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One-Electron Excitations vs. Collective Excitations in the 1D Falicov–Kimball Model with Hund Coupling at Half Filling

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The Falicov–Kimball model enriched with Ising-type Hund coupling between spins of itinerant electrons and magnetic ions is studied exactly on finite 1D rings. At half filling (one electron per site) and for the density of magnetic ions equal to 1/2 it is shown that many-electron collective excitations coupled to spin reorientations of the magnetic ions have much lower energy than single electron excitations. This property is caused by energy gaps formed at the Fermi levels in one-electron energy spectra of all relevant magnetic configurations of the ions. Consequently, low temperature properties of the system are not driven by one-particle, elementary electron excitations but many-particle collective excitations, where both electrons and spins of magnetic ions are involved. In addition, it is shown that many-body excitation spectra derived both from spin fluctuations and from charge fluctuations have a regular structure.

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1. Introduction

An inhomogeneous distribution of charge and/or magnetic moment observed in a number of correlated electron materials is intriguing, yet not fully understood phenomenon. One of the simplest model that describe the systems is the Falicov–Kimball model (FKM) supplemented with the Hund coupling between spins of itinerant and localized electrons [1–3].

The Hamiltonian of the model is

$$H = t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} d^{\dagger}_{i,\sigma} d_{j,\sigma} + U \sum_{i} n^{d}_{i} n^{f}_{i} - J \sum_{i} s^{z}_{i} S^{z}_{i} \,, \quad (1)$$

where $\langle i,j \rangle$ denotes the nearest neighbor lattice sites i and j, σ is a spin index, $d_{i,\sigma}$ ($d^{\dagger}_{i,\sigma}$) is an annihilation (creation) operator, n^{d}_{i} (n^{f}_{i}) is an occupation number of itinerant(localized) electron and s^{z}_{i} (S^{z}_{i}) stands for z-component of spin of itinerant (localized) electron. Any lattice site occupied (not occupied) by a localized electron corresponds to a magnetic (nonmagnetic) ion. The on-site interaction between an itinerant electron and a nonmagnetic ion is put to be equal to zero. On the other hand, the on-site interaction between an itinerant and localized electron is represented by two coupling constants: U, which is Coulomb-type and J, which reflects the Hund rule force. The hopping amplitude t is set equal to one, so we measure all energies in units of t. From here we refer to sites occupied (not occupied) by localized electrons as magnetic (nonmagnetic) ions and to itinerant electrons as electrons.

In our previous studies we established some basic rules of formation of charge and magnetic arrangement at zero temperature for various densities ρ_d and ρ_f of electrons and magnetic ions, respectively [1, 2]. To better understand the rules and to learn more about interactions between ions generated by their on-site coupling with electrons, here, for the first time we examine excited states in addition to the ground states. The investigations reveal existence of a regular structure of the excitations, from which a simple picture of forces, derived from the electrons that act on the ions, emerges.

In this contribution we focus merely on the 1D model at half filling (one electron per site, i.e. $\rho_d = 1$) for $\rho_f = 1/2$. In this particular case we found that in the ground state magnetic ions occupy every second lattice site (the checkerboard-type charge order) and spins of the nearest neighboring ions have opposite orientations (see Fig. 1).

Fig. 1. The ground state configuration of ions for $\rho_f = 1/2$ and $\rho_d = 1$. Magnetic ions are marked by arrows and nonmagnetic ones by black disks.

We discuss various sorts of excited states and their energy spectra in the next section.

2. Analysis of excitations

There are three different ways of perturbation of the ground state: single electron excitations, spin fluctuations or charge fluctuations.

For a given configuration of magnetic ions defined by their positions in the lattice (*charge distribution*) and their spin arrangement (*spin distribution*) the single electron energy levels are fixed. Then, the system can be excited by pushing up electrons from levels lying below the Fermi energy to above it (single electron excitations).

Here we determine the energy spectra by numerical diagonalization of the Hamiltonian (1) on finite 1D clusters, assuming the interaction parameters fulfill the following conditions: $5 \leq U \leq 10$ and $J = 0.2U$. It appears that for any charge and spin configuration of magnetic ions $\{w\}$ single electron energy levels are confined within two subbands separated by an energy gap at the Fermi level (this is in analogue to the universal Hubbard gap). The gaps depend on U, J and $\{w\}$, and within the assumed range of the coupling constants it increases nearly linearly with U (see Fig. 2).

