Kosterlitz Thouless Phase Transition

Exam Project for the course in Computational Physics

Antonio Santaniello

1 Decription of the phenomenon

The Kosterlitz-Thouless phase transition is a phase transition associated with the formation of topological defects, which are configurations of the field with non-trivial topology, constituting excited states of the system. It can be observed that for d (spatial dimensions) ≤ 2, there are no phase transitions associated with the breaking of continuous symmetry (this is known as the Mermin-Wagner theorem). In this case, it would be the spontaneous breaking of $U(1)$ symmetry due to the magnetization of the system. However, the system still exhibits a phase transition due to the formation of spin vortices. The latter is energetically disfavored but entropically favored. At low temperatures, the first contribution dominates, while at high temperatures, the second contribution and the proliferation of vortex creation lead to disorder in the system.
The energy of the system is given by:

$$E = -J \sum_{<ij>} (S_i^x S_j^x + S_i^y S_j^y).$$

Here, $\vec{S}_i$ represents the vector associated with the i-th spin. By substituting $S_i^x = \cos(\theta_i)$ and $S_i^y = \sin(\theta_i)$, the expression can be rewritten in terms of an angular variable:

$$E = -J \sum_{<ij>} cos(\theta_i - \theta_j).$$

In the limit as $a \to 0$, it becomes a field theory described by the map $\theta : [0, L]^2 \to S^1$ (J. Cardy, Scaling and Renormalization in Statistical Physics):

$$E \approx E_0 + K \int dxdy(\nabla\theta)^2.$$

The energy minimum is degenerate and is obtained for a configuration $\theta = const. \in [0, 2\pi]$. However, assuming that the theta field can have singularities (defects), new stationary configurations are obtained in this case, which are called vortices.
Here, we conventionally set $k_B = J = 1$.

2 Code Description

The code is written in Fortran and is based on the one used for the Ising model. It consists of a module and a program.

2.1 Module

The module consists of a function and 6 subroutines:

- The function "Delta E" calculates the energy difference between two system configurations and is used to calculate the probability of transitioning from one state to another (in the "metropolis" subroutine).
- The "initial" subroutine initializes the system, defining the values of the matrix "s" of size $L \times L$ (where L is declared as a parameter). The values are real numbers between 0 and 2π, corresponding to the angles associated with the spins at each site. Initialization can be done by choosing random values with a uniform distribution or by setting all entries to 0, and the choice is made using the character variable "in mode." Additionally, initial values for

energy and magnetization (a two-dimensional vector) are calculated. The subroutine takes an integer variable "N" as input, indicating the size of the $N \times N$ submatrix of "s" that is actually manipulated, allowing us to simulate smaller lattices.

- The "prob" subroutine defines the canonical weight and should be called whenever you want to change the system's temperature.
- The "metropolis" subroutine implements the Metropolis algorithm. During spin updates, the values of the angles are set between 0 and 2π. This is unnecessary for the calculation of physical quantities but simplifies the conditions for searching for vortices (in the "vortex" subroutine) since we don't have to consider all multiples of 2π. This subroutine also contains the dependence on "N" for the same reason as before.
- The "config" subroutine saves the spin configurations on a square lattice of size "N." The third and fourth variables in the file are used to define the spin vectors, which can be plotted using "gnuplot" with the "with vectors" command.
- The "vortex" subroutine calculates the number of vortices, which is done by summing the differences in angles along a clockwise 1x1 square.
- The "accum" subroutine (to be called after equilibration) accumulates variables to be averaged over time.

2.2 Program

The program itself consists of 4 main blocks that can be accessed via a character variable. These blocks are designed to perform specific tasks related to the problem requirements:

- "quench" implements temperature quench with a "do" loop that modifies the temperature. Exponential and linear cooling have been tested with no significant differences.
- "temp" calculates the required quantities within the specified interval.
- "fit" creates the necessary files for fitting magnetic susceptibility.
- "theta" calculates the variance of the angle with respect to the instantaneous magnetization.

If none of these blocks are entered using the respective character variable, the code performs a simple run of the algorithm at a fixed temperature and writes quantities of interest to a file.

3 Answers for the Task

(b)

For this part, lattices of varying side lengths from 4 to 32 with a step size of 4 were used. The Metropolis algorithm was employed with 1000 equilibration steps and 5000 data collection steps. To achieve an acceptance probability of around 40%, it is necessary to use a maximum angle (tmax) equal to $\theta_{max} = 0.6$ radians.

