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Phase diagram of the Kondo lattice model with a superlattice potential

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Abstract. We study the ground state of a Kondo lattice model where the free carries undergo a superlattice potential. Using the density matrix renormalization group method, we establish that the model exhibits a ferromagnetic phase and spiral phase whose boundaries in the phase diagram depend on the depth of the potential. Also, we observed that the spiral to ferromagnetic quantum phase transition can be tuned by changing the local coupling or the superlattice strength.

1. Introduction

Over the last few decades, cold atom setups have allowed the observation of Bose-Einstein condensates [1], BEC-BCS crossover of an attractive Fermi gas [2], and quantum phase transitions [3]. Now it is possible to emulate several condensed matter Hamiltonians with these setups, with the advantage of having full control over the parameters (kinetic energy, interactions, and density) and access to various dimensions [4].

The interplay between orbital and spin degrees of freedom is a crucial issue that determines the physical properties of manganese oxide perovskites and heavy-fermion materials [5]. Recently there has been interest in studying this competition in cold atom setups. The first proposal was made by Gorshkov et al. [6], who suggested the use of alkaline-earth atoms confined in optical lattices. Bauer et al. [7] proposed the use of a mixture of ⁴⁰K and ²³Na to generate a Kondo-correlated state, showing that the Kondo energy scale is accessible through current experimental techniques. Also, a new scheme for obtaining a SU(3) orbital Kondo effect with ultracold atoms was suggested by Nishida [8].

Recently, using ¹⁷³Yb atoms loaded into a 3D optical lattice, it was possible to observe a SU(6) Mott insulator state [9]. Also, Zhang et al. [10] achieved the first spectroscopic observation of SU(10) symmetry with ⁸⁷Sr atoms confined in a 2D optical trap. A one-dimensional realization of strongly-correlated liquids of ultracold fermions interacting repulsively within SU(*N*) symmetry, with a tunable number *N* of spin components, was reported by Pagano et al. [11].

Recently, Scazza et al. [12] confined ¹⁷³Yb atoms in two meta-stable electronic states and measured the spin-exchange contact interactions. This development will allow the emulation of two-orbital problems with cold atoms, such as for example the Kondo lattice model. An extension of this model with a harmonic potential for the free carries was studied recently [13,14], and it was found that in the ground state different insulating and metallic regions can coexist.



2. Model

In the present paper, we consider ^{171}Yb atoms, which have a total spin of $1/2$. Our setup consists of confining these atoms in the 1S_0 (g) and 3P_0 (e) states independently in two different optical lattice potentials with the same periodicity. Furthermore, it is reasonable to consider that there is a high Coulomb repulsion between the e atoms and that the collisions do not cause spin changes. Hence the delocalized g atoms experience an external potential due to confinement, while they interact locally with the localized e atoms through a Heisenberg-type term (see the setup in Figure 1). The Hamiltonian of this new Kondo lattice system is given by,

$$H = -t \sum_{i=1, \sigma}^{L-1} \left(\hat{c}_{i, \sigma}^\dagger \hat{c}_{i+1, \sigma} + \text{h.c.} \right) + \sum_{i=1}^L (J \mathbf{s}_i \cdot \mathbf{S}_i + V_i \hat{n}_i) \quad (1)$$

Where, $\hat{c}_{i\sigma}^\dagger$ creates an atom at site i in the electronic state 1S_0 and (nuclear) spin state σ . \mathbf{S}_i is a localized spin-1/2 operator, $\hat{n}_i = \sum_{\sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}$, and $\mathbf{s}_i = \frac{1}{2} \sum_{\alpha\beta} \hat{c}_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i,\beta}$ is the delocalized atom spin-density operator, $\boldsymbol{\sigma}$ being the vector of Pauli matrices. L is the lattice size, and J is the antiferromagnetic local exchange coupling. We fix our energy scale taking $t = 1$.

To observe new ingredients in the magnetic phase diagram of the Kondo lattice model, we consider that the free carries undergo a superlattice potential, which has the value $V_i = V$ for odd sites and $V_i = 0$ for even sites. Here V denotes the shift in the energy levels for each site.

For half-filling, this confinement potential leads to a quantum phase transition from a Kondo insulator spin liquid state without potential to a charge-gapped antiferromagnetic state with nonzero potential [15]. Now we will concentrate on fillings far away from half-filling and explore the ground state for low local couplings as a function of the superlattice potential.

To study the Hamiltonian (1), we considered $m = 600$ states per block within the finite-size algorithm of the density matrix renormalization group method (DMRG) [16] taking into account open boundary conditions. The discarded weight was around 10^{-6} or less.

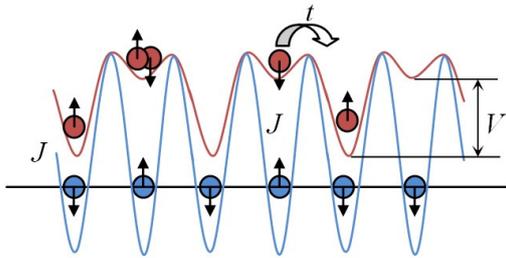


Figure 1. (color online) Schematic of the set-up. g atoms are red, and undergo a superlattice potential; e atoms are blue, and are fixed at each site.

