PHYSICS

MAGNETIC TRANSITION OF YTTERBIUM ATOMS CONFINED IN OPTICAL SUPERLATTICE WITH LOCAL FERROMAGNETIC INTERACTION

TRANSICIONES DE FASE MAGNÉTICA DE LOS ÁTOMOS DE ITERBIO CONFINADOS EN UNA SUPERRED ÓPTICA CON UNA INTERACCIÓN LOCAL FERROMAGNÉTICA

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ABSTRACT

Ramírez Diego-F, R. Franco, J. Silva-Valencia. Magnetic transition of ytterbium atoms confined in optical superlattice with local ferromagnetic interaction. Rev. Acad. Colomb. Cienc., 37 (1): 44-49, 2013. ISSN 0370-3908.

We used the density matrix renormalization group to study the ground state of ytterbium atoms (^{171}Yb) for the Hund lattice model, where the delocalized atoms are confined in a one-dimensional optical superlattice and his number is one third of the lattice sites. We found a paramagnetic-ferromagnetic quantum phase transition for any value of the potential strength. The local critical ferromagnetic coupling decreases as the superlattice potential increases.

Key words: Hund lattice model, ferromagnetic coupling, heavy fermions

RESUMEN

Nosotros usamos el grupo de renormalización de la matriz densidad para estudiar el estado base de los átomos de Iterbio (^{171}Yb) para el modelo de red de Hund, donde los átomos delocalizados son confinados en una superred óptica unidimensional y son un tercio de los sitios de la red. Nosotros hallamos una transición de fase magnética paramagnética-ferromagnética para algunos valores del potencial. El punto crítico del acoplamiento decrece cuando el potencial de la superred disminuye.

Palabras clave: Modelo de red de Hund, acoplamiento ferromagnético, fermiones pesados.

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1. Introduction

Ultracold atoms confined in an optical lattice (quantum simulation) offer a clean and simple system for the experimental investigation of quantum phase transitions. Bosonic [1] and fermionic [2, 3] models, and the spin Hamiltonians [4] can be controlled under novel conditions: dimensionality, interactions between particles through Feshbach resonances [5], independent periodic potential [6, 7] and different lattice topologies [8]. Moreover, Gorshkov et al. [9] showed that properties of fermionic alkaline-earth-metal atoms confined in an optical lattice allows the simulation of simple models, or condensed-matter Hamiltonians, such as the Kugel-Khomskii model [10], *SU(N)* Hubbard chains [11] and the Kondo lattice model [12, 13]. Motivated by these developments, we analyze ytterbium atoms confined in an optical superlattice using the Hund lattice model (HLM).

The Kondo lattice model (KLM) and its Hund lattice model (HLM) counterpart are canonical models for studying the interaction between a magnetic moment (localized) interacting via a contact Heisenberg exchange J with the spin of any conduction (delocalized) electron at each lattice site. For these models, the one-dimensional and three-dimensional ground-state phase diagram is determined by two para/meters: the ratio of the exchange coupling to the hopping (J/t), and the density of the conduction electrons n_c; with strong coupling the Kondo effect favors the singlet state, while with weak coupling the RKKY interaction tends to stabilize a magnetic order. Fig. 1 shows the phase diagram for the Hund model with numerical results, with a localized magnetic moment $S=1/2$, analogous to the KLM [14]. At half-filled $n=1$, characterized by a spin gap, the system exhibits a spin-liquid phase [15]. The ferromagnetic phase exists above the critical points (empty symbols). The phase beneath the critical points is much less understood; Ref. [14] shows two phases: the "spiral" phase characterized by two broad peaks in the local spin-spin correlation function, and the "island" phase, characterized by the ferrimagnetic condition. However, for intermediate coupling, there is another ferromagnetic state between the "paramagnetic" phase [16]. Moreover, Ref. [17] analyzes the paramagnetic phase in the KLM with alkaline-earth-metal atoms confined in an optical lattice. Based on the latest literature, which motivates the present paper, we assumed the "paramagnetic" term for this area.

For three-dimensional electronic structures, the KLM is applied to heavy-fermions material (with greatly enhanced effective mass), which exhibits an antiferromagnetic (AFM) exchange, favoring the antialignment between localized and delocalized particles. The HLM is applied to manganese oxide perovskites, with a ferromagnetic (FM) exchange moderated by Hund's rule coupling; a strong coupling favors the alignment of the three localized t_{2g} spins with the spin of the e_g conduction electron [23]. However, the experimental data of manganese oxide perovskites disagree with the model [27].

