# Homework 10, Statistical Mechanics: Concepts and applications
## 2019/20 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

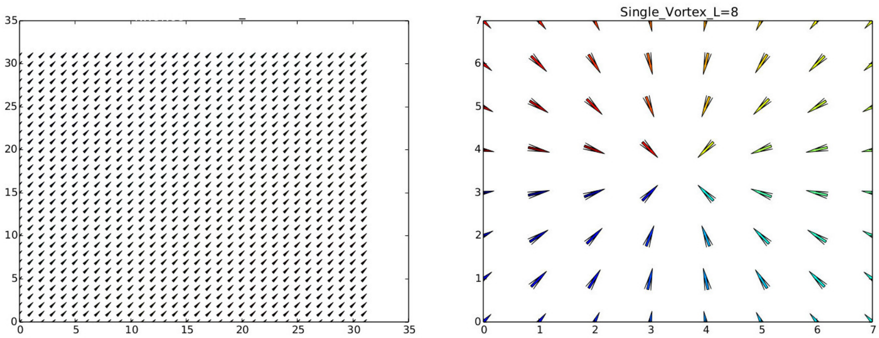


FIG. 1: No vortex (left) and single vortex (right) at zero temperature, in the $32 \times 32$ and $8 \times 8$ $XY$ models with open boundary conditions, respectively.

### 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 ground state, 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.

*The zero-vortex configuration is shown in Fig. 2. All of the spins point to an identical direction.*

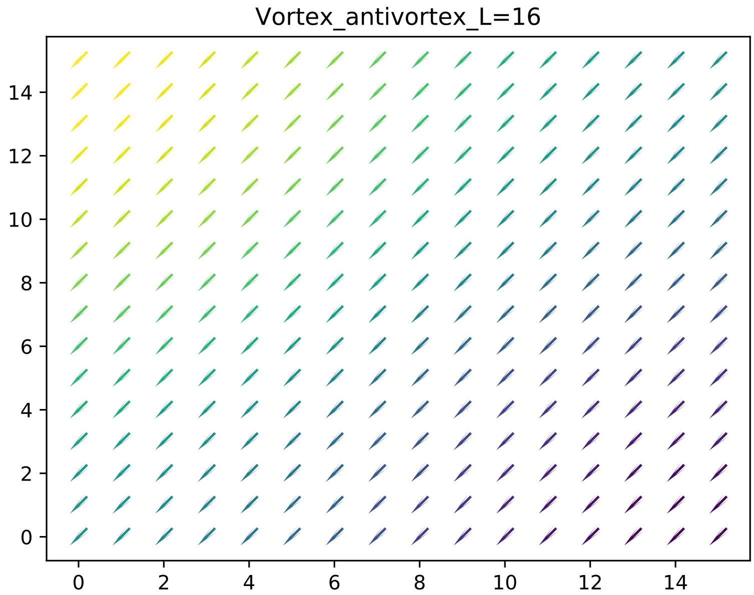


FIG. 2: Zero-vortex configuration when $L = 16$.

### 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.

*With* `vortex_pair.py`*, it is possible to plot the configuration with a(n) single (anti)vortex. The configurations may be found in Fig. 3 and Fig. 4. These configuration satisfies*

$$\oint_i \phi(i) - \phi(i-1) = \pm 2\pi \tag{1}$$

*where $\oint_i$ means all the sites on a closed loop enclosing the centre of the (anti)vortex. These sites are labelled by $i$, and neighboring sites have neighbouring indices. On the lattice, almost every spin aligns with its neighbors. If introducing a local fluctuation, i.e. change the direction of a single spin, the perturbed spin will finally point into the direction its neighbours point to. Thus, with the presence of an (anti)vortex, the local fluctuations will finally disappear.*

