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The electron correlation effect on the magnetic properties of quasi-one dimensional-materials on the base of graphitic nanoclusters with embedded transition metals

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It is well known, the phase diagrams of the nanostructured magnetic materials demonstrate a variety of low-spin and high-spin states. The switch ability of these states is the central point to potential applications in molecular spintronics and high-density magnetic data storage. In this work, we studied the energy spectrum and thermodynamics of quantum Heisenberg spin model for graphitic nanoribbons with periodically embedded heteroatoms and model chain magnets formed by triangular graphitic clusters. The exact diagonalization study, density matrix renormalization group and Quantum Monte-Carlo method based on stochastic series expansion approach were used for this purpose. We found that clusters with frustrated interactions could exhibit spin switching when the corresponding coupling parameters are changed. For several carbon nanoribbons, we found macroscopic ground state spin and intermediate magnetization plateau. We also studied the exact thermodynamics of infinite distorted nanoribbons described by the special case of Heisenberg-Ising model. Special attention was given to the doped systems described by single-band Hubbard model with strong electron repulsion at partial electron filling. Here we used cyclic spin permutation formalism to derive the corresponding low-energy lattice Hamiltonians. We found numerically the possibility of the spin switching with the change of model parameters. We also demonstrated that the correlated hopping terms, which are present in our Hamiltonians, may change significantly the lowest energy spectra of the corresponding magnets in comparison with the similar description within the framework of the t-J model.

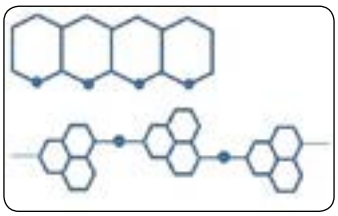

Figure 1: Graphitic clusters with embedded heteroatoms

Recent Publications

1. V O Cheranovskii, D J Klein, E V Ezerskaya and V V Tokarev (2018) Finite size effects in anisotropic U=∞ Hubbard ladder rings. Journal of Superconductivity and Novel Magnetism 31:1369-1373.
2. V O Cheranovskii, D J Klein, E V Ezerskaya and V V Tokarev (2017) Validity of t-J approximation for extended Hubbard model with strong repulsion. Low Temperature Physics 43:1622-1625
3. V O Cheranovskii, D J Klein, E V Ezerskaya, V V Tokarev (2017) Lowest energy states of Hubbard ladder model with infinite electron repulsion. Computational and Theoretical Chemistry 1116:112-116.
4. V O Cheranovskii, E V Ezerskaya, D J Klein and V V Tokarev (2017) Ground state spin of Hubbard model with infinite electron repulsion. Acta Physica Polonica Series a 131(4):916-918.
5. V O Cheranovskii and E V Ezerskaya (2015) Magnetic properties of the infinite U Hubbard model on one-dimensional frustrated lattices. Journal of Superconductivity and Novel Magnetism 28:773-776.

Biography

Vladyslav O Cheranovskii has completed his Doctor of Sciences in the year 1994 from Institute for Single Crystal. He is the Professor of V.N.Karazin Kharkiv National University, Department of Chemistry. He has published 49 papers recognized by Scopus and Web of Science databases. He is working in field of Solid State Physics and Quantum Chemistry. His main subject of interests includes strongly correlated electron system quantum theoretical simulation of electron structure and thermodynamics of nanomagnets.

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