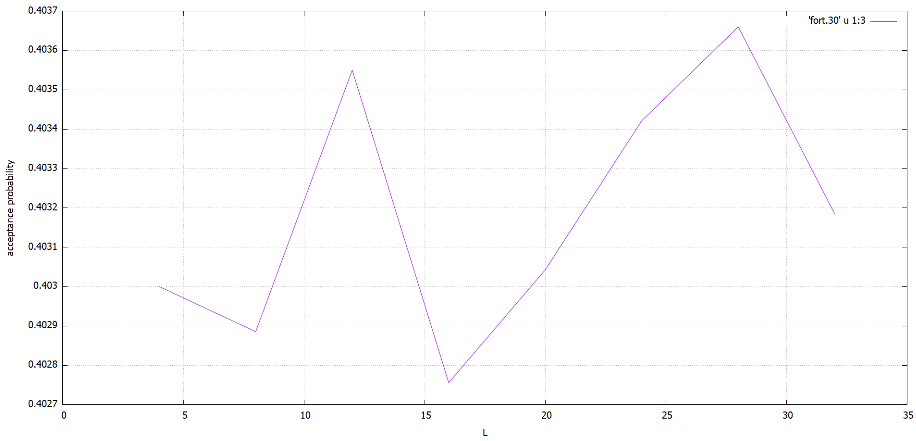

Figure 1: Acceptance probability as a function of N

From the graphs, it can be observed that there is a logarithmic divergence of the angular variance of magnetization with respect to the lattice size.

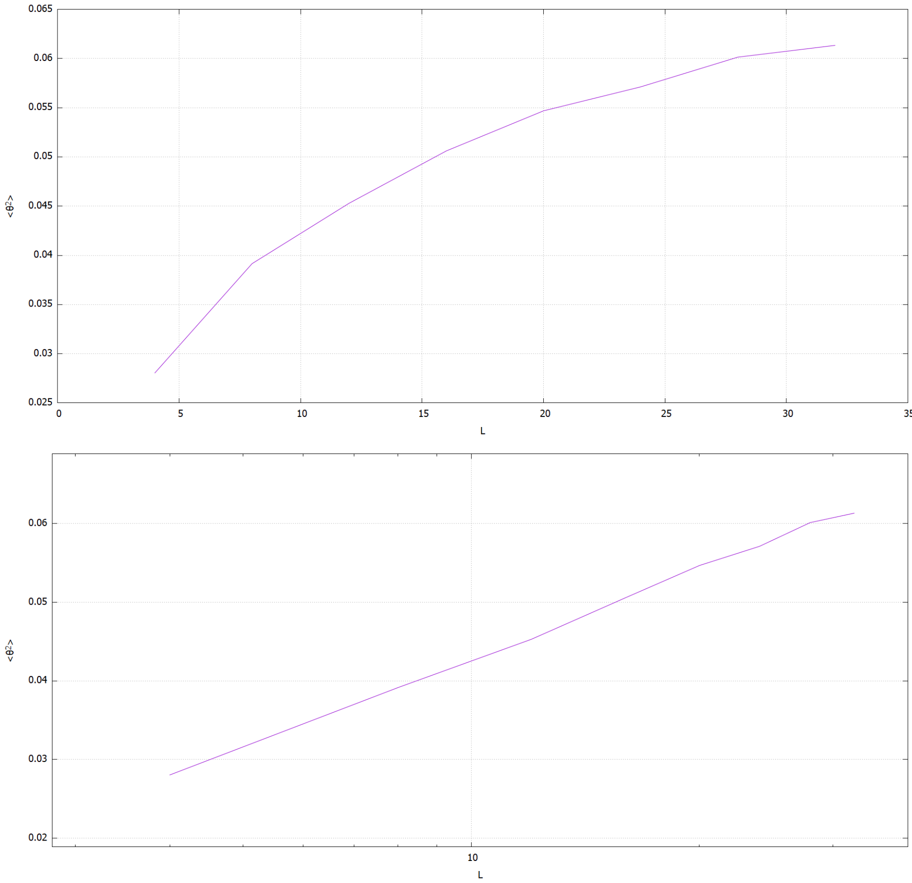

Figure 2: Mean square angle value in linear and logarithmic scale

(c)

The goal of this temperature quench is to bring the system to a stable excited state, corresponding to a local but not global energy minimum. To achieve this, the system is evolved rapidly, using 200 Monte Carlo sweeps for each temperature. The temperature is initially set at 600.5 and is decreased by 20 at each iteration until it reaches the desired value of 0.5. The value of L is fixed at 32, and the range of angle changes is set to $\theta_{max} = 1.2$ radians. It can be noticed that 4 positive and 4 negative vortices are formed. In general, the number of positive and negative vortices is equal.

