Journal of Physics: Conference Series **200** (2010) 012108 doi:10.1088/1742-6596/200/1/012108

Properties of the one-dimensional half-filled-band extended Hubbard model

F O Freire and C A Macedo[1]

Departamento de Fisica, Universidade Federal de Sergipe, 49100-000 Sao Cristovao, SE, Brazil

E-mail: cmacedo@.ufs.br

Abstract. With the aim of contributing to a better understanding of the finite-temperature properties of low-dimensional strongly correlated systems we study a one-dimensional half-filled-band extended Hubbard model with a term of exchange interaction between neighboring sites. We analyze the temperature dependence of the specific heat, internal energy, entropy, number of doubly occupied sites, magnetic susceptibility, spin-spin correlation functions, and also investigate a detailed diagram of magnetic correlations. We use the method of small-cluster exact diagonalization calculations with the application of the grand canonical ensemble and of extrapolation techniques to the infinite chain. Our results show that the examined model exhibits a rich structure of magnetic properties due to the competition between the onsite Coulombian repulsion and the exchange interaction.

1. Introduction

The Hubbard Model [1, 2] has been used to describe correlated fermions in a variety of circumstances, from high temperature superconductors to organic composites of heavy conducting fermions. In this work we use the extended Hubbard model [3-5], that is, we add a term of exchange interaction between neighboring sites to the model presented by Hubbard in his original paper.

Our Hamiltonian model is:

$$H = \sum_{<i,j>,\sigma} T_{ij} c_{i\sigma}^{+} c_{j\sigma} + \frac{U}{2} \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} - 4J \sum_{<i,j>} S_i^z S_j^z \tag{1}$$

where,

$$S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}).$$

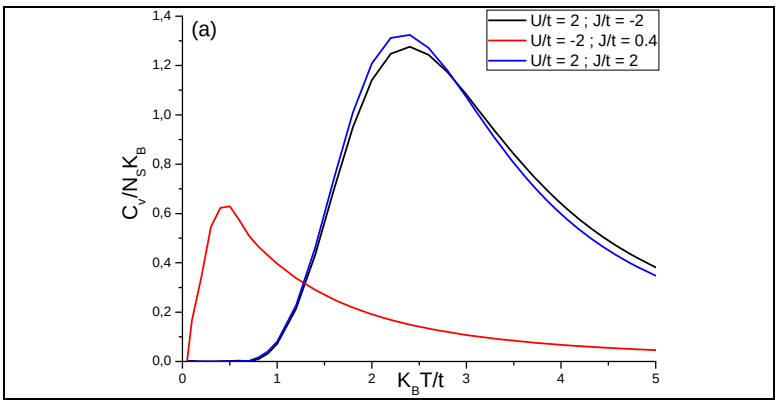
The Hamiltonian model (1) consists of three essential parts: the term that expresses the electron dynamics, characterized by the integral of electronic transference between neighboring sites, *t*; the onsite electron-electron repulsion, represented by energy *U* and the term of exchange interaction between magnetic moments of neighboring sites, characterized by the exchange term *J*.

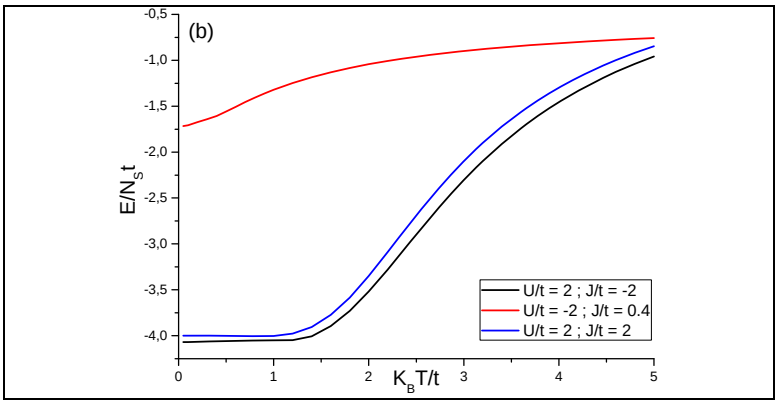
We choose the extended Hubbard model to better understand several phenomena that need to be further analyzed. A good example of this are ferromagnetic correlations which have yet to be better understood in the scope of the simple Hubbard model.

