.

In this paper, we focus on the transition points that separate the band and Mott insulator phases, using the spin and charge gaps and the structure factors.

2. Model

The Hamiltonian for the $AB_2$ chain is defined by:

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

(1)

Where $\hat{c}_{i,\sigma}^\dagger$ creates an electron at site $i$ with spin $\sigma$, $n_{i\sigma} = \hat{c}_{i,\sigma}^\dagger \hat{c}_{i,\sigma}$, and $n_i = n_{i\uparrow} + n_{i\downarrow}$. The parameter $t$ is the nearest-neighbour hopping amplitude (we take $t = 1$), $U$ is the on-site Hubbard interaction, and $\Delta_i$ is the difference in on-site energies. When we talk about the $AB_2$ chain, we have a unit cell with three sites, so two sites have an energy difference of $\Delta_i = 0$ and the other of $\Delta_i = -\Delta$, and this structure is repeated periodically.

On the other hand, for a fill equal to two electrons per unit cell, we have some limit cases for the $AB_2$ chain: for $U < \Delta$, the site $A$ is doubly occupied and the site $B$ is empty. This means that physically the lower band is filled and the others are empty, so the system behaves like a band insulator (BI). For $U > \Delta$ and for any value of $t$, in the Hubbard model we take a Mott insulator (MI) with $n = 1$. In the case of $n = 2$ and $U - \Delta > t$, the system adopts a form of modified MI state, called “correlated insulator” (CI), with almost exactly one particle per site and a charge gap of approximately $U - \Delta$ [5].

To study the ground state energy of our system, we calculate the spin ($\Delta_s$) and the charge ($\Delta_1$) gaps defined by

$$
\Delta_s = E_0(N, 1) - E_0(N, 0), \quad \Delta_1 = E_0(N + 1, 1/2) + E_0(N - 1, 1/2) - 2E_0(N, 0)
$$

(2)

Where $E_0(N, S_z)$ is the ground state energy for a lattice of size $L$ with $N$ particles in a spin sector $S_z$, $S_z$ being the $z$ component of the total spin [4]. With density matrix renormalization group, $\Delta_s$ can be calculated by the ground state energy in different subspaces $S_z$ in two different sweets, whereas for $\Delta_1$ we calculate the ground state energy in the subspaces with the corresponding particle numbers. In total, we work with four states.

Also, we decided to calculate the spin $S(k)$ and charge $N(k)$ structure factors, which indicates how the spin and charge are ordered in real space. For the ground state, the spin and charge structure factors can be defined by $S(k) = \frac{1}{L} \sum_{j,l} e^{ik(j-l)} \langle \mathbf{S}_j \mathbf{S}_l \rangle$ and $N(k) = \frac{1}{L} \sum_{j,l} e^{ik(j-l)} \langle \hat{n}_j \hat{n}_l \rangle$ respectively, where $\mathbf{S}$ is the spin operator, and $\hat{n}$ is the charge density operator. As for the spin ordering, if the spin structure factor exhibits a maximum at 0, the ordering is ferromagnetic; if the maximum is at $\pi$, it is antiferromagnetic. Otherwise, there will be a different ordering, maybe paramagnetic. Finally, for the charge ordering, the first peak in the charge structure factor indicates how much charge there is in the system, and the second peak shows how many electrons there are per unit cell. Therefore, we can determine the charge and spin distribution for our whole system.
3. Results

In order to numerically study the ground state of the $AB_2$ chain for two electrons per unit cell, we used the density matrix renormalization group method with 7 sweets and 300 states per block, and we obtained an error on the order of $10^{-9}$ or less, for system sizes $L = 18, 36, 54, 72, 90, \text{ and } 108$.

In Figure 1, we show the gap difference, $\Delta_1 - \Delta_s$, as a function of $U$ for three different values of $\Delta$. For all $\Delta$ values, we observe that there first exists a left-hand region in which the gap difference is equal to zero. This region grows as $\Delta$ increases. So the system is in a region type BI (as was noted by Torio [5]), because the spin and charge gaps are equal. Thus we obtain one site with double-occupation and the others with zero occupation. Also, we see that the gap difference increases rapidly within a short range 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 in which gaps are different and there is a particular ordering in the system. According to this Figure, we will have three phases in the system: a band insulator region, an Mott insulator region, and an intermediate phase between them.

