

Effect of the repulsion interaction on the ground-state of the Kondo lattice model with a superlattice potential

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Abstract. We investigate the ground-state of a new Kondo lattice model, where the free carriers interact repulsively between them and undergo an external superlattice potential. This model can be simulated with ¹⁷¹Yb atoms confined in optical lattices. We use the density matrix renormalization group method to evaluate the charge and spin gaps, and the structure factors. We found that the ground-state evolves from a Kondo spin liquid state to a charge-gapped antiferromagnetic state with zero spin gap, when the antiferromagnetic exchange increases. Also, we verify that the quantum critical point varies linearly with the repulsion and the exchange.

1. Introduction

The cold atoms community has been observed that the alkaline-earth atoms are useful to study the interplay of spin and charge degrees of freedom, therefore emulate some Hamiltonians that describe the physical properties of heavy fermions materials [1]. The first degenerate gas of alkaline-earth atoms was achieved by Fukuhara *et al.* [2]. After this, it was possible to observe the superfluid-insulator quantum phase transition with bosonic isotopes, and a Mott-insulator state with fermionic isotopes.

Daley *et al.* [3] recently proposed that the atoms in ¹S₀ (*g*) and ³P₀ (*e*) states can be confined independently in two different optical lattice potentials with the same periodicity. In this system, the collisions do not cause spin changes, because at low temperatures the scattering lengths are independent of the nuclear spins. Based on the above proposal, and encouraged by the possibility of studying the interplay between orbital and spin degrees of freedom, it was shown that using alkaline-earth atoms confined in an optical lattice it is possible to simulate the Kondo lattice model [4, 5], which can be obtained when the strong repulsion between *e* atoms is taken into account through a unit-filling constraint such that they are localized.

Using the mean field theory with a local density approximation, Foss-Feig *et al.* [6, 7] consider the free *g* atoms confined in a harmonic potential and interacting with localized *e* atoms in one and two dimensions. They modeled the system with the Kondo lattice model plus a quadratic potential term and observed that metallic regions and Kondo insulator domains with one *g* atom at each site coexist. A beyond mean field study of the 1D case was made using DMRG [8].



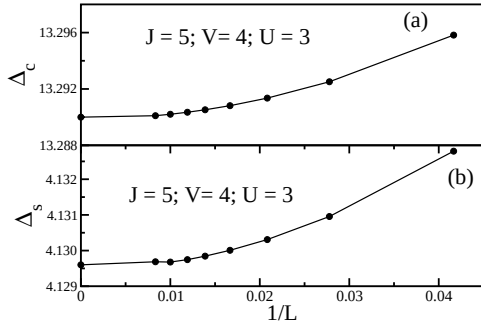


Figure 1. Charge (a) and spin (b) gaps for different lattice sizes. Here $V = 4$, $U = 3$ and $J = 5$.

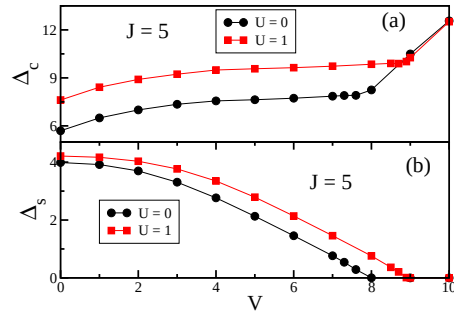


Figure 2. Thermodynamic limit of charge (a) and spin (b) gaps as a function of the superlattice potential strength.

The progress in the trapping technique allows the experimentalist to confine bosonic and fermionic atoms in different kinds of potentials: harmonic, superlattice, and anharmonic [9, 10, 11].

Here, we take into account the repulsive interaction between the g atoms, which experience a superlattice potential, while they interact locally with the e atoms through a Heisenberg type term.

