Rotational band structure of low-lying excitations in small Heisenberg systems

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A new class of magnetic compounds known as molecular magnets is attracting much attention. A very interesting species is the recently synthesised Keplerate structure \{Mo$_{72}$Fe$_{30}$\} [1], where embedded within a (diamagnetic) host molecule, 30 Fe$^{3+}$ paramagnetic ions (spins $s = 5/2$) occupy the sites of an icosidodecahedron and interact via isotropic, nearest-neighbour antiferromagnetic exchange. Investigations of the counterpart classical systems have shown that the classical ground state consists of three sublattices with relative angles of 120° between nearest-neighbour spins [2]. Employing this knowledge we propose to describe the low-temperature behaviour of \{Mo$_{72}$Fe$_{30}$\} by replacing the Heisenberg Hamiltonian by an approximate Hamiltonian [3]

$$H = -2J \sum_{u \neq v} \vec{S}(u) \cdot \vec{S}(v) \approx -\frac{J}{5} [\hat{S}^2 - (\hat{S}_A^2 + \hat{S}_B^2 + \hat{S}_C^2)] , \quad (1)$$

where $\vec{S}$ is the total spin operator and $\hat{S}_A$, $\hat{S}_B$, and $\hat{S}_C$ are the three sublattice spin operators. It has been noted for many spin arrays [4], especially bipartite systems, that such an approximation is very good at least for the lowest rotational band (minimal $E$ for each $\vec{S}$). We could show that the rotational band Hamiltonian accurately describes recent magnetisation measurements of \{Mo$_{72}$Fe$_{30}$\}, see figure and Ref. [3].

The present method, which is based on the approximate rotational band Hamiltonian (1), offers an insightful and quantitatively useful platform to describe the low-temperature behaviour of systems where the exact Heisenberg Hamiltonian cannot be diagonalized anymore.

I would like to thank M. Luban, R, Modler (Ames Lab), with whom this work was done, and K. Bärwinkel, H.-J. Schmidt, M. Exler, D. Mentrup (Osnabrück) and J. Richter (Magdeburg) for fruitful discussions.

References