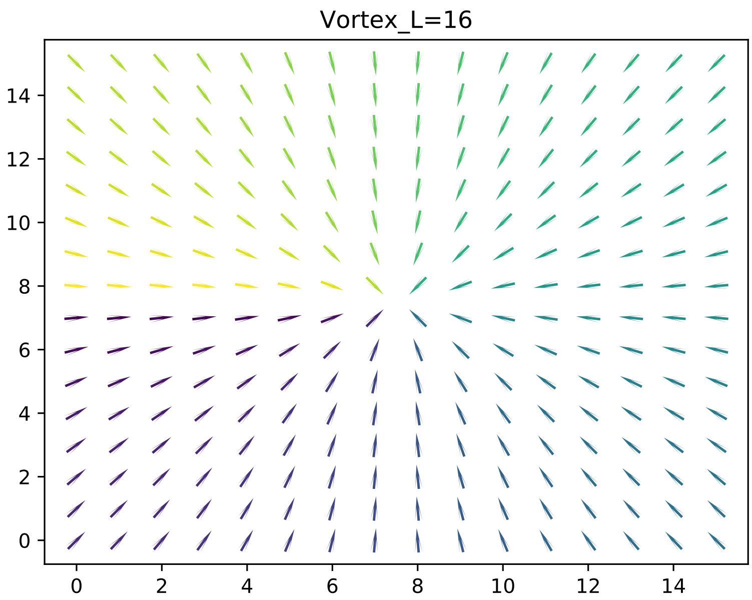


FIG. 3: A vortex in an $L = 16$ system.

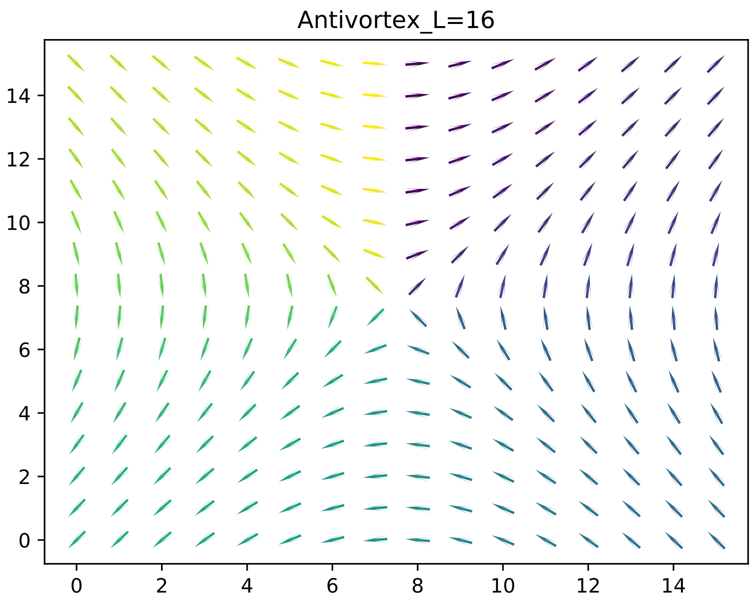


FIG. 4: An antivortex in an $L = 16$ system.

### 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

$$E_{\text{vortex}} = \pi J_R \log L + E_c \tag{2}$$

(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?

*The dependence of the energy of (anti)vortex on the system size is shown in Fig. 5. In the semi-log*

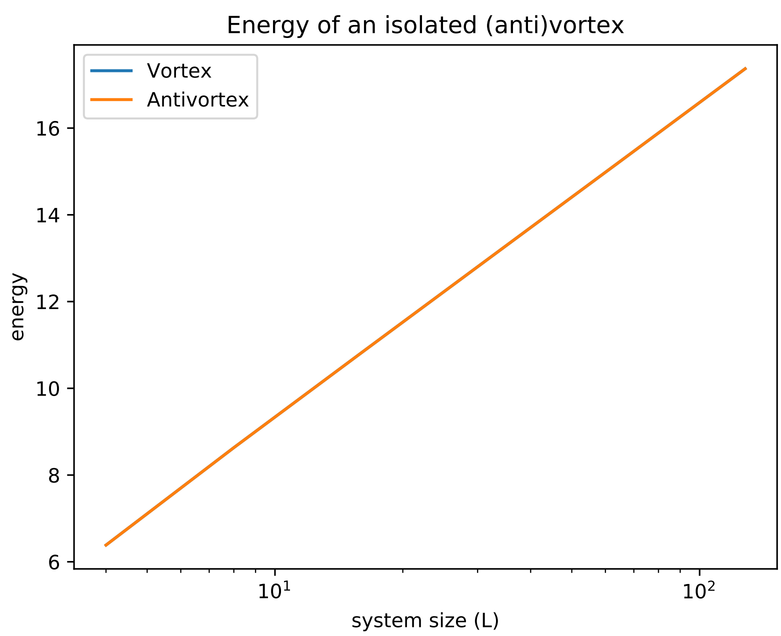


FIG. 5: Total energy of the system when (anti)vortex is presented. The curves overlap with each other. The numerical result supports the result given by analytic argument.