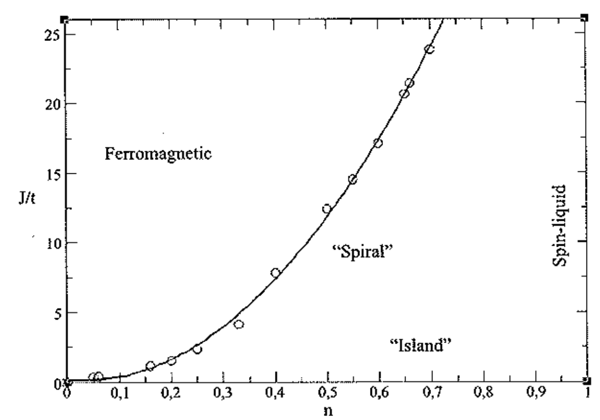

Figure 1. Magnetic phase diagrams of 1D Hund model. The ferromagnetic coupling increases with the filling. (Points taken from Ref. [14]).

Experimental investigation at low dimensionality in heavy fermion systems, reproduces the conditions of the KLM (Kondo effect vs. RKKY interaction) and offers the possibility of exploring the fundamental physics of the two-dimensional system [18]. Analogous to the 2D one, the 1D KLM and HLM will have a superlattice structure with nanofabrication techniques [19, 20]. However, to our knowledge these systems are not realized in condensed-matter systems. Nevertheless, it could be explored with the ytterbium atoms confined in a one-dimensional optical superlattice. Therefore, the new model has three parameters: the ratio of the exchange coupling and optical superlattice to the hopping-matrix element (J/t, V/t), and the density of the delocalized atoms (n). We analyzed a ground-state phase diagram of the HLM, where the number of delocalized atoms is one third of the system sites ($n=1/3$), using the density matrix renormalization group method DMRG [21].

We end this section with the features of the ytterbium atoms and the optical lattice. Section 2 explain the Hamiltonian model. Section 3 shows the result for the HLM, and section 4 summarizes our results.

Recently papers [16, 22] have used the KLM to explored the magnetic transition of ytterbium (Yb) atoms confined in optical lattice. The stables isotopes of this element are ^{168}Yb, ^{170}Yb, ^{171}Yb, ^{172}Yb, ^{173}Yb, ^{174}Yb and ^{176}Yb. For experimental studies of the Fermi gases two fermionic isotopes are used: ^{171}Yb and ^{173}Yb with nuclear spin $I = 1/2$ and $I = 5/2$ [11]. The first has two different internal states: $I = F = 1/2$, then $2F+1 = 2$. Hence, the ^{171}Yb can be used to simulated the KLM, which allows two degrees of freedom for each band, either spin up or spin down [23]. Furthermore, the atoms exhibits electronic state dependence: the metastable excited state $^3P_0$ and the ground state $^1S_0$, which posses no electron spin and thus no hyperfine interaction with the nuclear spin. Therefore, the nuclear spin strongly affects the interaction solely between these atoms [24, 25].

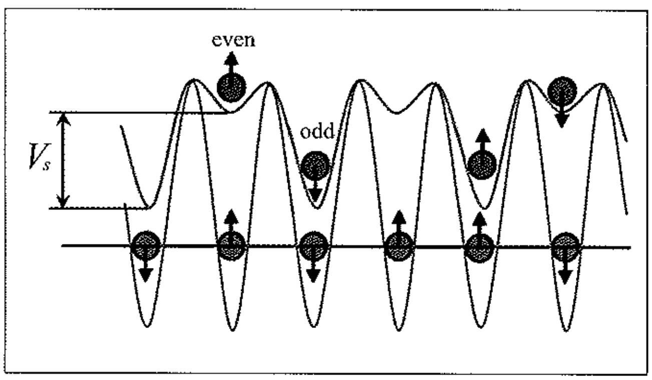

Figure 2. (Color online) HM plus a superlattice potential for delocalized atoms.

