Phenomenological modelling of molecular-based antiferromagnetic rings

P. Kozłowski\textsuperscript{a}, G. Kamieniarz\textsuperscript{a}, G. Musiał\textsuperscript{a}, W. Florek\textsuperscript{a}, M. Antkowiak\textsuperscript{a}, K. Jaśniewicz-Pacer\textsuperscript{a}, M. Haglauer\textsuperscript{a}, A. Caramico D'Auria\textsuperscript{b,c}, F. Esposito\textsuperscript{b}, D. Gatteschi\textsuperscript{d}

\textsuperscript{a}Faculty of Physics, A. Mickiewicz University, Poznań, Poland
\textsuperscript{b}Dipartimento di Scienze Fisiche, Universita di Napoli, Napoli, Italy
\textsuperscript{c}'Coherentia' CNR-INFM, Napoli, Italy
\textsuperscript{d}Dipartimento di Chimica, Universita di Firenze, Firenze, Italy

Two non-perturbative approaches: the direct exact diagonalization and quantum transfer matrix (QTM) techniques, applicable to Heisenberg spin systems modelling molecular rings, are described. The models include the single-ion anisotropy, alternating nearest-neighbour bilinear exchange coupling and the biquadratic term. Using these techniques and exploiting the Hamiltonian symmetry, we have performed calculations beyond the strong exchange limit for relatively large spin systems: (i) twelve spins $s = 1$ (Ni\textsubscript{12}) and (ii) eight spins $s = 3/2$ (Cr\textsubscript{8}). In both cases, the energy spectra in the presence of single-ion anisotropy, biquadratic exchange and magnetic field have been calculated using the direct exact diagonalization. The anisotropy-dependent splitting and spin-mixing as well as the field-dependent crossing of energy levels is presented and analysed. The efficiency and flexibility of QTM method is demonstrated for the spin $s = 3/2$ ring, including the exact magnetic torque calculations. The susceptibility and specific heat have been found to depend mainly on the mean value of the alternating couplings.

Subject category:
2. Quantum and Classical Spin Systems

Presentation mode:
oral

Corresponding author:
Piotr Kozłowski

Address for correspondence:
Faculty of Physics, A. Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

Email address:
kozl@amu.edu.pl