Spiral to ferromagnetic transition in a Kondo lattice model with a double-well potential

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Abstract. Using the density matrix renormalization group method, we study a system of ¹⁷¹Yb atoms confined in a one-dimensional optical lattice. The atoms in the ¹S₀ state undergo a double-well potential, whereas the atoms in the ³P₀ state are localized. This system is modelled by the Kondo lattice model plus a double-well potential for the free carries. We obtain phase diagrams composed of ferromagnetic and spiral phases, where the critical points always increase with the interwell tunneling parameter. We conclude that this quantum phase transition can be tuned by the double-well potential parameters as well as by the common parameters: local coupling and density.

1. Introduction

Heavy-fermion materials exhibit a rich variety of ground states, some of these being magnetic and others not. To explain some properties of these materials, the scientific community has used the periodic Anderson model and the Kondo lattice model [1]. The main problem for the experimental study of these materials is the absence of control of the parameters, which has stimulated a search for new ways to test the ideas involved in the above models, where the charge and spin degrees of freedom compete. Taking into account the success of cold-atom setups for studying quantum phenomena such as the superfluid-insulator quantum phase transition, Gorshkov et al. proposed using alkaline-earth atoms confined in cold-atom setups to emulate the Hamiltonians that describe the physical properties of heavy-fermion materials [2].

Recently, Nishida [3] suggested a new scheme for obtaining a SU(3) orbital Kondo effect with ultracold atoms, and Bauer et al. [4] proposed the use of a mixture of ⁴⁰K and ⁴¹Na to generate a Kondo-correlated state. Also, the realization of a one-dimensional system of fermions interacting repulsively with SU(N) symmetry, where N can be tuned [5] and the spin-exchange contact interactions between confined ¹⁷¹Yb atoms can be measured [6], has stimulated study of this subject.

Foss-Feig et al. [7] and Silva-Valencia et al. [8] follow Gorshkov’s proposal and consider that ¹⁷¹Yb atoms in ¹S₀ (g) and ³P₀ (e) states can be confined independently in two different optical lattice potentials with the same periodicity. If the collisions do not cause spin changes and the strong repulsion between e atoms is taken into account through a unit-filling constraint, then it is possible to simulate the Kondo lattice model [9] plus an external potential to the free carries. Considering a quadratic potential, they show that metallic regions and Kondo insulator domains with one g atom at each site coexist.

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2. Model and results

Yb atoms in a double-well potential [10] can be described by considering a kinetic term for the free atoms, which undergo the external potential, and a local interaction term between local and free atoms. Therefore the Hamiltonian is given by

\[
H = -\sum_{i,\sigma} \left( \hat{c}_{2i,\sigma}^\dagger \hat{c}_{2i,\sigma} + \hat{c}_{2i+1,\sigma}^\dagger \hat{c}_{2i+1,\sigma} + \text{h.c.} \right) + \sum_{i} (J_s i \cdot S_i + V \hat{n}_i) \tag{1}
\]

Where, \( \hat{c}_{i\sigma}^\dagger \) is the creation operator for an atom at site \( i \) in the electronic state \( ^1S_0 \) and (nuclear) spin state \( \sigma \). \( s_i \) and \( S_i \) are spin-1/2 operators for free and localized atoms, respectively, and \( \hat{n}_i = \sum_\sigma \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma} \) is the density operator. The shift in the energy levels between neighbor sites \( V \) is zero for odd sites and \( V \) for even sites. The intrawell tunneling is our energy scale and equal to one, whereas the interwell tunneling is \( t \). \( J \) is the antiferromagnetic local exchange coupling and the lattice size is \( L \).

Figure 1 shows a picture of our experimental setup, where the double-well potential for the free atoms 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. Note that \( V \) can be tuned by shifting one laser beam with respect to the other, and the inter and intrawell tunnelings can be adjusted independently through careful control of the intensities [11, 12]. Here we consider \( t \leq 1 \).

![Figure 1. Schematic of the set-up. g atoms are red, and undergo a double-well potential; e atoms are blue, and are fixed at each site. t is the interwell tunneling parameter.](image)

The ground state of the Hamiltonian (1) was studied using the density matrix renormalization group method (DMRG) method [13], taking into account open boundary conditions. We considered \( m = 400 \) states per block, and the discarded weight was around \( 10^{-6} \) or less.

To characterize the different phases of our model, we calculate the spin structure factor \( S(q) = \frac{1}{L} \sum_{j,k} e^{i\mathbf{q} \cdot \mathbf{r}_{jk}} \langle S_j^\dagger \cdot S_k \rangle \), where \( S_j^\dagger \cdot S_k \) is the total spin at site \( j \). This quantity gives us information about the order of the system. For instance, when the total spin at the sites without singlets points in the same direction, we have a ferromagnetic order, which is reflected by a maximum at the wavenumber zero. An antiferromagnetic order leads to a maximum at \( \pi \).

