Calculating critical temperatures for ferromagnetic order in two-dimensional materials

Magnetic order in two-dimensional (2D) materials is intimately coupled to magnetic anisotropy (MA) since the Mermin-Wagner theorem implies that rotational symmetry cannot be spontaneously broken at finite temperatures in 2D. Large MA thus comprises a key ingredient in the search for magnetic 2D materials that retain the magnetic order above room temperature. Magnetic interactions are typically modeled in terms of Heisenberg models and the temperature dependence on magnetic properties can be obtained with the random phase approximation (RPA), which treats magnon interactions at the mean-field level. In the present work we show that large MA gives rise to strong magnon-magnon interactions that lead to a drastic failure of the RPA. We then demonstrate that classical Monte Carlo (MC) simulations correctly describe the critical temperatures in the large MA limit and agree with RPA when the MA becomes small. A fit of the MC results leads to a simple expression for the critical temperatures as a function of MA and exchange coupling constants, which significantly simplifies the theoretical search for new 2D magnetic materials with high critical temperatures. The expression is tested on a monolayer of CrI3, which were recently observed to exhibit ferromagnetic order below 45 K and we find excellent agreement with the experimental value.