Homework 10, Statistical Mechanics: Concepts and applications
2016/17 ICFP Master (first year)

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In lecture 10 (Kosterlitz-Thouless physics 1/2: The XY (planar rotor) model), we studied in detail the basic topological excitations in this model, namely the vortices. These excitations exist next to the spin waves which are responsible for the destruction of long-range order, as we saw, in the lecture 10, in Wegner's solution of the harmonic model. Vortices and anti-vortices also provides the theme for the present homework session. For simplicity, we will restrict ourselves to zero temperature.

I. SIZE-DEPENDENCE OF THE VORTEX ENERGY

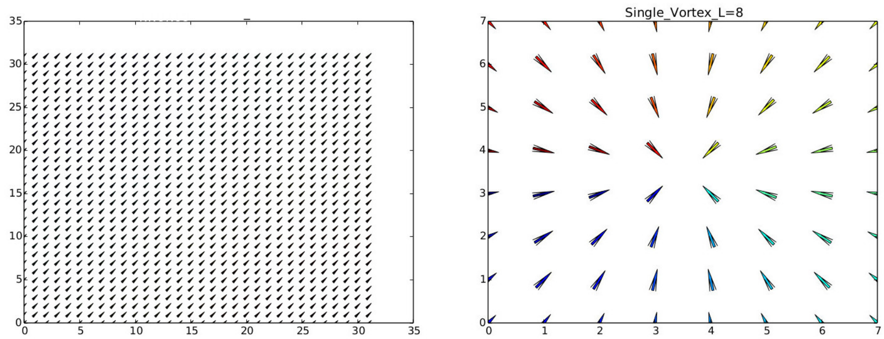

FIG. 1: No vortex (left) and single vortex (right) at zero temperature, in the 32×32 and 8×8 XY models with open boundary conditions, respectively.

A. Zero-vortex configuration

"Write" a computer program which generates a vortex-free configuration in an $L \times L$ lattice with open boundary conditions, relax the system to the groundstate, and take this energy to be zero (instead of writing the program yourself, simply generate such a configuration from the program `vortex_pair.py` made available on the website by putting both the vortex and anti-vortex to infinity). Make sure you understand how this program works.

B. Single-vortex configuration

Trivially modify the program `vortex_pair.py` to place a single vortex at the center of an $L \times L$ lattice, and compute the local minimum of the energy. To do so, you may for example put the vortex at the center, and the antivortex very far outside the lattice (for the initial configuration). Describe the configuration you observe and explain why it is stable with respect to local fluctuations.

1. Vortex and core energy

The theory of Kosterlitz and Thouless assumes that the excitation energy of a single vortex can be described by the formula

$$E_{\text{vortex}} = \pi J_R \log L + E_c \tag{1}$$

(where we suppose a lattice spacing of 1). From your converged data for different values of L, extract the value of the renormalized stiffness J_R and of the core energy. Can you confirm that the core energy does not scale with the system size? By analyzing the configurations you obtain, answer the following questions: Why is the energy of the vortex approximately a logarithm, in the first place, and why is there a constant core-energy correction to the logarithm?

II. DISTANCE-DEPENDENCE OF THE VORTEX-ANTIVORTEX PAIR ENERGY

One of the key aspects of the Kosterlitz-Thouless theory is the interaction between a vortex and an antivortex, which is given by the famous formula:

$$U_{ij}(r_{ij}) = -\pi J_R q_i q_j \log r_{ij} + 2E_c, \tag{2}$$

where q_i and q_j are the charges of the vortex and the anti-vortex, respectively. Use the program `vortex_pair.py` for a single system size, as for example $L = 128$ to compute the pair excitation energy as a function of the distance (in lattice sites) of the vortex-antivortex pair. Can you confirm that the pair energy is logarithmic in the pair separation?
NB: At the boundary of the system, the spins are not constant. This makes it impossible to compute the core energy. Don't worry about E_c.