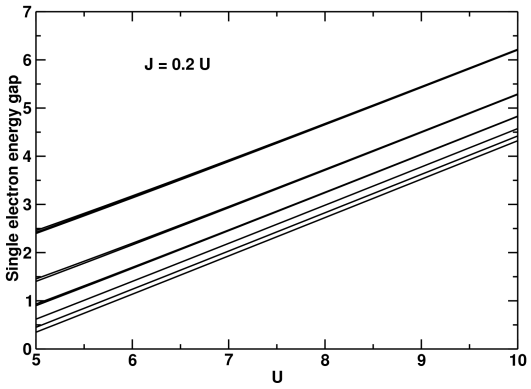

Fig. 2. Single electron energy gaps at the Fermi level of ferromagnetic phases with all possible charge distributions as a function of U.

In Fig. 2 we display values of the energy gaps as a function of U for all possible distributions of the ions (i.e. for all possible charge distributions) with spins of magnetic ions aligned ferromagnetically. The largest gap is found for the "checkerboard" phase and the smallest one for the segregated phase, where magnetic/nonmagnetic ions are clumped together.

Apart from single electron excitations, one can also excite the system by changing positions and/or spin orientations of magnetic ions. Then, the sequence of the ground state single electron energy levels is modified and the excitation energy is equal to a difference between the Fermi sea energy of the modified sequence and the sequence assigned to the ground state configuration, respectively. Since all electrons are involved in the process, these are many-body excitations. Indeed, any change (fluctuation) of spin or charge configuration of the ions results in a transformation of many-electron function.

Obviously, the many-electron excitations generated by changes of spin configurations (*magnetic excitations*) and those generated by changes of charge distributions (*charge excitations*), as well as single electron excitations, can be combined. However, energy scales associated with these distinct sorts of excitation are considerably different within the physically relevant range of the interaction parameter that we assumed here. The lowest energy is associated with many-body *magnetic excitations*. Much more is required for many-body *charge excitations*, but, if U is sufficiently large, the highest energy is related to single electron excitations. The noticed difference in the energy scales is consistent with findings reported in Ref. [4].

In our case of the 1D rings consisting of 16 sites occupied by 8 magnetic ions, there are 12870 possible charge arrangements, but due to symmetries only 436 of them are nonequivalent. For each charge configuration there are $2^8 = 256$ possible spin arrangements, but again, due to symmetries their number is substantially reduced. For the lowest in energy the charge checkerboard configuration there are merely 18 nonequivalent magnetic arrangements.

Fermi sea energies corresponding to these 18 magnetic arrangements form a sequence of 5 distinct groups, each of which is characterized by a fixed number of antiferromagnetic pairs of the nearest neighboring magnetic ions. Obviously, the number of different Fermi sea energies within each group is equal to the number of nonequivalent spin arrangements with a constant number of antiferromagnetic pairs. The lowest group consists of only one value, as the ground state configuration is a unique one with all the pairs antiferromagnetic (in our case there are 8 pairs). The second group contains nonequivalent phases with 6 antiferromagnetic pairs (2 pairs are ferromagnetic then), and in the groups corresponding to higher and higher energy the number of antiferromagnetic pairs decreases by 2 when passing from one group to the next in the sequence. The last group contains only one value equal to the Fermi sea energy of the ferromagnetic arrangement with no antiferromagnetic pairs.

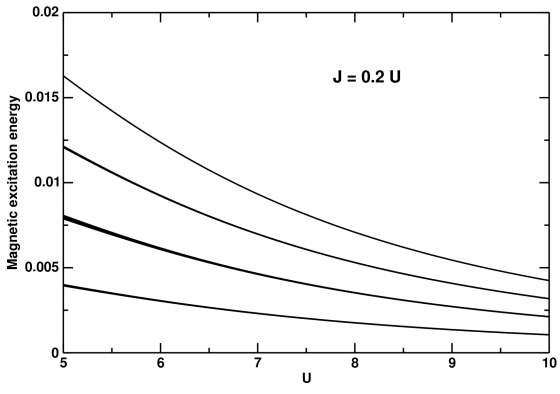

Fig. 3. Magnetic excitation energies as a function of U for the ground state "checkerboard" charge distribution. Starting from below, the consecutive groups of lines correspond to an increasing (by two) number of ferromagnetically aligned pairs of spins of the nearest neighboring magnetic ions. Energy of the ground state antiferromagnetic phase is represented by the horizontal axis, and energy of the ferromagnetic phase represents the uppermost line.

In Fig. 3 we display excitation energies of the whole electron system originating from changes of magnetic configurations as a function of U for the ground state checkerboard-type charge distribution. One can notice that differences between maximum and minimum energy within each of the group of the exited states, as well as differences between mean energies of the consecutive groups decrease with U. Within the considered range of the parameters the former are much smaller than the later.