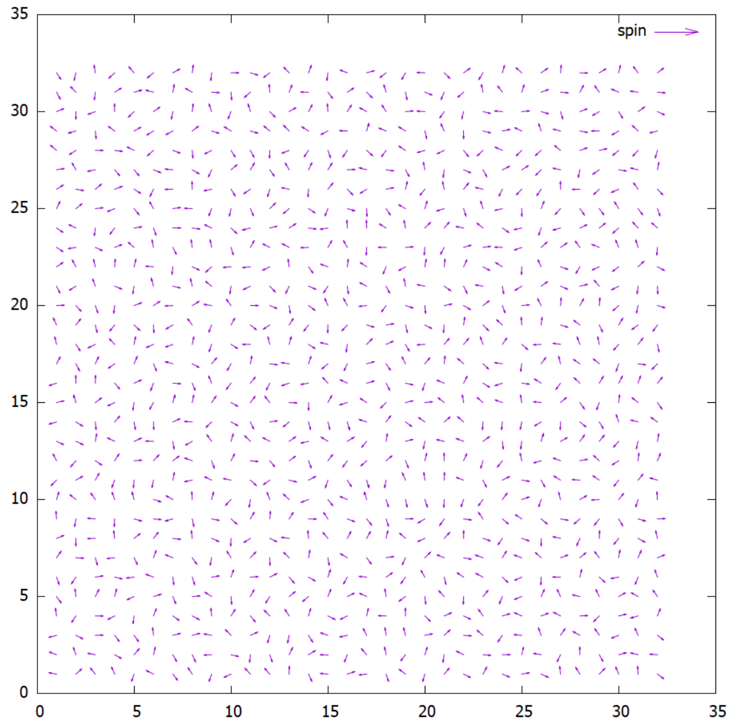

Figure 3: Initial configuration

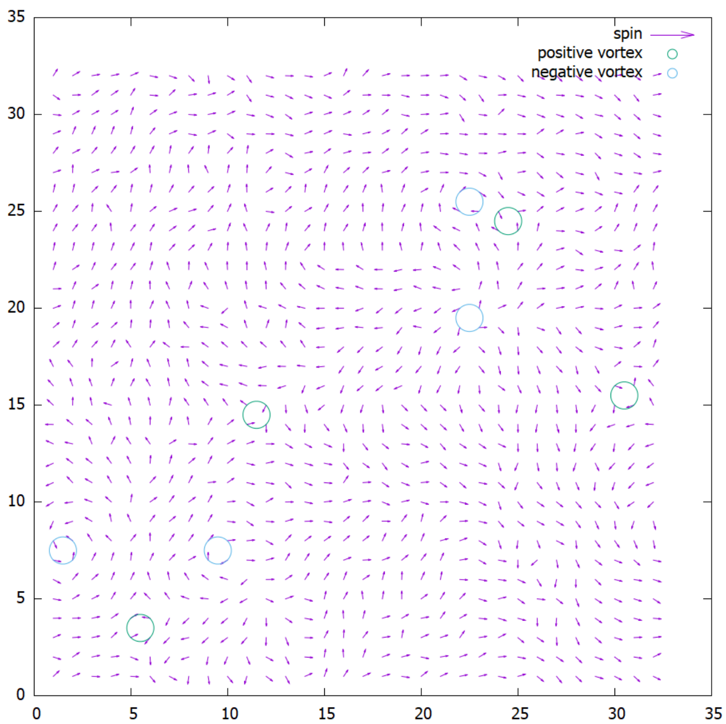

Figure 4: Final configuration at T=0.5

By further lowering the final temperature of the quench, the vortex configurations become more noticeable. Below is the result obtained at $T = 0.05$ with the remaining parameters unchanged.

