Abstract

Role of the Orbital Ordering on Molecular Magnet $Mn_{12}Ac$

Liang-Jian ZOU

Condensed Matter Group
The Abdus Salam International Centre for Theoretical Physics
P. O. Box 586
Trieste 34100
Italy

zou@ictp.trieste.it

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Molecular magnets exhibit many novel nanostructure magnetic properties and potential application, while most of the present studies concentrate on the collective spin dynamics and quantum magnetic tunneling of molecular spin based on a phenomenal Heisenberg spin model, the spin is the only relevant freedom degree. This work focus on the microscopic origin of the spin interaction in molecular magnets $Mn_{12}Ac$, we find the orbital freedom degree plays roles in the $S = 10$ groundstate and the spin dynamics. Starting from the orbital-degenerate Hubbard model, we obtain the superexchange magnetic coupling matrix for different orbitals between Mn ions by the second-order perturbation approach, orbital-dependent couplings among Mn ions stablize the $S = 10$ configuration as realistic ground state and the groundstate energy gap by the exact diagonalization. Therefore the anisotropic spin interaction in $Mn_{12}Ac$ is attributed to the spatial-symmetry-broken orbital interaction, the orbital dynamics is thus involved in the spin dynamics.

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