Our main goal in this paper is to determine the evolution of the quantum phases of the model with the intrawell tunneling \( t \) when the other parameters of the model are fixed. The Kondo lattice model Hamiltonian is obtained by equation (1) considering \( t = 1 \) and \( V = 0 \). It is well known that for a global density \( \rho = 0.25 \), the critical point is located around \( J_c/t \approx 0.60 \), i.e. for values larger than \( J_c \) the ground state is ferromagnetic and the spin structure factor has a maximum at \( q = 0 \). For smaller values, the ground state is “spiral”, which means that the magnetic order is unclear, and the localized spins can show diverse alignments along the lattice, characterized by a non-definite position of the maximum of \( S(q) \) [14].

Now we consider the double-well potential and the spin structure factor as a function of the wave number, shown in Figure 2, where the global density is constant and equal to \( \rho = 0.25 \). Considering a local coupling \( J = 0.35 \) and with \( V = 0 \), we know that the ground state will be of the spiral type when \( t = 1 \), and this type remains for \( t = 0.6 \), as shown in Figure 2(a). When the potential is more deeper (\( V = 2 \)), we observe that the maximum of the spin structure factor is at \( q = 0 \), which indicates that the ground state is ferromagnetic (see Figure 2(b)).
Fixing the parameter $V$ and decreasing the local coupling, we observe in Figure 2(c) that the maximum at $S(q)$ is offset from zero, indicating a spiral state. Note that the spiral states in Figure 2(a) and (c) are different, i.e. the magnetic order is not the same, and the maximum positions are different. If the depth of potential increases, for instance $V = 4$ in Figure 2(d), the maximum of the spin structure factor is at $q = 0$, indicating that the ferromagnetic state is recovered. We observe that the local coupling and the depth of potential generate localization of the free atoms, which allows the formation of singlets, leading to the possibility of tuning the ferromagnetic to spiral quantum phase transition by changing the local coupling or $V$ when the interwell tunneling and the density are fixed.

Maintaining the depth of potential at $V = 0$, we expect that as $t$ increases the free atoms will tend to move to the neighbor sites, which hinders the formation of singlets, leading to the need to consider larger values of the local coupling for obtaining a ferromagnetic state. This fact is corroborated in Figure 3, where we show the local coupling versus the interwell tunneling for a global density $\rho = 0.25$. For $V = 0$, we note that the ferromagnetic phase decreases as the interwell tunneling grows. The critical points that separate the ferromagnetic and spiral phases for each value of the interwell tunneling grow monotonously. This behavior remains the same for other values of the depth of potential, $V = 2$ and 4. However, the localization effect of the depth of the potential causes the area of the ferromagnetic phase in the phase diagram to increase with the depth of the potential.

The spin structure factor for atoms in a double-well potential with parameters $t = 0.3$ and $V = 2$ is shown in Figure 4 for different values of the local coupling and the global density. For a constant global density $\rho = 0.25$, we observe that for local couplings $J = 0.1$ and $J = 0.2$ the ground state of the system is spiral and ferromagnetic, respectively, as shown in Figure 4(a) and (b). Keeping the same local coupling as in Figure 4(b) but increasing the number of free atoms, we obtain a larger density, for instance $\rho = 0.40$, and we note that the ground state changes (see Figure 4(c)). Now we have a spiral with a very complex structure: note that none of wavevectors dominate, as happened before for other parameter values. To obtain a ferromagnetic state, we need a larger value of the local coupling when the density is $\rho = 0.40$; for instance, we show in Figure 4(c) that for $J = 0.4$, the maximum of $S(q)$ is at $q = 0$, and the ground state is ferromagnetic.

In Figure 5, we show the phase diagram of the model for the densities $\rho = 0.25$ and $\rho = 0.40$ when the depth of potential is fixed at $V = 2$. We observe that the critical points increase monotonously as a function of the interwell tunneling regardless the global density. For each
value of the interwell tunneling, we see that for larger densities a larger local coupling is necessary in order to obtain a ferromagnetic state, because more atoms lead to a larger double occupation probability, which makes the formation of singlets difficult, and we have to localize the atoms by increasing the local coupling. Above the lines in Figure 5, we have a ferromagnetic phase, and below them, we have a spiral phase.

3. Conclusions

Ytterbium atoms in the $^1S_0 \ (g)$ state that undergo a double-well potential interacting with localized Ytterbium atoms in the $^3P_0 \ (e)$ state were studied using the DMRG method. This one-dimensional system was modeled by the Kondo lattice model plus a double-well potential for the free atoms. For the parameters considered here, we found a ferromagnetic and a spiral phase, which compete in the phase diagram. The ferromagnetic area increases as the density decreases, and the depth of potential grows. The quantum phase transition between these phases can be tuned by varying the local coupling, the depth of the potential, the interwell tunneling, or the density when three of these parameters are fixed.

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Figure 4. The spin structure factor for different parameters. The double-well parameters are $t = 0.3$ and $V = 2$.

Figure 5. Phase diagram as a function of the interwell tunneling. The double-well parameters are $t = 0.3$ and $V = 2$. 