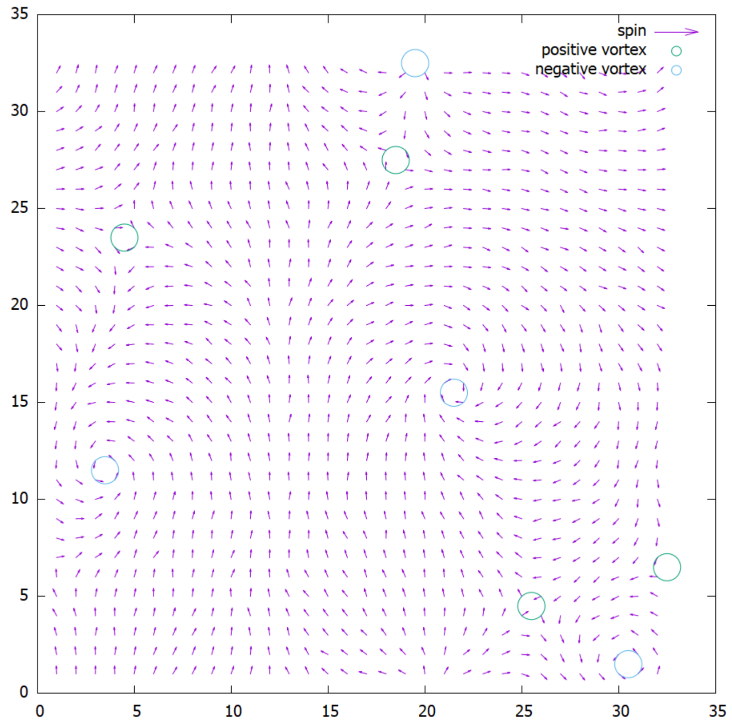

Figure 5: Final configuration at T=0.05

(d)

For this part, the parameters were set as follows: L=32, $\theta_{max} = 1.4$ radians, $nequil = 1000$, $nmcs = 5000$. The average energy per site increases with temperature, as the spins tend to become disordered, pointing in random directions due to thermal agitation. The specific heat shows a peak, which is located approximately between $T = 1.0$ and $T = 1.2$. The vorticity increases with temperature. The duality between positive and negative vortices resembles that of particles and antiparticles. Using this interpretation, we can associate an energy with a vortex, characterizing the cost of excitation compared to the ordered configuration. When the number of vortices is small, the system can be treated as a gas of non-interacting particles, and the abundance of vortices is determined by the canonical weight associated with the energy of creating such a state: $e^{-\beta E_{KT}}$. It can be observed from Figure 9 that the logarithm of vorticity increases linearly for small temperature values.

