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An Introduction to Computer Simulation Methods Third Edition (revised)
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or Edition II of the previous book (By Gould and Tobochnik only)

Project 17.25. Kosterlitz-Thouless transition in the planar model

The planar model (also called the x-y model) consists of spins of unit magnitude that can point in any direction in the x-y plane. The energy or Hamiltonian function of the planar model in zero magnetic field can be written as

$$E = -J \sum_{i,j=nn(i)} \left[s_{i,x}s_{j,x} + s_{i,y}s_{j,y} \right], \qquad (17.64)$$

where $s_{i,x}$ represents the x-component of the spin at the ith site, J measures the strength of the interaction, and the sum is over all nearest neighbors. We can rewrite (17.64) in a simpler form by substituting $s_{i,x} = \cos\theta_i$ and $s_{i,y} = \sin\theta_i$. The result is

$$E = -J \sum_{i,j=nn(i)} \cos(\theta_i - \theta_j), \qquad (17.65)$$

where θ_i is the angle that the ith spin makes with the x axis. The most studied case is the two-dimensional model on a square lattice. In this case the mean magnetization $\langle \mathbf{M} \rangle = 0$ for all temperatures $T > 0$, but nevertheless, there is a phase transition at a nonzero temperature, T_{KT}, the Kosterlitz-Thouless (KT) transition. For $T \leq T_{KT}$, the spin-spin correlation function $C(r)$ decreases as a power law for increasing r; for $T > T_{KT}$, $C(r)$ decreases exponentially. The power law decay of $C(r)$ for all $T \leq T_{KT}$ implies that every temperature below T_{KT} acts as if it were a critical point. We say that the planar model has a line of critical points. In the following, we explore some of the properties of the planar model and the mechanism that causes the transition.

a. Write a Monte Carlo program to simulate the planar model on a square lattice using periodic boundary conditions. Because θ and hence the energy of the system is a continuous variable, it is not possible to store the previously computed values of the Boltzmann factor for each possible value of ΔE. Instead, of computing $e^{-\beta \Delta E}$ for each trial change, it is faster to set up an array `w` such that the array element `w(j)` $= e^{-\beta\Delta E}$, where `j` is the integer part of $1000\Delta E$. This procedure leads to an energy resolution of 0.001, which should be sufficient for most purposes.

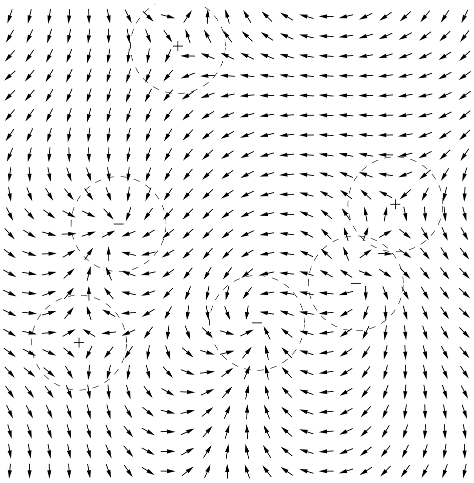

Figure 17.7: A typical configuration of the planar model on a 24×24 square lattice that has been quenched from $T = \infty$ to $T = 0$ and equilibrated for 200 Monte Carlo steps per spin after the quench. Note that there are six vortices. The circle around each vortex is a guide to the eye and is not meant to indicate the size of the vortex.

b. One way to show that the magnetization $\langle \mathbf{M} \rangle$ vanishes for all T is to compute $\langle \theta^2 \rangle$, where θ is the angle that a spin makes with the magnetization $\mathbf{M}$ at any given instant. (Although the mean magnetization vanishes, $\mathbf{M} \neq 0$ at any given instant.) Compute $\langle \theta^2 \rangle$ as a function of the number of spins N at $T = 0.1$, and show that $\langle \theta^2 \rangle$ diverges as $\ln N$. Begin with a 4×4 lattice and choose the maximum change in θ_i to be $\Delta\theta_{\mathrm{max}} = 1.0$. If necessary, change θ_{max} so that the acceptance probability is about 40%. If $\langle \theta^2 \rangle$ diverges, then the spins are not pointing along any preferred direction, and hence there is no mean magnetization.

c. Modify your program so that an arrow is drawn at each site to show the orientation of each spin. We will look at a typical configuration and analyze it visually. Begin with a 32×32 lattice with spins pointing in random directions and do a temperature quench from $T = \infty$ to $T = 0.5$. (Simply change the value of β in the Boltzmann probability.) Such a quench should lock in some long lived, but metastable vortices. A vortex is a region of the lattice where the spins rotate by at least 2π as your eye moves around a closed path (see Fig. 17.7). To determine the center of a vortex, choose a group of four spins that are at the corners of a unit square, and determine whether the spins turn by $\pm 2\pi$ as your eye goes from one spin to the next in a counterclockwise direction around the square. Assume that the difference between the direction of two neighboring spins, $\delta\theta$, is in the range $-\pi < \delta\theta < \pi$. A total rotation of $+2\pi$ indicates the existence of a positive vortex, and a change of -2π indicates a negative vortex. Count the number of positive and negative vortices. Repeat these observations on several configurations. What can you say about the number of vortices of each sign?

d. Write a subroutine to determine the existence of a vortex for each 1×1 square of the lattice. Represent the center of the vortices using a different symbol to distinguish between a positive and a negative vortex. Do a Monte Carlo simulation to compute the mean energy, specific heat, and number of vortices in the range from $T = 0.5$ to $T = 1.5$ in steps of 0.1. Use the last configuration at the previous temperature as the first configuration for the next temperature. Begin at $T = 0.5$ with all $\theta_i = 0$. Draw the vortex locations for the last configuration at each temperature. Use at least 1000 Monte Carlo steps per spin at each temperature to equilibrate and at least 5000 Monte Carlo steps per spin for computing the averages. Use an 8×8 or 16×16 lattice if your computer resources are limited, and larger lattices if you have sufficient resources. Describe the T dependence of the energy, specific heat, and vorticity (equal to the number of vortices per area). Plot the logarithm of the vorticity versus T for $T < 1.1$. What can you conclude about the T-dependence of the vorticity? Explain why this form is reasonable. Describe the vortex configurations. At what temperature can you find a vortex that appears to be free, that is, a vortex that is not obviously paired up with another vortex of opposite sign?

e. The Kosterlitz-Thouless theory predicts that the susceptibility χ diverges above the transition as

$$\chi \sim A\, e^{b/\epsilon^{\nu}}, \tag{17.66}$$

where ϵ is the reduced temperature $\epsilon = (T - T_{KT})/T_{KT}$, $\nu = 0.5$, and A and b are nonuniversal constants. Compute χ from the relation (17.14) with $\mathbf{M} = 0$ because the mean magnetization vanishes. Assume the exponential form (17.66) for χ in the range $T = 1$ and $T = 1.2$ with $\nu = 0.7$, and find the best values of T_{KT}, A, and b. (Although the analytical theory predicts $\nu = 0.5$, simulations for small systems indicate that $\nu = 0.7$ gives a better fit.) One way to determine T_{KT}, A, and b is to assume a value of T_{KT} and then do a least squares fit of $\ln \chi$ to determine A and b. Choose the set of parameters that minimizes the variance of $\ln \chi$. How does your estimated value of T_{KT} compare with the temperature at which free vortices first appear? At what temperature does the specific heat have a peak? The Kosterlitz-Thouless theory predicts that the specific heat peak does not occur at T_{KT}. This result has been confirmed by simulations (see Tobochnik and Chester). To obtain quantitative results, you will need lattices larger than 32×32.