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

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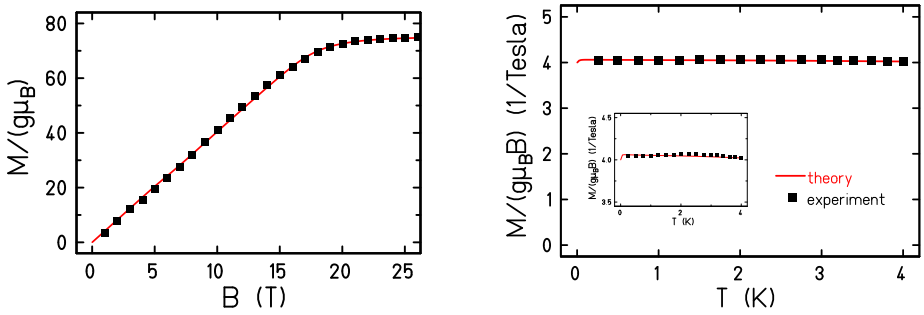
A new class of magnetic compounds known as molecular magnets is attracting much attention. A very intersting species is the recently synthesised Keplerate structure $\{Mo_{72}Fe_{30}\}$ [1], where embedded within a (diamagnetic) host molecule, 30 Fe^{3+} paramagnetic ions (spins $s = 5/2$) occupy the 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^o 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]

$$\underset{\sim}{H} \;=\; -2\,J \sum_{u\neq v} \underset{\sim}{\vec{s}}(u)\cdot\underset{\sim}{\vec{s}}(v) \approx -\frac{J}{5}\left[\underset{\sim}{\vec{S}}^2 - \left(\underset{\sim}{\vec{S}}_A^2 + \underset{\sim}{\vec{S}}_B^2 + \underset{\sim}{\vec{S}}_C^2\right)\right], \qquad (1)$$

where $\underset{\sim}{\vec{S}}$ is the total spin operator and $\underset{\sim}{\vec{S}}_A$, $\underset{\sim}{\vec{S}}_B$, and $\underset{\sim}{\vec{S}}_C$ 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 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.



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