*plot, the plotted relation is almost strictly linear. This means that the energy scales as* $\log(L)$*. Fitting shows that the intersection in the semi-log plot is roughly* $2$*, which means that a part of the energy does not scale with the size of the system.*

*The energy of the vortex could be estimated in the following way. If a site is far from the center of the vortex, the interaction between this site and its neighbors is of the order of*

$\cos(\Delta\phi) \sim (\Delta\phi)^2$. *With eq. (1) and the symmetry of the system,* $\Delta\phi \sim 1/r$, *where* $r$ *is the distance between the site and the centre of the vortex. Thus, the total energy*

$$E_{vortex} \sim \int_0^L (1/r)^2 2\pi r dr \sim \log(L)$$

*However, when* $r \sim 1$ *(Recall the distance between two neighbouring sites is set to 1. This is also the cut-off scale of this model), the approximations break down. At the centre of a vortex, the configuration would always be roughly the same, regardless of the size of the system or the spins far from the centre. Thus, the contribution of these sites should be irrelevant to the size of the system. And it is the constant core energy of the vortex.*

## 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:

$$U_{ij}(r_{ij}) = -\pi J_R q_i q_j \log r_{ij} + 2E_c, \tag{3}$$

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 $E_c$.

*The energy of vortex on the system size is shown in Fig. 6. In the semi-log plot, the curve shows a flawed linear relation. The divergence between numerical analytic result has mainly two origins. Firstly, when the vortex and anti-vortex almost overlap, their contributions will cancel each other and the total energy will be close to 0. Thus, at small distances, the energy of a vortex-antivortex pair grows rapidly. Besides, when the distance is too large, some sites, which contributes to the total energy, will not be taken into account, since the size of the system is fixed. Thus, at large distances, eq. (3) is also not expected to work in the current problem. In practice, confirming eq. (3) is more difficult than confirming eq. (2).*

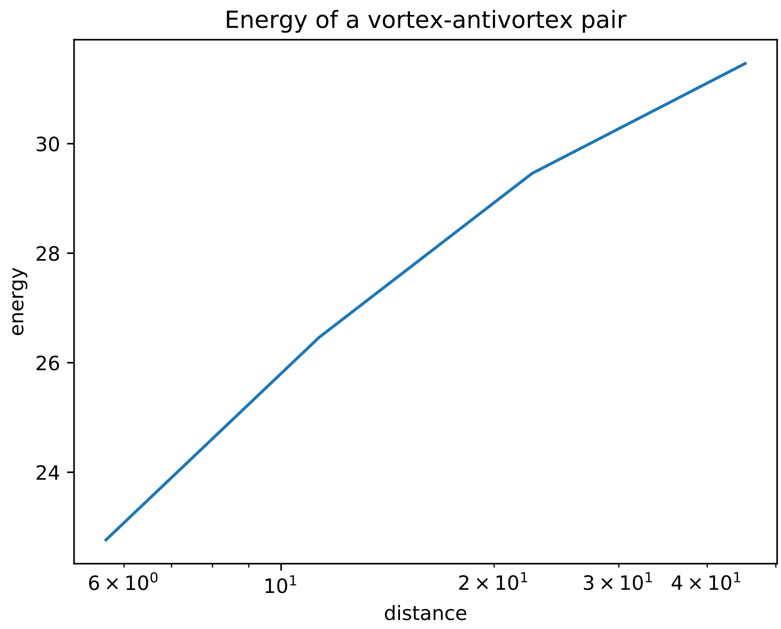


FIG. 6: Total energy of the system when a vortex-antivortex pair is presented in the system ($L = 128$). For distances shown in the plot, eq. (3) is roughly true.