ESpinS: A program for classical Monte-Carlo simulations of spin systems

Abstract

In this talk, we introduce the ESpinS code, which is for investigating the thermodynamic properties of spin systems. We first explain the Hamiltonian spin and the Monte Carlo method and then explain the replica-exchange method. In the following, we will go into the details of the code, and at the end, several examples will be given to show the abilities of the code in the simulation of spin systems. In addition to Heisenberg interactions, other interactions such as Dzyaloshinskii–Moriya are implemented in the ESpinS code. The code can calculate many properties such as energy histogram, neutron scattering structure, etc. Also, in this code, the magnetic order parameters can be defined according to each system. The code works with both the local update and replica-exchange algorithms. The central part of this code is written in Fortran 90 language and can be run in serial and parallel. Creating the input file is very simple, and the user does not need to define the complexity of a spin Hamilton.

This code is available as open-source on the Github site (https://github.com/nafiserb/ESpinS), containing several examples and the manual.