4th exam item

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Abstract

Thermodynamic simulations, Ising-model and the Metropolis algorithm

1 Introduction

Not only do thermodynamic simulations have important practical applications, but they also give us insight into what is "dynamic" in thermodynamics. In the following few pages we are going to dwelve into how to calculate thermodynamic properties of complex systems, give a brief summary of the Metropolis algorithm and its applications. The theory forms the basis for field- theoretic calculations of quantum chromodynamics, some of the most fundamental and most time-consuming computations in existence.

2 The Ising-model

Ferromagnets contain finite-size domains in which the spins of all the atoms point in the same direction. When an external magnetic field is applied to these materials, the different domains align and the materials become "magnetized." Yet as the temperature is raised, the total mag- netism decreases, and at the Curie temperature the system goes through a phase transition beyond which all magnetization vanishes.

To handle this behaviour we can develop the most simple model: a **chain of spins**. As our model we consider N magnetic dipoles fixed in place on the links of a linear chain. Because the particles are fixed, their positions and momenta are not dynamic variables, and we need worry only about their spins. We assume that the particle at site i has spin s_i , which is either up or down:

$$s_i \equiv s_{z,i} = \pm\frac{1}{2}$$

Each configuration of the N particles is described by a quantum state vector:

$$|\alpha_j\rangle = |s_1, s_2, ..., s_N\rangle = \left\{ \pm\frac{1}{2}, \pm\frac{1}{2}, ... \right\}, \quad j = 1, ..., 2^N$$

Since fixed particles cannot be interchanged, we do not need to concern ourserlves with the symmtery of the wave function.

The energy of the system arises from the interaction of the spins with each other and with the external magnetic field B . We know from quantum mechanics that an electron's spin and magnetic moment are proportional to each other, so a magnetic dipole–dipole interaction is equivalent to a spin–spin interaction. We assume that each dipole interacts with the external magnetic field and with its nearest neighbor through the potential:

$$V_i = -J\vec{s_i}\vec{s_{i+1}} - g\mu_b\vec{s_i}\vec{B}$$

Here the constant J is called the *exchange energy* and is a measure of the strength of the spin– spin interaction. The constant g is the *gyromagnetic ratio*, that is, the proportionality constant between a particle's angular momentum and magnetic moment. The constant $\mu_b = e\hbar/(2m_e c)$ is the Bohr magneton, the basic measure for magnetic moments.

Even for small numbers of particles, the 2^N possible spin configurations gets to be very large ($2^{20} > 10^6$), and it is expensive for the computer to examine them all. Realistic samples with $\approx 10^{23}$ particles are beyond imagination. Consequently, statistical approaches are usually assumed, even for moderate values of N.

The energy of the system in state α_k is the expectation value of the sum of the potential V over the spins of the particles:

$$E_{\alpha_k} = \langle \alpha_k | \sum_i V_i | \alpha_k \rangle = -J \sum_{i=1}^{N-1} s_i s_{i+1} - B\mu_b \sum_{i=1}^{N} s_i$$

If we turn off the external magnetic field there will be no preferred direction in space and the average magnetization should vanish even though energetically most adventageous state would be all spins aligned. To resolution of the paradox is that the system is unstable at $B = 0$. Some properties must be calculated differently. For example magnetization should be calculated $\langle | \sum_i s_i | \rangle$ and not $\langle \sum_i s_i \rangle$, with no preferred direction.

The equilibrium alignment of the spins depends critically on the sign of the exchange energy J . If $J > 0$, the lowest energy state will tend to have neighboring spins aligned. If the temperature is low enough, the ground state will be a ferromagnet with all the spins aligned. If $J < 0$, the lowest energy state will tend to have neighbors with opposite spins. If the temperature is low enough, the ground state will be a antiferromagnet with alternating spins.

A fascinating aspect of magnetic materials is the existence of a critical temperature, the *Curie temperature*, above which the gross magnetization essentially vanishes. Below the Curie temperature the quantum state of the material has long-range order extending over macroscopic dimensions; above the Curie temperature there is only short-range order extending over atomic dimensions. Even though the 1-D Ising model predicts realistic temperature dependences for the thermodynamic quantities, the model is too simple to support a phase transition. However, the 2-D and 3-D Ising models do support the Curie temperature phase transition.

3   Some statistical mechanics

Statistical mechanics starts with the elementary interactions among a system's particles and constructs the macroscopic thermodynamic properties such as specific heats. The essential assumption is that all configurations of the system consistent with the constraints are possible. In some simulations the problem is set up such that the energy of the system is fixed. The states of this type of system are described by what is called a *microcanonical ensemble*. In contrast, when the temperature, volume, and number of particles remain fixed, we have what is called a *canonical ensemble*.

When we say that an object is at temperature T , we mean that the object's atoms are in thermodynamic equilibrium at temperature T such that each atom has an average energy

proportional to T. Although this may be an equilibrium state, it is a dynamic one in which the object's energy fluctuates as it exchanges energy with its environment (it is thermodynamics after all). Indeed, one of the most illuminating aspects of the simulation we shall develop is its visualization of the continual and random interchange of energy that occurs at equilibrium.

The energy E_{α_j} of state α_j in a canonical ensemble is not constant but is distributed with probabilities $P(\alpha_j)$ given by the Boltzmann distribution:

$$P(E_{\alpha_j}, T) = \frac{e^{-E_{\alpha_j}/k_B T}}{Z(T)}$$

$$Z(T) = \sum_{\alpha_j} e^{-E_{\alpha_j}/k_B T}$$

Here k is Boltzmann's constant, T is the temperature, and $Z(T)$ is the partition function, a weighted sum over states. Note that the sums $Z(T)$ are over the individual states or configurations of the system. Another formulation is to sum over the energies of the states of the system and includes a density-of-states factor $g(E_i)$ to account for degenerate states with the same energy. While the present sum over states is a simpler way to express the problem (one less function), we shall see that the sum over energies is more efficient numerically. In fact, in this section we even ignore the partition function $Z(T)$ because it cancels out when dealing with the ratio of probabilities.

References