The optical lattice is formed by the interference of two or more laser beams. The electric field provided by the oscillating light from a laser, interacts with the dipole moment in the atoms, creating a trapping potential [26] $V(x) \sim I \sin(2x\lambda)$, where I is the intensity and λ the wavelength of the laser beam. Therefore, the atoms can be trapped in a bright interference pattern. Thus, independent storage associate with the ground state $^1S_0$ (g) and transport associate with the metastable excited state $^3P_0$ (e) are created, where the ytterbium atoms can be trapped in two different optical lattice potential with the same periodicity. Furthermore, it is possible to form periodic 1D, 2D and 3D spatial structures and different kinds of potentials can be constructed: harmonic, anharmonic and superlattice. This last kind consists of a superposition of two laser beams along the same direction with different wavelengths, obtaining different periodicities and potential depth on the sites. In Fig. 2, the optical superlattice (red line) is associate with the $^1S_0$, and the other optical lattice (blue line) is associate to the $^3P_0$.

2. Model

The separation and the deepth of the sites and supersites (even and odd in Fig. 2) throughout the optical superlattice define the interaction between the ultracold fermionic atoms and give rise to strongly a correlated system, which can be analyzed with the Anderson lattice Hamiltonian, the Hubbard model and the KLM. If a short-range superlattice potential is applied to this last model, the system can be simulated by means of localized atoms (blue line, Fig. 2) coupled with the delocalized atoms at the sites and supersites (red line, Fig. 2), where no interaction exists between them. Moreover, the model may exhibit two cases for the coupling: the "Kondo" model with $J < 0$ (antiferromagnetic) and the "Hund" model with $J > 0$ (ferromagnetic). In the present paper, we analyzed the last case where the delocalized atoms are confined in a one-dimensional optical superlattice whose Hamiltonian has the form:

$$\begin{aligned} H &= -t\sum_{i,\sigma}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} + \text{h.c}\right) \\ &\quad -J\sum_{i,\sigma,\beta}\left(\hat{c}^{\dagger}_{i,\alpha}\hat{\boldsymbol{\sigma}}_{\alpha\beta}\hat{c}_{i,\beta}\cdot\mathbf{S}_i\right) \\ &\quad +\sum_{i,\sigma}V_i\hat{n}_{i,\sigma} \end{aligned} \tag{1}$$

The first term represent the kinetic energy of delocalized atoms hopping between nearest-neighbor sites, where $\hat{c}^{\dagger}_{i,\sigma}\left(\hat{c}_{i+1,\sigma}\right)$ are the creation (annihilation) operators for one atom at the site i with spin $\sigma(=\uparrow,\downarrow)$ and t is the hopping amplitude. The second term represent the local Heisenberg interaction, where J is the coupling Hund, $\hat{\boldsymbol{\sigma}}$ is the Pauli matrix and $\mathbf{S}_i$ is a localized spin operator 1/2. We assume that t is set to 1.

The third term represents the one-dimensional optical superlattice potential. Here, $\hat{n}_{i,\sigma} = \hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i,\sigma}$ represent the local density of the delocalized atoms. V_i determines the optical superlattice potential, being the difference between the odd and even sites defined with two sites periodicity. In the present paper, $V_s = V$; therefore, $V_i = V$ for odd sites and $V_i = 0$ for even sites (Fig. 2), which denotes the shift in the energy levels for each site. When $V_s = 0$ Eq. 1 returns to the HLM Hamiltonian.

Since we study a one-dimensional many-body system in the ground state, the density matrix renormalization group method (DMRG) is applied in order to study the Hamiltonian (1), when the number of delocalized atoms is one third of the localized atoms.

3. Result

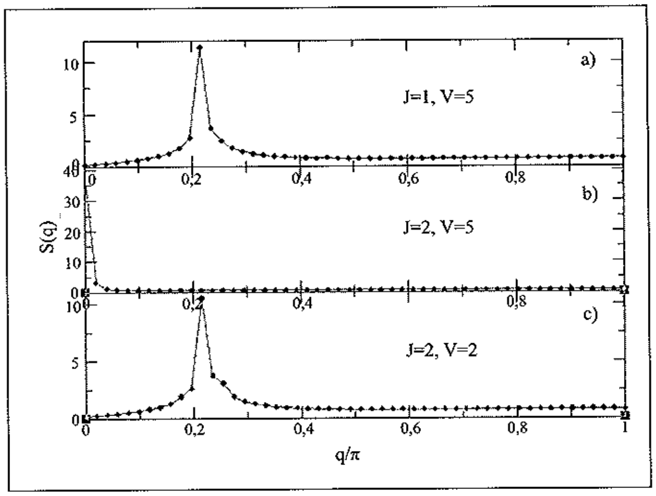

Figure 3. (Color online). Spin structure factors of ytterbium (Yb) atoms in a superlattice potential with lattice size $L = 102$, and $N = 34$ delocalized atoms. a) and c) represent a paramagnetic phase at $J = 1$, $V = 5$ and $J = 2$, $V = 2$. b) exposed a ferromagnetic phase at $J = 2$, $V = 5$.