2. Model and results

Using the ^{171}Yb atoms, we can emulate the Kondo lattice model plus a external potential, which Hamiltonian is given by

$$H = -t \sum_{i\sigma} \left(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{h.c.} \right) + \sum_i \left(U n_{i,\uparrow} n_{i,\downarrow} + J \mathbf{S}_{ic} \cdot \mathbf{S}_{if} + V_i (n_{i,\uparrow} + n_{i,\downarrow}) \right), \quad (1)$$

where, $c_{i\sigma}^\dagger$ creates an atom at site i in the electronic state 1S_0 , and (nuclear) spin state $\sigma = \uparrow$ or $\downarrow$. $n_{i\sigma}$ is the local density operator of delocalized atoms with spin σ , and the spin operator of localized (delocalized) atoms is $\mathbf{S}_{if}$ ($\mathbf{S}_{ic}$). Finally, we consider a superlattice confinement potential, which is zero for even sites and nonzero (V) for odd sites of the lattice. This potential can be created through the superposition of two optical lattices of different frequencies, with the frequency of one optical lattice being double that of the other.

We set the hopping integral $t = 1$ and adopt the density matrix renormalization group method [12] maintaining $m = 400$ states per block.

In this paper, we consider a local antiferromagnetic coupling between the localized and delocalized atoms, and we analyze the case when the number of delocalized atoms matches the lattice size. Without superlattice potential ($V_i = 0 \forall i$), this system has a finite charge and spin gaps for different values of the exchange (J) and repulsion (U). Calculating the the ground state energy for the S^z sector of a lattice with L sites, we obtain the spin gap $\Delta_s = E_g(S^z = 1, N = L) - E_g(S^z = 0, N = L)$. The charge gap is given by $\Delta_c = E_g(S^z = 0, N = L+2) - E_g(S^z = 0, N = L)$. To characterize the ground-state, we calculate the charge structure factor $N(q) = \frac{1}{L} \sum_{j,k} e^{iq(j-k)} \langle n_j n_k \rangle$, and also the spin structure factor $S(q) = \frac{1}{L} \sum_{j,k} e^{iq(j-k)} \langle \mathbf{S}_j^T \cdot \mathbf{S}_k^T \rangle$, where $\mathbf{S}_j^T = \mathbf{S}_{jc} + \mathbf{S}_{jf}$ is the total spin. Without superlattice potential, the spin structure factor is nonzero and constant indicating that the ground-state is composed by a local singlet in each site, whereas the charge structure factor has a strong peak at $q = 0$ indicating the homogeneous distribution of charge in the lattice.

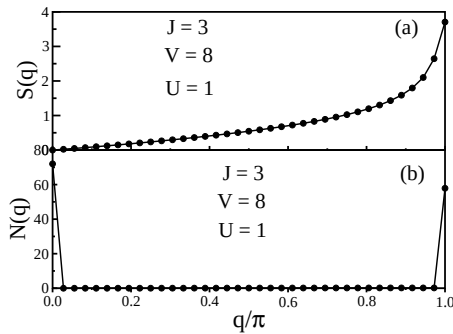


Figure 3. The spin (a) and charge (b) structure factors in the charge gapped antiferromagnetic state.

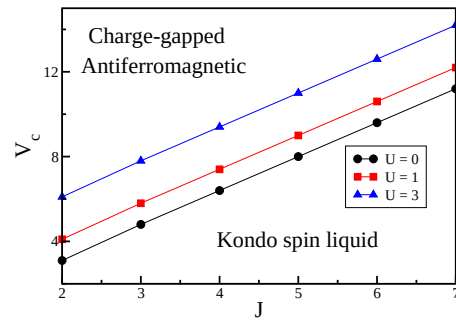


Figure 4. Phase diagram of ^{171}Yb atoms in a superlattice potential with constant repulsion interaction.

We show in Fig. 1 the spin and charge gaps for different lattice sizes of ^{171}Yb atoms in a superlattice potential of strength $V = 4$. The antiferromagnetic coupling is $J = 5$ and the repulsion between the g atoms is $U = 3$. We observed that the charge gap decreases as the lattice size increases; however, for larger sizes this behavior is slow, indicating that at the thermodynamic limit this quantity can be finite (see Fig. 1(a)). To determine the thermodynamic limit of the charge gap, we fit the curve to the following expression $\Delta(L) = \Delta(\infty) + \frac{\alpha}{L} + \frac{\beta}{L^2}$, where α and β are constants [13]. By adjusting the curve in Fig. 1(a) to the above expression, we obtain that the charge gap in the thermodynamic limit is $\Delta_c(J = 5, V = 4, U = 3) = 13.2900$, which is larger than the value without repulsion interaction $\Delta_c(J = 5, V = 4, U = 0) = 7.5624$.