3. Results

Today, it is well known that the one-dimensional Kondo lattice model ($V_i = 0 \forall i$ in Hamiltonian (1)) exhibits a very rich phase diagram away from half filling. For a large local coupling, the ground state is ferromagnetic, whereas for small couplings the local spins exhibit a special magnetic order called the “island” phase by Garcia et al. [17]. Between these phases there is a spiral phase, where the magnetic order is unclear. The main difference between these phases is the magnetic order, which can be determined by calculating the spin structure factor $S(q) = \frac{1}{L} \sum_{j,k} e^{iq(j-k)} \langle \mathbf{S}_j^T \cdot \mathbf{S}_k^T \rangle$ of the ground state, where \mathbf{S}^T is the total spin (free plus local) operator. This quantity exhibits a maximum at $q = \rho\pi$ ($q = 0$) in the island (ferromagnetic) phase, ρ being the density of the free carries. If we start with a certain phase and begin to change the parameters of the system, a critical point will be the parameter value for which $S(q)$ reaches its maximum value at the characteristic position of a different phase.

In Figure 2 (a), we show the spin structure factor for the original Kondo lattice model for $J = 1$, and it exhibits a maximum at $q/\pi < \rho$; therefore the ground state of the system

is spiral. If we keep the local coupling and turn on the superlattice potential, for instance $V = 1$, we note that the maximum of $S(q)$ moves to zero, indicating that the ground state is ferromagnetic (Figure 2(b)). The superlattice potential causes a phase transition from the spiral to the ferromagnetic phase. Fixing the superlattice potential and decreasing the local coupling, we expected that the size of the singlet formed by delocalized and localized atoms would increase and the ferromagnetic order would not be favored, which we can observe in Figure 2(c) for $J = 0.8$, where the spin structure factor indicates a spiral ground state. In this case, another small peak appears, indicating an additional underlying magnetic order in the system. Now, the phase transition is due to the local coupling. The superlattice potential favors the localization of the atoms; therefore, the formation of singlets, i. e. a further increase in the superlattice potential, brings the system back to a ferromagnetic phase (Figure 2(d)). The above discussion allows us to conclude that the system undergoes a quantum phase transition from the spiral to a ferromagnetic state, which can be tuned by varying the local coupling or the potential strength. We believe that this phase transition is continuous.

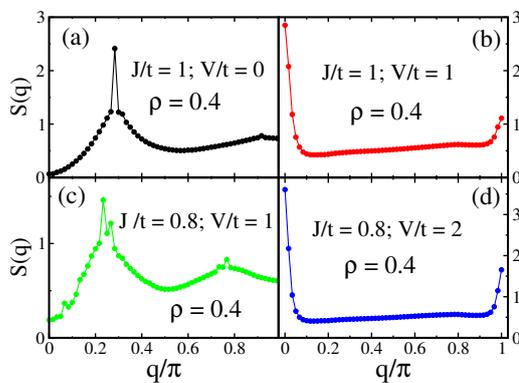


Figure 2. (color online) Spin structure factors for $\rho = 0.4$ with different parameters J/t and V/t .

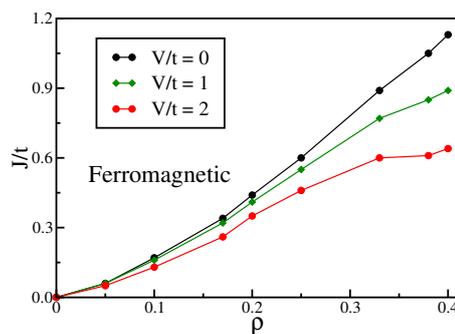


Figure 3. Phase diagram as a function of the density for $V = 0, 1$ and 2 . The lines are visual guides.

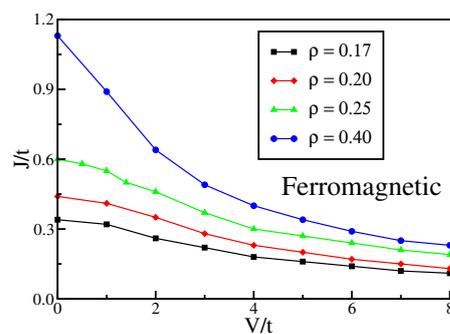


Figure 4. Phase diagram as a function of the strength. The lines are visual guides.

The boundary between the spiral and the ferromagnetic phase of the original Kondo lattice model is shown in Figure 3 (black points). As is well known, the critical coupling increases with the density [18]. Also, we show the boundary between these phases for $V = 1$ (green points) and $V = 2$ (red points). For both superlattice potentials, we observed that the critical points take low values for any density. This tendency increases as the overall density rises. In Figure 4, we plot the local critical coupling as a function of the superlattice strength for some densities.

We observe that the critical points take lower values as the potential increases; i.e., for a fixed density the critical points decrease monotonously, separating the ferromagnetic and the spiral phases. This behavior is expected, due to the localization generated by the potential, which reduces the spatial extension of the singlets and leads to a lower value of the local coupling in order to obtain ferromagnetism. For any density, we note that the decrease of the critical points is greater for low- and intermediate -strength potentials; however, for higher values, the critical points vary very slowly, indicating the difficulty of redistributing the carriers in the system.

4. Conclusions

Using the density matrix renormalization group method, we studied the ground state of a Kondo lattice model with a superlattice potential, which can be emulated in an optical lattice setup. For densities lower than $\rho = 0.4$, we found that the spiral to ferromagnetic phase transition can be tuned by varying the local coupling or the superlattice potential. We observed that all phases are robust enough to survive at the thermodynamic limit.

We conclude that the external superlattice potential will determine the ground state once the density and the local coupling are defined. The critical points that separate the different phases of this model decrease monotonously as a function of the potential strength, reflecting the localization effect. Our calculations lead us to think that these transitions are of second order, although a bosonization calculation can help to confirm this.

Acknowledgments

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