The magnetic phase diagram of the KLM and Hund models for a partially filled system has been calculated through the spin structure factor [14], defined as the local spin-spin correlation function and its Fourier transform. We used this argument for the same purpose, which can be written as:

$$S(q) = \frac{1}{L}\sum_{j,k} e^{iq(j-k)} \left\langle \mathbf{S}_j^T \cdot \mathbf{S}_k^T \right\rangle \tag{2}$$

L represent the lattice sites and $\mathbf{S}_j^T = \sum_{\alpha,\beta} \hat{c}_{j,\alpha}^{\dagger} \sigma_{\alpha\beta} c_{j,\beta}^{\dagger} + \mathbf{S}_j$ is the total spin at the site j (Fig. 2). When Eq. 2 shows a peak at $q = 0$, the system indicates an alignment of the total spin or *ferromagnetic state*. The paramagnetic state exhibits a maximum at a q-value between 0 and π.

The Hund model for the case $n = 1/3$ exhibits a ferromagnetic phase at $J \geq 5$ (Fig. 1), which is highlighted for a maximum value or peak of $S(q)$ at $q = 0$. However, we observed this phase at $J = 5$ when the model is subjected to a superlattice potential. This can be seen in Fig.3b, in which we consider $J = 2$ and $V = 5$, for $L = 102$ sites and $m = 200$ states per block. The confinement of the delocalized atoms at the odd sites increases with the potential, reducing the tunneling and the kinetic energy and favoring local ferromagnetic coupling.

If the local ferromagnetic coupling is fixed and the potential decreases, we expect that the system will show a paramagnetic phase when $J = 2$. Fig. 3c shows the maximum spin structure factor at $q \approx 0.2$ for $V = 2$, indicating that the system evolves to a paramagnetic phase.

Now, we vary the ferromagnetic coupling and fix the potential. Comparing the figures 3a and 3b, the maximum value of $S(q)$ has a paramagnetic order at $J = 1$ and a ferromagnetic order at $J = 2$, for $V = 5$. This occurs by means of Hund's rule coupling, in which if J increased the delocalized atoms force the localized atoms to align in the same direction favoring the ferromagnetic phase. Therefore, the probability of the delocalized atoms being aligned parallel to the localized atoms at each site increases.

With Fig. 3, we conclude that the system evolves from a paramagnetic to ferromagnetic phase, which can be tuned by varying the local coupling or the potential strength.

The weight of the peak of the spin correlation $S(q)_{max}$ represents the magnetic order of the system. In Fig.4a, the potential is fixed and the coupling changes. For $J = 1$ (red line), $S(q)_{max}$ increases slowly and is finite at the thermodynamic limit, indicating that the paramagnetic state is stable. For a larger coupling (blue line), the maximum of the spin structure factor increases as a function of the lattice size. For these parameters, the system is in a ferromagnetic state; hence this result indicates to us that the system remains in this state and that the magnetic order is not due to the finite size effects.

Keeping in mind Fig 3, we explored several values of the potential and the coupling, indicating a magnetic phase transition. In Fig 5, we change the potential, finding the points of the coupling at which the transition occurs; in this figure, we demonstrate the propagation of the ferromagnetic area when the potential is increased. Furthermore, we analyzed the situations when $V = 0$ and $V \to \infty$. The first case represents the HLM without potential, in which the transition phase occurs at $J \geq 5$ (Fig. 1). The critical point in Fig. 5 is $J_c(V = 0) = 4.964 \pm 0.085$, which is in agreement with the previous result [19]. The second case indicates that the ferromagnetic phase can be obtained for low values of the coupling, where the critical point at which the transition occurs acquires a constant value.