For $\Delta = 10$ and $U = 1$, in Figure 2(a) we are in the band insulator region, which indicates that there are two electrons at one site (site A) and zero electrons at the other (site B), which characterizes this region. In Figure 2(b), we are in the Mott insulator region (with $U = 18$), and we have an electron at site A and another electron between two sites B. Thus we know that the system has two phases with different charge and spin ordering.

![Figure 1. Gap difference $\Delta_1 - \Delta_s$ as a function of $U$ for $L = 72$.](image1)

![Figure 2. Charge Density for: (a) BI and (b) MI.](image2)

In order to separate the phases, we need to find the critical point where the phase transitions occur. So we calculate the spin and charge structure factors. However, the charge structure factor is not shown in our results, because this does not give clear information about where the phase transition is. In Figure 3, we show the spin structure factor as a function of the momentum $k/\pi$ for $\Delta = 2$ and $\Delta = 20$ with two values of $U$. We can see in Figure 3(a) that the structure factor shows an increasing and continuous behavior, indicating that there does not exist a particular ordering in the system. If we increase the value of $U$ (for instance $U = 5.3$ in Figure 3(b)), we see that the spin structure factor exhibits a maximum at $k = 2\pi/3$, which indicates a particular charge ordering for equal or larger values of $U$ than this. If we consider $\Delta = 20$ for $U = 18$, we are in the intermediate phase, where the spin structure factor $S(k)$ does not exhibit a maximum value (Figure 3(c)), so we don’t have a correlated phase. However, if we increase the value of $U$ to 22.4 or larger, the behavior changes, indicating that we have a maximum value of $S(k)$, as we see in Figure 3(d).

We observe that the point where we have a maximum in the spin structure factor $S(k)$ depends on the size of the lattice. In order to find the transition point, we have to extrapolate to the...
thermodynamic limit, as in Figure 4. We can clearly see that as the size of the lattice grows, the transition point rises, and finally, using the extrapolation, we found, for $\Delta = 2$, that the critical point is $U_s = 5.96$. However, the value determined by Torio et al. was $U_s \approx 8.2$ for $\Delta = 2$.

As can be seen, our values and theirs diverge, which reflects the finite size effects, because they used small lattices, while our results indicate the transition points at the thermodynamic limit.

Also, the values for $\Delta = 10$ behave in a manner similar to $\Delta = 2$. We found the transition point at $U_s = 12.6$, so we can say that at the thermodynamic limit, the critical points will exhibit a crescendo behavior as function of $\Delta$.

4. Conclusions
We studied the $AB_2$ chain model using the density matrix renormalization group method and we were able to clearly identify two phases: a band insulator and a Mott correlated insulator. Therefore, we speculated that there is an intermediate phase between them.

We corroborated that the gap difference is zero for the band insulator phase. Also we showed that, the spin structure factor allows calculating the transition point where the Mott correlated phase begins.

Finally, we determined the transition points at the thermodynamic limit, and we saw that the position of the points rises as a function of $\Delta$.

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References
[1] Demishev S V, Chernobrovkin A I, Glushkov V V, Grigorieva A V, Goodilin E A, Ohta H, Okubo S, Fujisawa M, Sakurai T, Sluchanko N E, Samarin N A and Semeno A V 2011 Phys Rev B 84 094426
[2] Bethe H 1931 Zeitschrift für Physik 71 205
[3] Esslinger T 2010 Annu Rev Condens Matter Phys 1 129
[4] Manmana S R, Meden V, Noack R M and Schönhammer K 2004 Phys Rev B 70 155115
[5] Torio M E, Aligia A A, Japaridze G I and Normand B 2006 Phys Rev B 73 115109
[6] Yamamoto S 2001 Phys Rev B 64 140102(R)
[7] Messer M, Desbuquois R, Uehlinger T, Jotzu G, Huber S, Greif D, Esslinger T 2015 (ArXiv:1503.05549)