NUMERICAL SIMULATION OF MESOSCOPIC RINGS

G. Kamieniarz and R. Matysiak
Computational Physics Division, Institute od Physics
A. Mickiewicz University, ul. Umultowska 85,
61-614 Poznan, Poland

9.7 cm

Magnetic properties of large clusters of metal ions are investigated as they should change gradually from those typical of simple paramagnets to those observed for bulk magnets. In this communication we present the first application of the transfer-matrix method worked out in the framework of quantum statistical mechanics to characterize the susceptibility behaviour of the Mn_6 cluster ($[Mn(hfac)_2NITPh]_6$) with six alternating spins $S = 5/2$ and $S = 1/2$. We find the estimate of the coupling constant $J/k_B = 350 \pm 10[K]$. For Ni_{12} cluster ($[Ni_{12}(O_2CMe)_{12}(chp)_{12}(H_2O)_6(THF)_6]$) we have also developed a group-theoretical approach so that the matrix representation of the Hamiltonian can be reduced and exactly diagonalized on the supercomputing platforms.

13.4 cm

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Corresponding author :
G. Kamieniarz

Address for correspondence :
Computational Physics Division, Institute od Physics
A. Mickiewicz University, ul. Umultowska 85,
61-614 Poznan, Poland

Email address :
gjk@pearl.amu.edu.pl