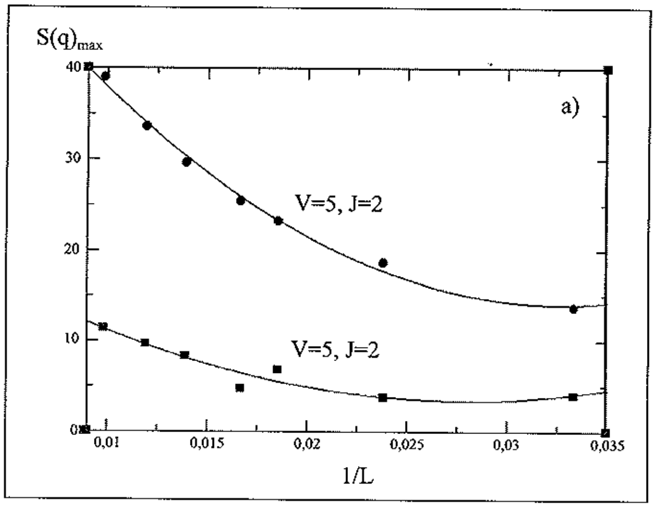

Figure 4. (Color online) The peak weight $S(q)$ a) for the ferromagnetic ($J=2$) and paramagnetic ($J=1$) cases at $V=5$.

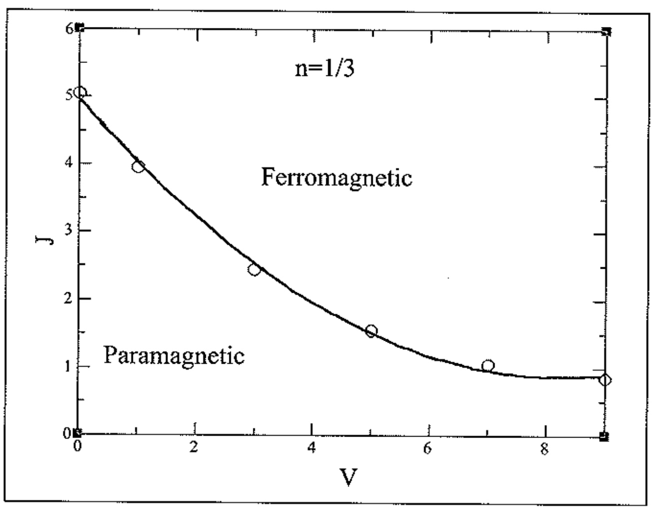

Figure 5. (Color online). Magnetic phase diagram of Ytterbium atoms for the Hund model with superlattice potential. The number of the delocalized atoms is a third of the localized magnetic moment: $n=1/3$.

Conclusions

We considered the number of delocalized atoms to be one third of the lattice size, and adopted the density matrix renormalization group technique to find the ground-state wave function of the Hund model plus a superlattice potential. We showed the magnetic phase diagram, in which the system increases the ferromagnetic phase with the potential, while the critical coupling decreases. This is caused by Hund's rule coupling, in which if the coupling is strong, an alignment of the delocalized spin with localized spin exists. Furthermore, the spin structure factor exhibits a ferromagnetic ordering of the total spins if the coupling increases for any value of the potential, favoring the ferromagnetic phase. Moreover, the ferromagnetic or paramagnetic ordering is maintained at the thermodynamic limit $L \to \infty$.

References

[1] **Greiner, M., Mandel, O., Esslinger, T, Hänsch, T. W., Bolch, I**, 2002, Quantum phase transition from a superfluid to a Mott insulator in a gas of ultracold atoms, Nature 415, 39.

[2] **Schneider, U., Hackermüller, L., Will, S., Best, Th., Bloch, I., Costi, T.A., Helmes, R. W., Rash, D.**, 2008, Metallic and Insulating Phases of Repulsively Interacting Fermions in a 3D Optical Lattice, Science 322, 1520.

[3] **Jördens, R., Strohmaier, N., Günter, K., Moritz, H., Esslinger, T.**, 2008, A Mott insulator of fermionic atoms in optical lattice, Nature 455, 204.

[4] **Jané, E., Plenio, M. B., Jonathan, D.**, 2002, Quantum-information processing in strongly detuned optical cavities, Phys. Rev. A 65, 050302.

[5] **Courteille, Ph., Freeland, R. S., Heinzen, D. J.**, 1998, Observation of a Feshbach Resonance in Cold Atom Scattering Phys. Rev. Lett. 81, 69.

[6] **Markus, O., Greiner, M., Widere, A., Rom, T., Haensch T. W., Bloch, I.**, 2013, Coherent transport of neutral atoms in spin-dependent optical lattice potentials, cond-mat/0301169

[7] **Jaksch, D., Cirac, J. I., Zoller, P.**, 2002, Dynamically turning off interactions in a two-component condensate, Phys. Rev. A 65, 033625.

