

In this paper, we consider an isolated trimer (an triangular cluster [2]) that is located, for example, in a polymer matrix or in a colloidal solution and that is in equilibrium with its environment. Our goal is to investigate the electronic structure of a trimer and to establish the dependence of the chemical potential on the intersite Coulomb interaction and changes in hopping integrals for a variable number of particles [3].

We solve the above problems for three limiting cases in the Hubbard model [3]: the on-site Coulomb repulsion is less than ($U < W$), approximately equal to ($U \approx W$), and much greater than ($U \gg W$) the conduction band width.

The eigenvalue spectrum and the corresponding state vectors by exact diagonalization, based on which we determined the trimer magnetization $M = \sum_i^N (n_{i,\sigma} - n_{i,-\sigma})$ has been calculated [3]. At constant volume, the chemical potential is defined via the change in the system's energy, $\mu = -\Delta E/\Delta n$, when the number of particles changes from three to two.

During research for the trimer with the variable number of electrons the range of the intersite Coulomb interaction and an interval of the magnetic fields, changing energy level splitting near the chemical potential, by more than an order have been found. The removal of the magnetic degeneracy in the trimer under the influence of the intersite Coulomb interaction and the formation of a singlet pairs of electrons under trimer deformation have been established.

This work was supported by the Ministry of Education and Science of the Russian Federation as part of the "Development of the Scientific Potential of Higher School" Program (project nos. 2.1.1./401, 2.1.1/930) and the Russian Foundation for Basic Research (project nos. 09-02-00554-a, 09-02-92001-NNS-a, 10-02-00507, 10-02-00787, 11-02-90709-mob_tr).

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24PO-J2-3

THERMODYNAMIC AND SPECTROSCOPIC STUDY OF QUASI-ONE-DIMENSIONAL MIXED-SPIN SYSTEM $(Y_{1-x}Nd_x)_2BaNiO_5$

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The crystal structure (*Immm*) of the R_2BaNiO_5 (R =rare earth or Y) compounds contains spin-S=1 chains composed by flattened NiO_6 octahedra sharing their corners. The chains are interconnected through the R^{3+} and Ba^{2+} ions. While Y_2BaNiO_5 is a typical Haldane gap system [1], members of the family R_2BaNiO_5 containing magnetic R^{3+} ions order antiferromagnetically. The Neel temperature range from 12 K ($R=Tm$) to 61 K ($R=Dy$). In the series of compounds $(Y_{1-x}Nd_x)_2BaNiO_5$ T_N depends on x .

The magnetic properties of $(Y_{1-x}Nd_x)_2BaNiO_5$ ($x = 1, 0.25, 0.15, 0.05$) were studied by means of spectroscopic, magnetic susceptibility, and specific heat measurements in the temperature range

0.3–350 K. We have found three peculiarities in magnetic behavior of the compounds studied. First, the magnetic ordering is manifested by the λ -type anomaly in the temperature dependence of the specific heat $C(T)$ and by the splitting of Nd^{3+} Kramers doublets, $\Delta(T)$, in the optical spectra. The Neel temperature decreases with decreasing concentration of neodymium and, for $x=1$ and $x=0.25$, is in good agreement with the available neutron scattering data [2]. The observed $\Delta(T)$ also decreases with decreasing x , which results in a reduced magnetic moment of the neodymium subsystem..

Second, the Schottky anomaly is present below T_N in the temperature dependence of both specific heat and magnetic susceptibility $\chi(T)$. It is caused by a temperature-driven population of the upper component of the split ground Kramers doublet of Nd^{3+} . The value of the splitting $\Delta(T)$ found from the spectra was used to calculate contributions of the Nd subsystem into magnetic susceptibility and specific heat. To fit the experimental data, the Nd - Ni and Nd - Nd interactions had to be taken into account.

Third, an extra anomaly was observed in the $\chi(T)$ and $C(T)$ dependences at about 3 K in every compound. We tentatively assign this peculiarity to the presence of nickel-chain breaks. We give an estimate for the contribution from the triplet state originating from an extra spin of a chain segment split by internal and external magnetic fields.

We argue that the behavior of nickel subsystem differs from that of ordinary antiferromagnets. At high temperatures, while the contribution of the Nd subsystem into magnetic susceptibility follows the Curie-Weiss law, the Ni subsystem behaves like the Haldane-gap system, the contribution of which is independent of the concentration x (in contrast to the rare-earth subsystem).

Support of the RAS under the Programs for Basic Research is acknowledged.

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24PO-J2-4

MAGNETIC INTERACTIONS IN DELAFOSSITES

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The delafossite structure compounds provide good examples of antiferromagnets on a triangular lattice giving an evidence of the influence of geometrical frustration on these magnetic systems. These compounds are quasi two-dimensional and are highly frustrated between neighbouring triangular layers as well as within a layer. Delafossites demonstrate complex step-like magnetization curves at low temperatures in applied external magnetic field.

Among delafossites CuFeO_2 , which is a naturally occurring mineral, was historically the first known compound of this type [1]. Its natural structure is characterized by the space group $R\bar{3}m$ formed by two-dimensional triangular lattice layers stacked rhombohedrally along the c axis [2]. Another compound discussed AgFeO_2 has two polytypes of crystal structures, that is, $R\bar{3}m$ and $P6_3/mmc$ [3].

In present work we have done *ab initio* magnetic structure calculation of the hexagonal polytype $P6_3/mmc$ of AgFeO_2 and a similar hypothetical structure for CuFeO_2 to obtain magnetic interaction parameters. This trick makes it possible to simplify drastically the calculation of the magnetic