In Fig. 1(b), we can see the spin gap as a function of the lattice size. Using the expression for the gap, we obtained that the spin gap at the thermodynamic limit is $\Delta_s(J = 5, V = 4, U = 3) = 4.1296$, again this value is larger than the value without repulsion interaction. Note that the spin and charge gaps increase with the repulsion when we consider the ^{171}Yb atoms confined in a superlattice potential, a similar result was found by Shibata *et al.* [13] for the homogeneous Kondo lattice model with a Coulomb interaction between the conduction electrons, however for our system the effect of the repulsion on the charge gap is stronger than on the spin gap.

For the parameters of Fig. 1, we obtained a ground-state with finite charge and spin gaps, hence this state is a Kondo spin liquid state, i. e. despite that the charge redistribution generates by the superlattice potential, the local repulsion and the strong exchange guarantee the formation of a singlet in each site of the lattice.

We are interested in finding new ground-states, i. e. to identify quantum phase transitions. For this reason, we evaluate the thermodynamic limit of the spin and charge gaps as a function of the strength of the optical superlattice potential. In Fig. 2, we show our results when the exchange and the repulsion are fixed to $J = 5$ and $U = 0, 1$ respectively. We observe that the spin gap decreases as the strength of the optical potential increases and vanishes at different values depending of the repulsion parameter(see Fig. 2(b)). Regardless the repulsion value, the system goes from a spin gap state to a spin gapless one, the critical point for $U = 1$ ($U = 0$) is $V_c(U = 1) = 9.0 \pm 0.1$ ($V_c(U = 0) = 8.0 \pm 0.1$). In Fig. 2(a), we note that the charge gap change his behavior at the critical point, after this, the charge increases linearly with the potential strength. Before the critical point the charge gap increases slowly and the difference between the curves with and without repulsion is almost the same, on the contrary to the spin gap, where the difference increases with the strength of the superlattice potential.

To understand the above results, we must to consider that the superlattice potential generates a redistribution of charge in the lattice, the even (odd) sites tends to be doubly occupied (empty)

for a critical value and the localized atoms order antiferromagnetic, under this conditions the effective local coupling vanishes and the delocalized and localized chains of atoms are disconnected. The repulsion effect prevent the double occupation and we have to increase the charge redistribution to overcome the repulsion barrier.

We conclude that for any repulsion value, the system suffers a quantum phase transition at the critical point: the system goes from a Kondo insulator phase with finite charge and spin gaps to a antiferromagnetic insulator phase with only a charge gap. The latter phase is characterized by non-local coupling and a superlattice ordering of the charge, with a site doubly occupied and the neighbor site empty when the strength is that high.

In Fig. 3, we show the charge and spin structure factors for ^{171}Yb atoms in a superlattice potential in the charge-gapped antiferromagnetic state ($J = 3$, $V = 8$, $U = 1$). We observe that the spin structure factor $S(q)$ is an increasing function with a pronounced maximum at $q = \pi$, which is consistent with the fact that the spin gap is zero and the localized atoms are in antiferromagnetic ordering (see Fig. 3(a)). The charge structure factor [Fig. 3(b)] vanishes for all values of q except at $q = 0$ and $q = \pi$, indicating that we have a superlattice charge ordering, characterized by empty and fully occupied sites.

3. Conclusions

We studied the ground-state of ^{171}Yb atoms confined in a one-dimensional optical superlattice, such that it simulates a Kondo lattice model with a superlattice potential. We found a quantum phase transition when the number of delocalized atoms matches the lattice size. This transition take place from the Kondo insulator state characterized by local singlets to a charge-gapped antiferromagnetic state without singlets. The latter state is characterized by an antiferromagnetic ordering of localized atoms, non-local effective coupling and a superlattice ordering of the charge, with a site doubly occupied and the neighbor site empty. We obtained that for any value of the repulsion the dependence of the critical strength potential V_c versus J is linear (see Fig. 4). Given a repulsion value, the line divides the phase diagram into two parts: the bottom, in which the system is in the well-known Kondo insulator phase, and the top, where the system is in the charge-gapped antiferromagnetic state. The evolution of the critical points is consistent with the expresion $V_c(J, U) = 3J/2 + U$.

Acknowledgments

The authors are thankful for the support of Universidad Nacional de Colombia (under grant DIB No. 15309) and the Brazilian agency CNPq.

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