Theoretical investigation of advanced magnetocaloric materials

Contact: Mike ZHITOMIRSKI DRF//INAC/PHELIQS/GT mike.zhitomirsky@cea.fr 04 38 78 43 30

PhD may follow: Yes

Summary :

An external magnetic field affects the entropy of a magnetic system and provokes temperature variations which can be used for magnetic refrigeration. Such an alternative cooling technology is increasingly important nowadays for space telescopes, particle physics experiments and quantum computing. The existing adiabatic demagnetization refrigerators utilize paramagnetic salts, which have limited capacity for temperatures above 1 K. Recently, two new families of magnetocaloric materials suitable for applications in the 1-4 K temperature range have been proposed: geometrically frustrated spin systems and dipolar magnets. We plan to study the magnetocaloric properties of such materials using large scale Monte Carlo simulations of realistic spin models appropriate for the known, Gd3Ga5O12 and GdLiF4, as well as for the prospective, Yb2Ti2O7 and Yb3Ga5O12, magnetocaloric materials. The theoretical study will benefit from a collaboration with the on-going experimental work at INAC.

Full description :

Computer simulations play an increasingly important role in the way scientists acquire knowledge about Nature. The Monte Carlo methods developed in the past 50 years have revolutionized the field of Statistical Mechanics. Initially used to study ideal simple models, the modern Monte Carlo techniques can be applied to real physical systems. This project is focused on the theoretical investigation of the magnetocaloric properties for a number of magnetic materials. Apart from the fundamental interest, this investigation has an important applied component related to the field of low-temperature magnetic refrigeration.

Actual performance of the adiabatic demagnetization refrigerators is determined by the ordering temperature of a refrigerant material. Therefore, the magnetocaloric properties can be improved by using magnetic materials with so called frustrated lattices, whose geometry precludes a simple magnetic ordering. In the past, we have developed the very efficient hybrid Monte Carlo algorithm and used them to study various properties of geometrically frustrated magnets. The initial task to be carried by student on this project is to develop a computer code for lattices with partial filling of magnetic sites. Such magnetic materials can be prepared by chemical substitution of nonmagnetic impurities. The modified code will be used to investigate the effect of nonmagnetic dilution with the aim to optimize the magnetocaloric properties of real materials. A complementary fundamental study will be devoted to the order from disorder effect in dilute frustrated magnets, which consists in selection of exotic types of magnetic order in degenerate frustrated magnets solely by the structural disorder.

Another class of magnetic solids with suppressed ordering transition includes materials with strongly reduced exchange interactions like in GdLiF4. Still, the dipole-dipole interactions between magnetic ions are always present and affect the material properties. Such materials have a great technological potential for magnetic refrigeration. To uncover this potential one needs to understand their basic physical properties. The student's task will include the analytic computations of the possible magnetic ground states of a dipolar magnet in zero and applied magnetic fields focusing on GdLiF4. In addition, the Monte Carlo codes have to be modified to take account of the long-range nature of the dipole interactions. Those will be used for theoretical investigation of the phase transitions and phase diagrams in two- and three-dimensional of dipolar magnets.

Requested skills :

Basic knowledge of programming and solid state physics