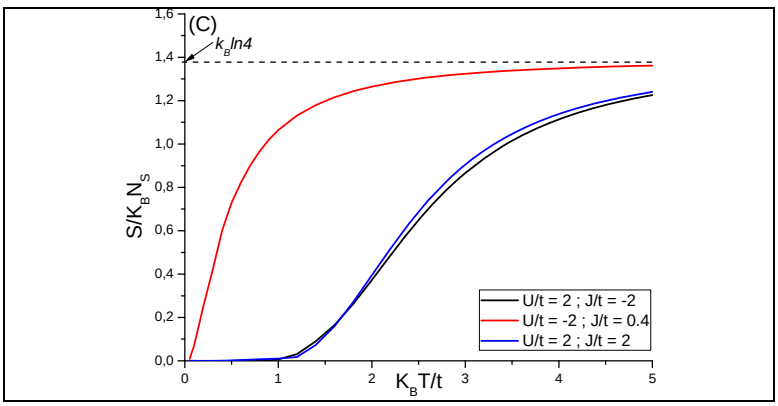
2. Thermodynamic Properties

In order to calculate the thermodynamic properties we use small-cluster exact-diagonalization calculations with the application of the grand canonical ensemble and of extrapolation techniques to the infinite chain as showed in references [6, 7]. Actually we have calculated all eigenvalues and eigenfunctions for chains with 2 to 6 sites.

We show in figure 1 the temperature dependence of the calculated specific heat, internal energy, entropy, number of doubly occupied sites, and magnetic susceptibility for typical values of (*U/t; J/t*) of the system in question. We also obtain a detailed diagram of magnetic correlations.







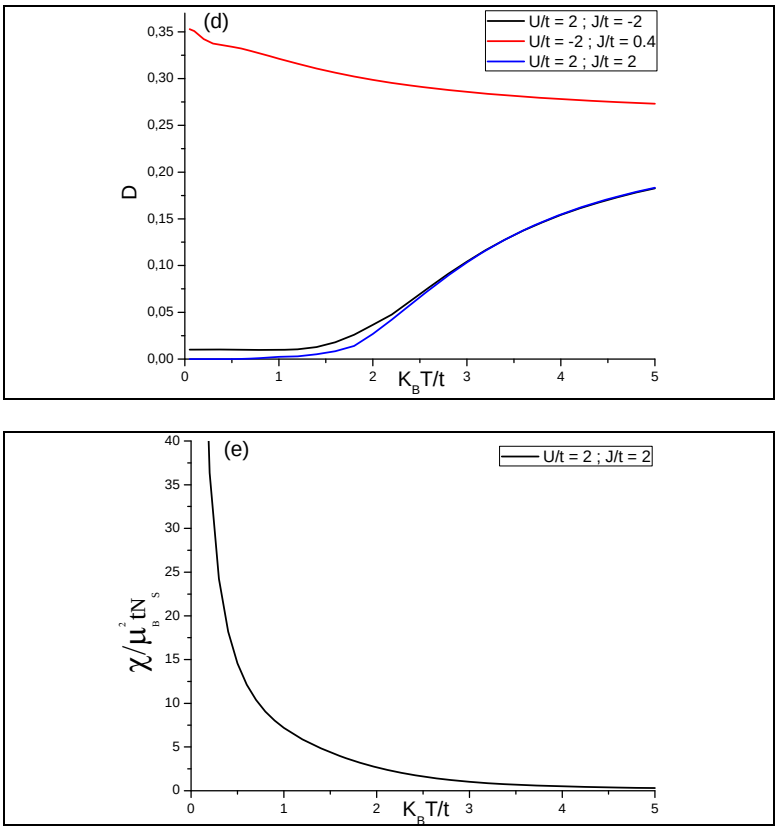


Figure 1. The thermodynamic properties of an infinite chain for typical values of *(U, J)*. (a) Specific heat; (b) Internal energy; (c) Entropy; (d) Number of doubly occupied sites; (e) Magnetic Susceptibility.