[8] **Guidoni, L., Verkerk, P.**, 1998, Direct observation of atomic localization in optical superlattices, Phys. Rev. A 57, R1501 (1998); Gorlitz, A., Kinoshita, T., Hansch, T. W., Hemmerich, A., 2001, Realization of bichromatic optical superlattices, ibid. 64, 011401.

[9] **Gorshkov, A.V., Hermele, M., Gurarie, V., Xu, C., Julienne, P.S., Ye, J., Zoller, P., Demler, E., Lukin, M.D., Rey, A.M.**, 2010, Two-orbital Su(N) magnetism with ultracold alkaline-earth atoms, Nature Phys. 6 289.

[10] **Kugel, K.I., Khomskii, D.I.**, 1973, Crystal Structure and magnetic properties of substance with orbital degenerecy, Sov. Phys. JETP 37 725.

[11] **Manmana, S.R., Hazard, K. R. A., Chen, G., Feiguin, A.E., Rey, A. M.**, 2011, SU(N) magnetism in chains of ultracold alkaline-earth-metal atoms: Mott transitions and quantum correlations Phys. Rev. A 84 043601.

[12] **Tsunetsugu, H., Sigrist, M., Ueda, K.**, 1997, The ground-state phase diagram of the one-dimensional Kondo lattice model, Rev. Mod. Phys. 69 809.

[13] **Shibata, N., Ueda, K., 1999** J. Phys.: Condens. Matter 11 R1.

[14] **Garcia, D. J., Hallberg, K., Alascio, B., Avignon, M.**, 2004, Spin Order in One-Dimensional Kondo and Hund Lattices, Phys. Rev. Lett. 93, 177204.

[15] **Tsunetsugu, H., Hatsugai, Y., Sigrist, M.**, 1992, Spin-liquid ground state of the half-filled Kondo lattice in one dimension Phys. Rev. B 46, 3175.

[16] **Peters, R., Kawakami, N.**, 2012, Ferromagnetic state in the one-dimensional Kondo lattice model, Phys. Rev. B 86, 165107.

[17] **Foss-Feig, M., Hermele, M., Gurarie, V., Rey, A. M.**, 2010, Pro-

bing the Kondo lattice model with alkaline-earth-metal atoms, Phys. Rev. A 81, 053624.

[18] **Shishido, H., Shibauchi, T., Yasu, K., Kato, T., Kontani, H., Terashima, T., Matsuda, Y.**, 2010, Tuning the Dimensionality of the Heavy Fermion Compound CeIn3, Science 372, 980.

[19] **Kim, S., Razegi, M.**, 2001: Advances in quantum dot structures. In: Processing and Properties of Compound Semiconductors, ed. by Willardson, K., Weber, E.R., Academic, New York.

[20] **Babak Ziaie, Antonio Baldi, Massood Z. Atashbar**, 2010: Introduction to micro-/Nanofabrication. In: Springer Handbook of Nanotechnology, ed. by Bhushan, B., Springer Berlin Heidelberg.

[21] **White, S. R.**, 1992, Density matrix formulation for quantum renormalization groups, Phys. Rev. Lett. 69, 2863.

[22] **Silva-Valencia, J., Franco, R., Figueira, M.S.**, 2013, Quantum phase transition of alkaline-earth fermionic atoms confined in an optical superlattice Physics Letters A. 377, 643.

[23] **Gulacsi, M.**, 2004, The one-dimensional Kondo lattice model at partial band filling, Advances in physics 53, 769.

[24] **Hayes, D., Julienne, P. S., Deutsch, I. H.**, 2007, Quantum Logic via the Exchange Blockade in Ultracold Collisions, Phys. Rev. Lett. 98, 070501.

[25] **Daley, A. J. , Boyd, M. M., Ye, J., Zoller, P.**, 2008, Quantum Computing with Alkaline-Earth-Metal Atoms, Phys. Rev. Lett. 101, 170504.

[26] **Grimm, R., Weidemuller, M. Ovchinnikov, Y. B.**, 2000, Optical dipole traps for neutral atoms. Adv. At. Mol. Opt. Phys. 42, 95-170.

[27] **Millis, A. J., Littlewood, P. B., and Shraiman, B. I.**, 1995, Phys. Rev. Lett., 74, 5144.