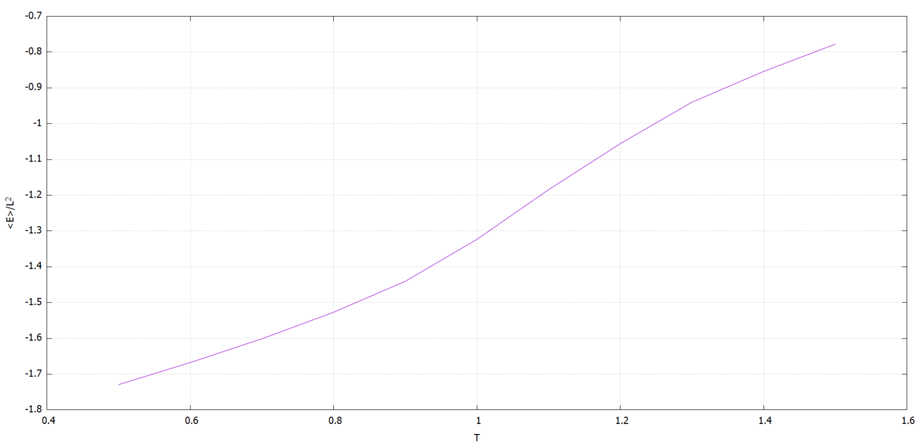

Figure 6: Average energy as a function of temperature

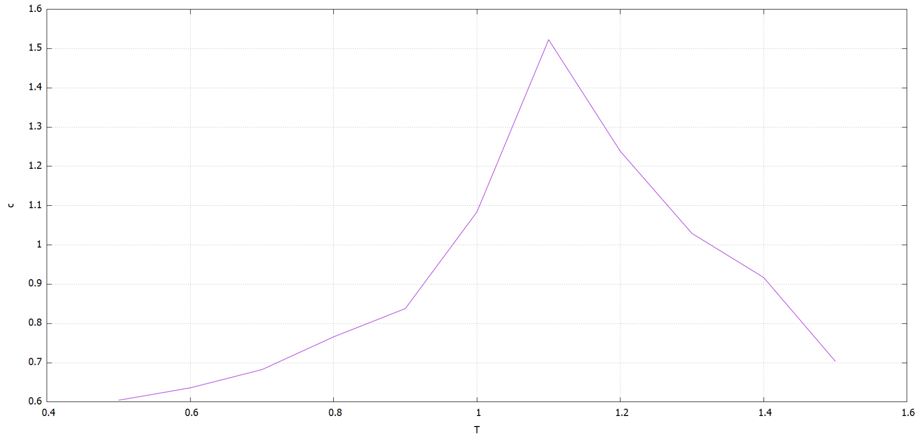

Figure 7: Specific heat as a function of temperature

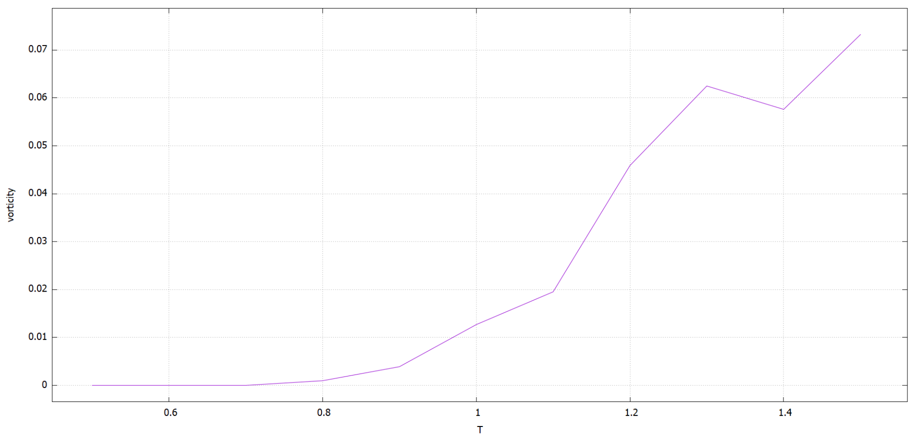

Figure 8: Vorticity as a function of temperature

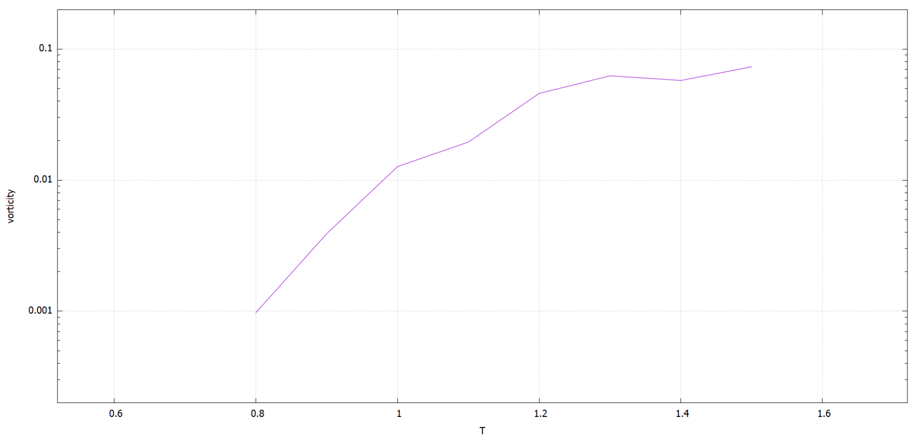

Figure 9: Logarithm of vorticity as a function of temperature

From the temperature-dependent configurations, it can be inferred that the first temperature at which free vortices are observed is approximately $T \approx 1.2$.

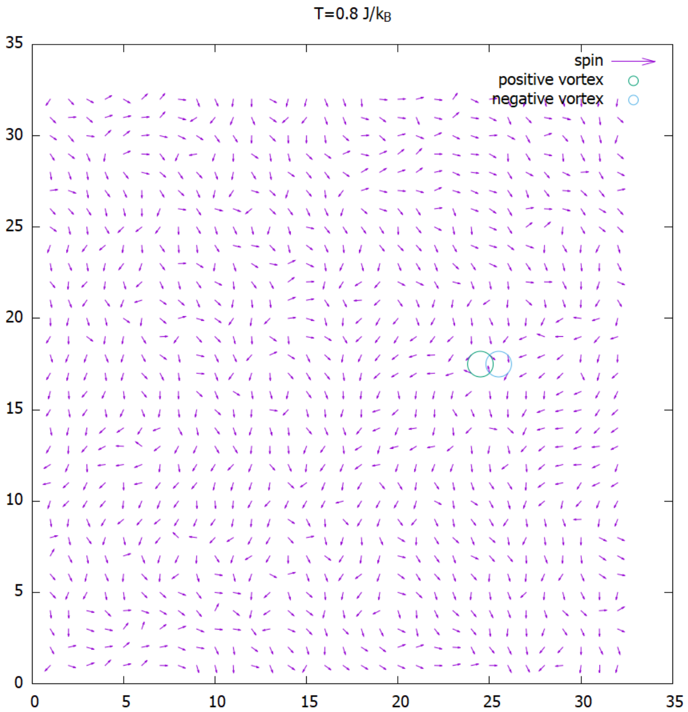

Figure 10:

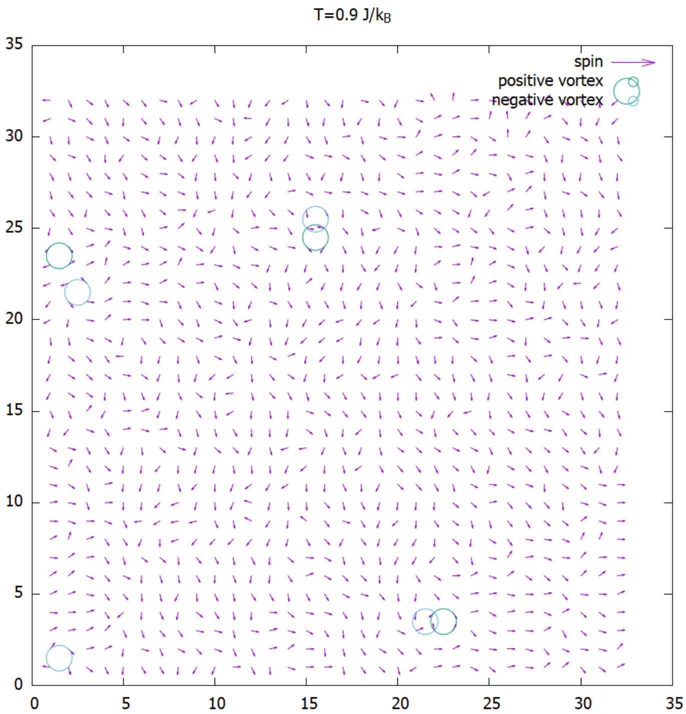

Figure 11:

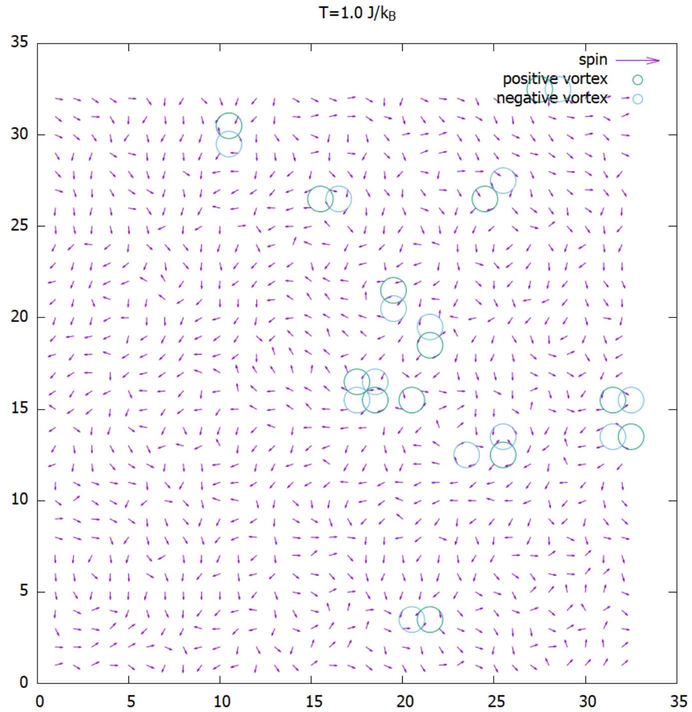

Figure 12:

