Roman Schnalle: Short visit Ref. No. 1073

"spin wave theory of highly symmetric molecules"

Purpose of the visit

Magnetic molecules are of great interest because of the possibility of an experimental study of low-dimensional quantum magnetism as well as of the much simpler description by theory. To describe thermodynamic properties of huge molecules one has to think about theoretical methods which are able to give reliable information about these systems, especially frustrated ones.
The purpose of the visit was to investigate in general whether spin wave theory is applicable for highly symmetric molecules. Since generalized spin wave theory does not belong to the methods used in Osnabrück so far, the major aim of the visit was to become more familiar with this technique.

Description of the work carried out during the visit

The application of finite-size spin wave theory (compare Takahashi, Phys. Rev. B 40, 2494 (1989) to frustrated magnetic molecules was discussed in order to understand technical as well as physical details of calculating thermodynamical properties.

Description of the main results obtained

The low-temperature thermodynamic properties of a possible magnetic molecule consisting of 12 spins of quantum number ½ occupying the sites of a cuboctahedron were calculated.

Future collaboration with host institute

The collaboration with Timothy Ziman and Olivier Cepas in Grenoble will be continued. It is planned to compare results from calculations of different magnetic systems and to do further calculations of more complex systems.

Projected publications/articles resulting or to result from the grant

The results are used within a diploma thesis at the University of Osnabrueck. The possibilities and restrictions of calculating thermodynamic properties by using spin wave theory will be investigated by comparing spin-wave results and results from exact numerical diagonalization. The use within other publications is also proposed.

Other comments (if any)

I would like to thank the ESF for founding the visit and Timothy Ziman as well as Olivier Cepas for fruitful discussions.