1st INTERNATIONAL SYMPOSIUM DSCMBS-2014

"Dushanbe Symposium on Computational Materials and Biological Sciences"

Book of Abstracts

S.U. Umarov Physical-Technical Institute, Academy of Sciences of the Republic of Tajikistan

&

Joint Institute for Nuclear Research, Dubna, Russia

1st INTERNATIONAL SYMPOSIUM DSCMBS-2014

"Dushanbe Symposium on Computational Materials and Biological Sciences"

Dushanbe, September 23 – 28, 2014

Book of Abstracts

Edited by
Kholmirzo T. Kholmurodov
and Khikmat Kh. Muminov

Dushanbe – 2014

QUADRUPOLE EXCITATIONS IN SPIN TUNELLING IN MAGNETIC NANOMOLECULES

Khikmat Kh. Muminov, Yusef Yousefi

S.U. Umarov Physical-Technical Institute of the Academy of Sciences of the Republic of Tajikistan, 299/1 Aini Ave, Dushanbe 734063, Tajikistan

A single-molecule magnet (SMM) is a molecule that behaves as an individual nanomagnet. Because of their small size and precise characterizeability, molecular nanomagnets exhibit many fascinating quantum phenomena, such as macroscopic quantum tunneling of magnetization and Berry-phase interference. They straddle the quantum mechanical and classical worlds, residing in a middle ground that is of abiding interest to physicists. In addition, SMMs may find application in high-density magnetic storage or as qubits, the processing elements in quantum computers. The spin of an SMM ranges from a few to many times that of an electron; the corresponding magnetization of the individual magnets is minuscule. The molecules readily crystallize so that a typical sample contains 10^{15} or more identical magnetic clusters in (nearly) identical crystalline environments. At the same time, the SMMs are relatively far apart so that the magnetic exchange between them is small, and they interact only very weakly with each other. To a very good approximation, a crystalline sample thus behaves at low temperatures as an ensemble of well characterized, identical, noninteracting nanoscale magnets. Although the symmetry and the magnitude of spin anisotropy, as well as the hyperfine fields, dipolar interactions, and other properties, vary substantially from one SMM to another, most exhibit the same overall behavior.

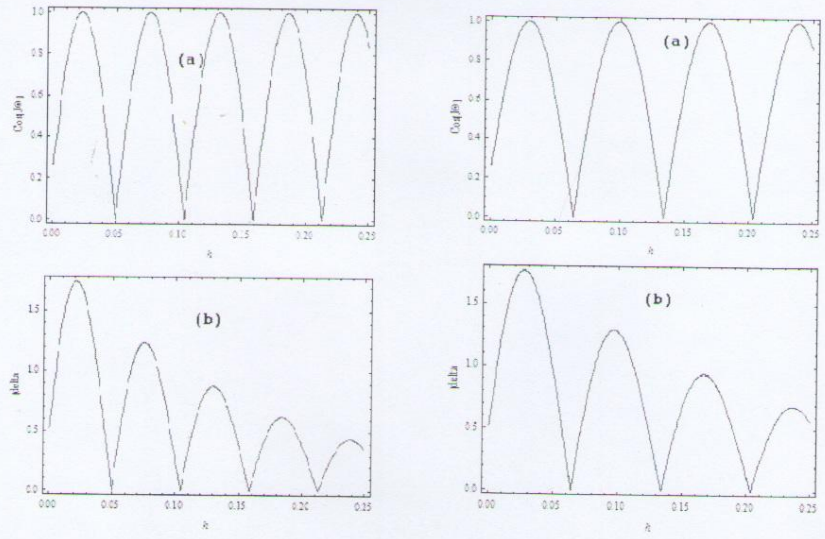
The molecule Fe_8 (proper chemical formula: $[Fe_8O_2(OH)_{12}(tacn)_6]^{8+}$) is magnetic, and forms good single crystals.

Spin-orbit and spin-spin interactions destroy complete rotational invariance, and give rise to anisotropy with respect to the crystal lattice directions. A variety of experimental techniques (electron spin resonance, ac susceptibility, magnetic relaxation, Mossbauer spectroscopy, neutron scattering) indicates [3-6] that their data can be very fit by the following model Hamiltonian

$$H = -k_1 J_z^2 + (k_1 - k_2) J_x^2 - k_4 (J_+^4 + J_-^4) - g\mu_B \vec{S}\vec{h}. \qquad (1)$$

The parameter g, k_1 and k_2 are known through variety experimental evidence [7]. with J = 10, $k_1 \approx 0.338$ K, and $k_2 \approx 0.246$ K. $k_4 \approx 2.9 \times 10{-}5$ K . The anisotropy energy is equivalent to a field of ≈ 2.5 T. The g factor is very close to 2.

Spin tunneling effects in nano-particle Fe_8 is studied by instanton calculation technique using the SU(3) generalized spin coherent states as a trial function. Energy level splitting is calculated by use of the spin coherent states path integrals and their dependence on the excitation of quadrupole dynamics is shown. In this case, it arises due to the presence of a Berry like phase in action, which gives rise to an interference between tunneling trajectories (instantons). It is established that the use of SU(3) generalized spin coherent states not only change the location of the quenching points, but also decreases the number of these points, which is in accordance.



a) b)

(a).Tunnel splitting oscillation cos(JΘ) versus h and (b). Tunnel splitting amplitude Δ versus h for Hamiltonian H_0 in SU(3) group

(b).Tunnel splitting oscillation cos(JΘ) versus h and (b). Tunnel splitting amplitude Δ versus h for Hamiltonian H in SU(3) group

Reference

1. B. Barbara and E. M. Chudnovsky, Phys. Lett. A 145, 205 (1990).
2. Advanced Research Workshop on quantum tunneling of magnetization- QTM, 94, Grenoble and Chichilianne, France, June27-July2, 1994.
3. A. Garg, Europhys. Lett. 22, 205 (1993).
4. K. Wieghardt, K. Pohl, Angew. Chem. Int. Ed. Engl. 23, 77 (1984).
5. C. Deifs et al., Inorg. Chem. 32, 3099 (1993).
6. A. L. Barra, P. Debrunner, D. Gatteschi and R. Sessoli, Europhys. Lett. 35,133 (1996).
7. C. Sangregorio, T. Ohm, C. Paulsen, R. Sessoli and D. Gatteschi, Phys. Rev. Lett. 78, 4645 (1997).