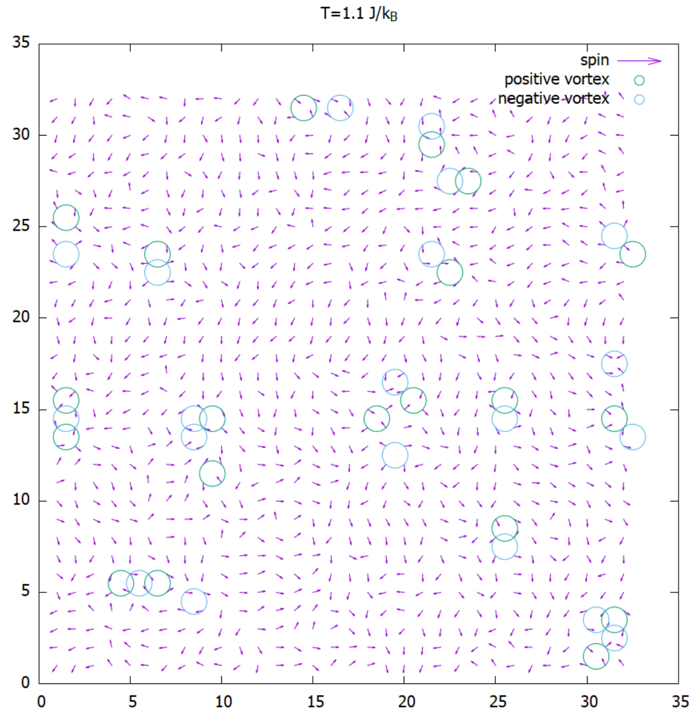

Figure 13:

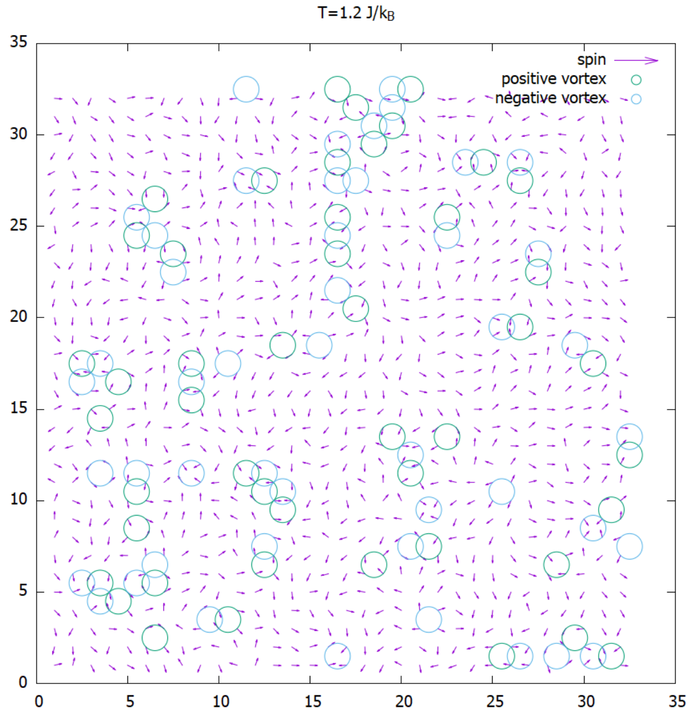

Figure 14:

(e)

Following the suggestion in the text, susceptibility is fitted with $<\vec{M}>=0$:

$$\chi = \frac{<\vec{M}^2>}{k_B T}.$$

For the fit, 25 temperature values equidistantly spaced between 1 and 1.2 were used. The parameters were fixed at: $L = 32$, $nmcs = 10000$, $\nu = 0.7$, $T_{KT} = 0.89$. The fit function used is $f(x) = a + b/\left(\frac{x-T_{KT}}{T_{KT}}\right)^{\nu}$, with parameters a and b, and with $T_{KT} = 0.89$[1]. The results obtained through gnuplot are: $a = 1.66 \pm 0.22$, $b = 1.046 \pm 0.074$, where a corresponds to $log(A)$ in equation (17.66). Finally, the fit was repeated, fixing the found parameter a and varying T_{KT} and b. The values obtained are: $b = 1.105 \pm 0.070$, $T_{KT} = 0.879 \pm 0.014$.

[1] Tobochnik and Chester, Monte Carlo study of the planar spin model.