We observe that in the curves of figure 1(c), at high temperatures, the entropy of the system tends always to $k_B ln4$, due to the total number of eigenstates being 4^N. In figure 1(d) we see that the curves of positive U (blue and black) present null or almost null initial values, indicating that at low temperatures the system is quite located, that is, it has very little doubly occupied sites because the repulsive coulombian interaction, and the exchange interaction, impair *D*. In the red curve, *D* presents high initials values which occur because *U* is negative, thus favoring double occupation in the system. In figure 1(e) we note that the susceptibility presents a typical behavior of systems with ferromagnetic correlation.

Using the spin-spin correlation function L_δ as defined in [8] we analyze the thermal dependence of the functions L_1, L_2 and L_3 for different values of *(U, J)*. We delineate a complete diagram of magnetic correlations for one dimensional system by using the extrapolation technique, also obtaining the result for the infinite chain. We have the goal of investigating the magnetic nature of the studied systems, because these correlation functions can supply information on the short-range magnetic order at temperatures nearing ground state. Figure 2 shows the diagram of the magnetic correlations for $T = 0.0001t/k_B$.

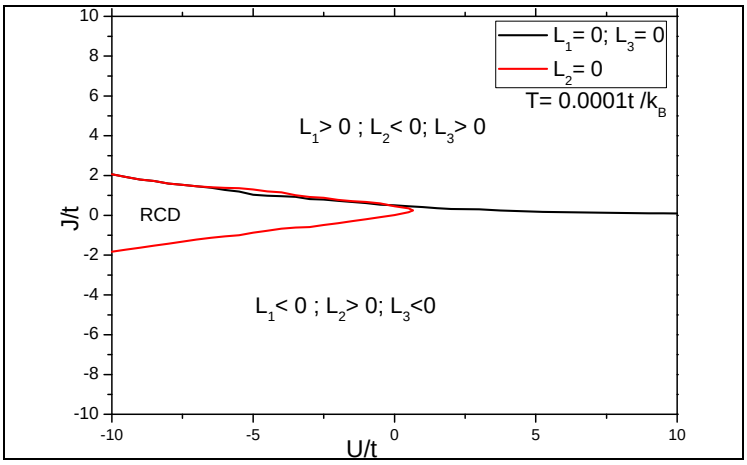


Figure 2. Diagram of short-range magnetic correlations for an infinite chain.

From figure 2 we determine three regions:

(a) $L_1 > 0$, $L_2 > 0$ and $L_3 > 0$, region of ferromagnetic correlations;
(b) $L_1 < 0$, $L_2 > 0$ and $L_3 < 0$, region of antiferromagnetic correlations;
(c) $L_1 < 0$, $L_2 < 0$ and $L_3 > 0$, but presenting very small values, that is, region of negligible correlations.

3. Conclusion

The results obtained for all cases are consistent and show the importance of considering the exchange interaction between neighboring sites in the study of ferromagnetic and antiferromagnetic systems for improving the understanding of the magnetic state of the system. Our results show that the examined extended Hubbard model exhibits a rich structure of magnetic properties due to the competition between the onsite Coulombian repulsion and the exchange interaction, including short-range ferromagnetic, antiferromagnetic, and insignificant spin-spin correlation regions.

References

[1] Hubbard J 1963 *Proc. R. Soc. London* A **276** 238
[2] Essler F H L, Frahm H, Göhmann F, Klümper A and Korepin V E 2005 *The One-dimensional Hubbard Model* (Cambridge: Cambridge University Press)
[3] El-Jaick L J, Toper A and Gomes A A 1980 *Phys. Stat. Sol.* (b) **99** 397
[4] Hirsch J E 1997 *Phys. Rev.* B **56** 11022
[5] Hirsch J E 2003 *Phys. Rev.* B **67** 035103
[6] Macedo C A, Azevedo L G and Souza A M C 2001 *Phys. Rev.* B **64** 184441
[7] Macedo C A and Souza A M C 2002 *Phys. Rev.* B **65** 153109
[8] Shiba H and Pincus P A 1972 *Phys. Rev.* B **5** 1966