2. Computer-Simulation Methods

Computer-simulation methods are by now an established tool in many branches of science. The motivations for computer simulations of physical systems are manifold. One of the main motivations is that one eliminates approximations. Usually, to treat a problem analytically (if it can be done at all) one needs to resort to some kind of approximation; for example, a mean-field-type approximation. With a computer simulation we have the ability to study systems not yet tractable with analytical methods. The computer simulation approach allows one to study complex systems and gain insight into their behaviour. Indeed, the complexity can go far beyond the reach of present analytic methods.

Because they can be used to study complex systems, computer-simulation methods provide standards against which approximate theories may be compared. At the same time, they allow the comparison of models with experiment, and provide a means of assessing the validity of a model.

There is yet another feature. Computer simulations can fill the gap between theory and experiment. Some quantities or behaviours may be impossible or difficult to measure in an experiment. With computer simulations such quantities can be computed.

At the outset of a simulation stands a well-defined model of a physical system. We are interested in computing properties of the physical system. Our point of view is that the properties or observables appear as averages over some sample space. For example, in the percolation problem (Sect.1.1) the threshold p_c is the average probability of percolation over the space of all configurations. In the spring problem (Sect.1.2) the temperature is computed as the average kinetic energy along the generated path.

For the main part we shall assume that a system under consideration has a model Hamiltonian $\mathcal{H}$. We denote a state of the system by $\mathbf{x} = (x_1,...,x_n)$, where n is the number of degrees of freedom. The set of states constitutes the available phase space Ω. The property A to be calculated will be a function of the states of the system. As mentioned above, our point of view is statistical mechanical. What we need to specify in order to compute the property A is a distribution function f(.). The quantity A is then given by

$$\langle A \rangle = Z^{-1} \int_{\Omega} A(\mathbf{x}) f(\mathcal{H}(\mathbf{x})) d\mathbf{x} \,, \tag{2.1}$$

where

$$Z = \int_{\Omega} f(\mathcal{H}(\mathbf{x}))d\mathbf{x} .$$

This is the *ensemble average* with the partition function Z. The distribution function f specifies the appropriate ensemble for the problem at hand.

The ensemble average is, however, not accessible in computer simulations. In such simulations the quantity A is evaluated along a path in phase space. Take the spring problem. We are not going to evaluate the temperature for a large number of similar systems, rather, we propagate the particle along a trajectory in phase space and evaluate the kinetic energy along the path. What we are computing is a *time average*

$$\bar{A}_t = (t-t_0)^{-1} \int_{t_0}^{t} A(\mathbf{x}(\tau))d\tau . \tag{2.2}$$

The question arising is: Are the two averages the same? For this we must invoke *ergodicity*, allowing the replacement of ensemble averages by time averages

$$\langle A \rangle = \bar{A}_{\infty} . \tag{2.3}$$

At this point, one of the two major limitations of computer-simulation methods arises. Clearly a computer simulation cannot follow a path over an infinite time. The *observation time is limited* to a finite path length so that actually the available phase space is sampled. One has to be content with

$$\bar{A} \simeq \langle A \rangle . \tag{2.4}$$

For some problems the finite observation time may be considered infinite. Consider, for example, the computation of a molecular system where the observation time is much larger than the molecular time. What we also have to take into account is the statistical error [2.1-3].

We are led to the question of how we are going to propagate the system through phase space. This is the point where we distinguish two methods. The approaches developed here are:

(i) deterministic methods, and
(ii) stochastic methods.

We look first at the deterministic methods. The idea behind these is to use the *intrinsic dynamics* of the model to propagate the system. One has to set up equations of motion and integrate forward in time. For a collection of particles governed by classical mechanics this yields a trajectory $(\mathbf{x}^N(t),\mathbf{p}^N(t))$ in phase space for the fixed initial positions $\mathbf{x}_1(0),...,\mathbf{x}_N(0)$ and momenta $\mathbf{p}_1(0),...,\mathbf{p}_N(0)$.