

Menu Project. Dilation symmetry in phase transitions

When a gas of molecules makes the transition to the liquid state, there can be spatial fluctuations of density that become much larger than the size of the molecules. This type of transition is known as a second-order phase transition. The purpose of this project is to exhibit this fluctuation behavior in a computer simulation, using a simple model of the gas that captures the phase-transition behavior. To do it, you need to understand the Metropolis algorithm for sampling an ensemble of configurations of a system in thermal equilibrium. This is discussed in Gould and Tobochnik, Second Edition, Chapter 17. I describe it briefly below.

Unlike the self-avoiding chain ensemble discussed in class, most systems in thermal equilibrium have a distinct bias in the probability of different configurations c . A system in thermal equilibrium, such as a gas or liquid that has been in a constant environment for a long time, has a definite temperature T . By T , we mean the absolute temperature expressed in energy units. At the absolute zero of temperature, $T = 0$; at room temperature T has a value of $1/40$ electron volts, or $1.6 \times 10^{-19}/40$ joules. Each configuration c of a gas has an energy $E(c)$. Every system at temperature T has a well-defined bias in the probability $P(c)$ of encountering configuration c in a random sample: for any pair of configurations c and c' ,

$$P(c')/P(c) = \exp(-E(c')/T) / \exp(-E(c)/T). \quad (1)$$

There is a straightforward way to make random changes in a configuration that give this thermal bias in $P(c)$. It is called the Metropolis algorithm and is discussed in Gould and Tobochnik. It is a way of choosing the conditional probabilities $q(c, c')$ of going from some initial configuration c to another one c' . Thus it is a generalization of our method for sampling random self-avoiding chains. In class we saw that if $q(c, c') = q(c', c)$ then after many samplings, $P(c') = P(c)$. This is the same as the thermal equilibrium bias above in the limit where all allowed c 's have energies $E(c)$ much smaller than T . Here is the generalization: If there is a bias in q , it produces a corresponding bias in P . That is, if $q(c, c') = Xq(c', c)$, then $P(c') = XP(c)$. If we select $X = \exp((E(c') - E(c))/T)$, the resulting $P(c)$ satisfy Eq. (1). This can be shown by straightforward algebra. (Beware of lingering sign errors I might have made. Verify with Gould and Tobochnik.)

The Ising model is a lattice gas model. The system is a square L by L lattice of cells, each of which may be in one of two states: occupied or empty. It is conventional to assign a number s_i to each cell i such that $s_i = 1$ means the cell is occupied and $s_i = -1$ means the cell is empty. Thus a configuration can be specified by listing the $\{s_i\}$. Gases undergo phase transitions because the molecules feel attractive interactions. In the Ising model we express this attraction in the simplest possible way: any neighboring pair of occupied sites is assigned a fixed energy $-J$; any neighboring pair of empty sites is assigned an energy $-J$ as well. Any pair of unequal sites is assigned an energy $+J$. Thus like neighbors are energetically favored: they increase the probability of the configuration. For further details, see Gould and Tobochnik. There is no kinetic energy in this gas. As it turns out, kinetic energy is not important for describing the average spatial properties of phase transitions.

This project consists of writing Java programs that implement Problems 17.5 in Gould and Tobochnik, 2nd edition. This is named "Equilibration of the two-dimensional Ising model". You can probably expand your lattice to 64 by 64 or 128×128 , for more dramatic results. Demonstrate that your program works properly by showing that it samples the 16 configurations of the 2 by 2 model with the correct probabilities.

Fractal properties: select a site near the center of the lattice. Compute the average value of s within a square box of radius R around this site. Use $R = 3, 5, 9, 17, \dots$. Denote these averages as $S(R)$. Find the average of each $S(R)$ over many independent configurations. A power-law dependence of $S(R)$ indicates dilation symmetry, as discussed in class. Such symmetry is supposed to occur in a sufficiently large system at its liquid-gas transition temperature. Look for this behavior in your system and report the exponent for any power law you find.