The Fermi sea energies corresponding to nonequivalent 436 charge arrangements (distributions of magnetic ions) are also divided into distinct groups, but their number is equal to 8 in our case. Each of the group is now characterized by a fixed number of pairs with the nearest lattice sites occupied by ions of the same sort.

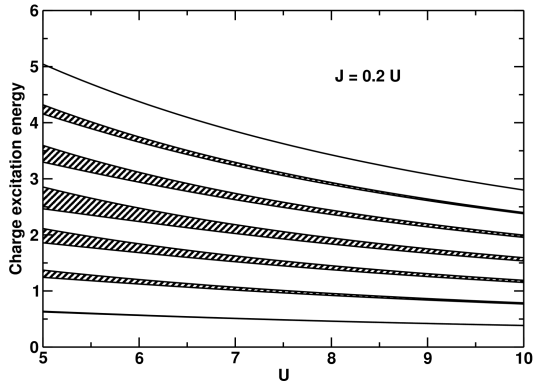

Fig. 4. Charge excitation energies of ferromagnetic phases as a function of U. Starting from below, the consecutive parts of the spectrum (the shaded regions) correspond to an increasing number (by two) of the nearest neighboring pairs of ions of the same sort. Each shaded region refers to phases with various distributions of a given number of the pairs. Energy of the checkerboard phase (without such a pair) is represented by the horizontal axis, and energy of the segregated phase represents the uppermost line.

In Fig. 4 we display excitation energies of the whole electron system originating from changes of charge configurations of the ferromagnetic phases as a function of U. Here again, differences between maximum and minimum energy within each of the group of excited states as well as differences between mean energies of the consecutive groups decrease with U. And the former are smaller than the later.

3. Conclusions

From our analysis of the FKM with Hund coupling for $\rho_f = 1/2$ and $\rho_d = 1$ it appears that the lowest temperature physics is governed merely by spin fluctuations of magnetic ions associated with modifications of many-electron Fermi sea functions. With an increase of temperature charge fluctuations related to displacements of the ions (also associated with modifications of the Fermi sea functions) come into play. Finally, when temperature is high enough, single electron excitations above energy gaps at the Fermi level start to contribute. Since all single electron energy gaps increase with U, whereas energies related to magnetic and charge fluctuations decrease with U, the role of single electron excitations becomes smaller and smaller at low temperature when U increases.

Perhaps the most striking feature of energy spectra of many-electron magnetic and charge excitations noticed during these studies is their structure. Both these spectra are composed of separated parts characterized by fixed numbers of the nearest neighboring pairs of either ferromagnetically arranged spins, in the case of magnetic excitations, or by ions of the same sort, in the case of charge excitations. The higher part of magnetic excitation spectrum, more ferromagnetic pairs of magnetic ions occur. Similarly, the higher part of charge excitation spectrum, more pairs of ions of the same sort occur.

What is more, with an increase of U mean distances between consecutive parts of the magnetic spectrum tend to the same value $\Delta_{\rm m}(U)$ whereas mean distances between consecutive parts of the charge spectrum tend to another value $\Delta_{\rm ch}(U)$. Then, if U is large enough, $\Delta_{\rm m}(U)$ measures an energy of a single spin flip and $\Delta_{\rm ch}(U)$ measures a repulsion energy of two ions of the same sort. Consequently, the resulting action of itinerant electrons produces the Ising-type interaction between localized spins and the repulsion between ions of the same sort. The conclusion related to the magnetic interactions is in agreement with the large U expansion results, where the FKM appears to tend to the Ising model [5].

Even though these preliminary studies are performed on finite 1D clusters only, we expect that the regularities will be found also in higher dimensions and in infinite systems. We plan to continue the research on the subject in our future work.

Acknowledgments

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References

[1] R. Lemański, *Phys. Rev. B* **71**, 035107 (2005).

[2] R. Lemański, J. Wrzodak, *Phys. Rev. B* **78**, 085118 (2008); R. Lemański, *Phys. Status Solidi B* **242**, 409 (2005); *Phys. Status Solidi B* **243**, 347 (2006); *J. Magn. Magn. Mater.* **310**, e327 (2007).

[3] P. Farkašovský, H. Čenčariková, *Eur. Phys. J. B* **47**, 517 (2005); M. Žonda, *Mod. Phys. Lett. B* **21**, 467 (2007); H. Čenčariková, P. Farkašovský, N. Tomašovičová, M. Žonda, *Phys. Status Solidi B* **245**, 2593 (2008).

[4] M. Maśka, K. Czajka, *Phys. Rev. B* **74**, 035109 (2006).

[5] M. Barma, V. Subrahmanyam, *Phase Transit. B* **16**, 303 (1989).