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

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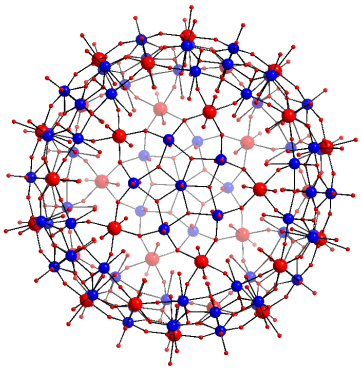
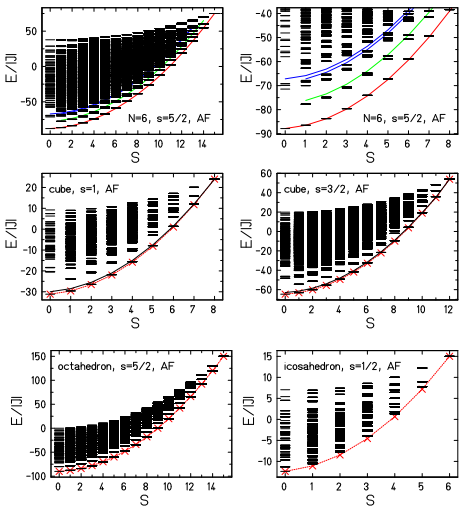


A new class of magnetic compounds known as molecular magnets is attracting much attention. These compounds can be synthesized as single crystals of identical molecular units, each containing several paramagnetic ions that mutually interact via Heisenberg exchange, $\hat{H} = -2\,J \sum_{(u<v)} \hat{\vec{s}}(u) \cdot \hat{\vec{s}}(v)$. A very interesting species is the recently synthesized Keplerate structure $\{Mo_{72}Fe_{30}\}$, 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.

Employing the sublattice structure we propose to describe the low-temperature behaviour of $\{Mo_{72}Fe_{30}\}$ by an approximate Hamiltonian

$$\hat{H} \approx -\frac{D\,J}{N}\left[\hat{\vec{S}}^2 - \left(\hat{\vec{S}}_A^2 + \hat{\vec{S}}_B^2 + \hat{\vec{S}}_C^2\right)\right] ,$$

where $\hat{\vec{S}}$ is the total spin operator and $\hat{\vec{S}}_A$, $\hat{\vec{S}}_B$, and $\hat{\vec{S}}_C$ are the three sublattice spin operators. It has been noted for many spin arrays, especially bipartite systems, that such an approximation is very good at least for the lowest rotational band (minimal E for each S) – a behaviour known as Landé interval rule.



The rotational band Hamiltonian accurately describes recent magnetisation measurements of $\{Mo_{72}Fe_{30}\}$. In addition we can predict the magnetic field values where resonances of the spin-lattice relaxation rate at low temperatures should occur; (*J. Schnack, M. Luban, and R. Modler, Europhys. Lett. (2001), submitted*).
The present method, which is based on the approximate rotational band Hamiltonian, offers an insightful and quantitatively useful platform to describe the low-temperature behaviour of systems where the exact Heisenberg Hamiltonian cannot be diagonalized anymore. Further research will concentrate on frustration effects in this system.