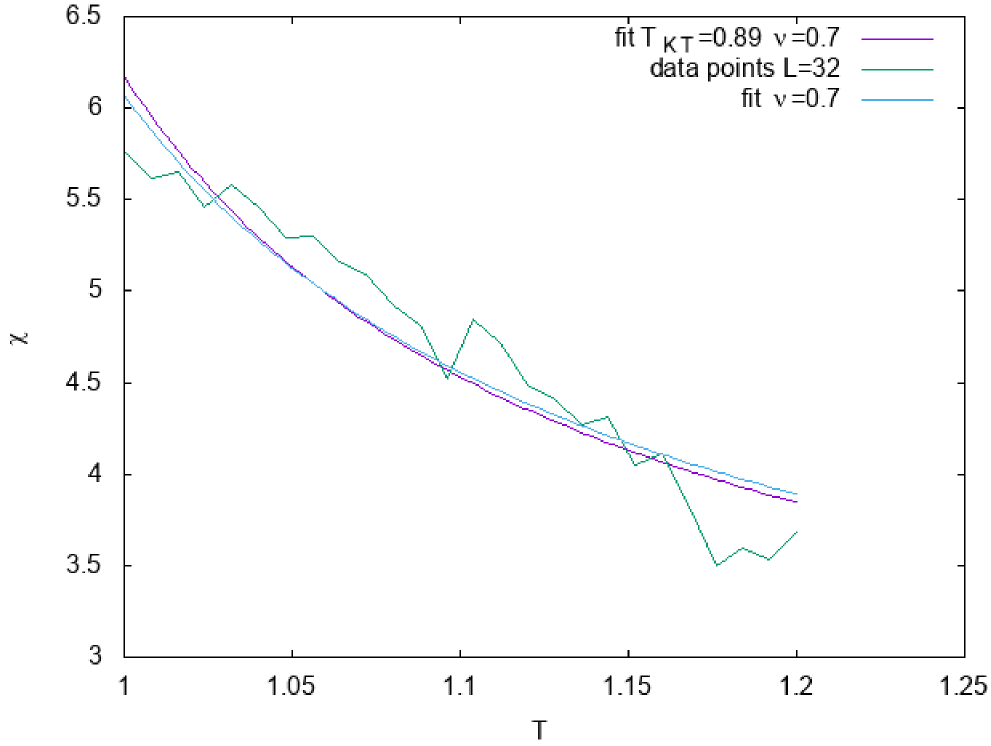

Figure 15: Function fitted to the data

A better fit is obtained in the range [1.1, 1.3], moving further away from the critical temperature.

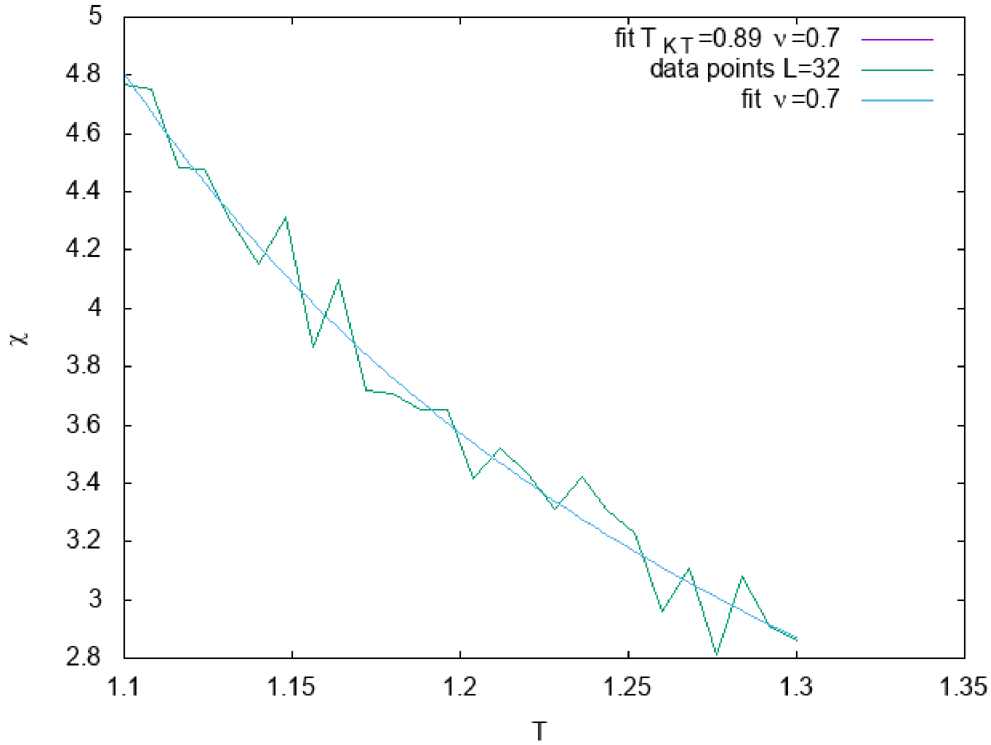

Figure 16: Alternative fit

In this case, the two types of fits coincide, and $T_{KT} = 0.89 \pm 0.01$ is estimated. This temperature value differs from the specific heat peak and the vortex decoupling temperature, which are compatible with each other.