



Figure 1.1 What is the meaning of the sine function?

performed using symbolic manipulation programs. The calculation of Feynman diagrams, which represent multidimensional integrals of importance in quantum electrodynamics, has been a major impetus to the development of computer algebra software that can manipulate and simplify symbolic expressions. Maxima, Maple, and Mathematica are examples of software packages that have symbolic manipulation capabilities as well as many tools for numerical analysis. Matlab and Octave are examples of software packages that are convenient for computations involving matrices and related tasks.

As the computer plays an increasing role in our understanding of physical phenomena, the *visual representation* of complex numerical results is becoming even more important. The human eye in conjunction with the visual processing capacity of the brain is a very sophisticated device. Our eyes can determine patterns and trends that might not be evident from tables of data and can observe changes with time that can lead to insight into the important mechanisms underlying a system's behavior. The use of graphics can also increase our understanding of the nature of analytical solutions. For example, what does a sine function mean to you? We suspect that your answer is not the series, $\sin x = x - x^3/3! + x^5/5! + \dots$, but rather a periodic, constant amplitude curve (see Figure 1.1). What is most important is the mental image gained from a visualization of the form of the function.

Traditional modes of presenting data include two- and three-dimensional plots including contour and field line plots. Frequently, more than three variables are needed to understand the behavior of a system, and new methods of using color and texture are being developed to help researchers gain greater insights into their data.

An essential role of science is to develop models of nature. To know whether a model is consistent with observation, we have to understand the behavior of the model and its predictions. One way to do so is to implement the model on a computer. We call such an implementation a *computer simulation* or simulation for short. For example, suppose a teacher gives \$10 to each student in a class of 100. The teacher, who also begins with \$10 in her pocket, chooses a student at random and flips a coin. If the coin is heads, the teacher gives \$1 to the student; otherwise, the student gives \$1 to the teacher. If either the teacher or the student would go into debt by this transaction, the transaction is not allowed. After many exchanges, what is the probability that a student has s dollars? What is the probability that the teacher has t dollars? Are these two probabilities the same? Although these particular questions can be answered by analytical methods, many problems of this nature cannot be solved in this way (see Problem 1.1).

One way to determine the answers to these questions is to do a classroom experiment. However, such an experiment would be difficult to arrange, and it would be tedious to do a sufficient number of transactions.

A more practical way to proceed is to convert the rules of the model into a computer program, simulate many exchanges, and estimate the quantities of interest. Knowing the results might help us gain more insight into the nature of an analytical solution if one exists. We can also modify the rules and ask "what if?" questions. For example, would the probabilities change if the students could exchange money with one another? What would happen if the teacher was allowed to go into debt?

Simulations frequently use the computational tools of numerical analysis and visualization, and occasionally symbolic manipulation. The difference is one of emphasis. Simulations are usually done with a minimum of analysis. Because simulation emphasizes an exploratory mode of learning, we will stress this approach.

Computers are also involved in all phases of a laboratory experiment, from the design of the apparatus to the *collection and analysis of data*. LabView is an example of a data acquisition program. Some of the roles of the computer in laboratory experiments, such as the varying of parameters and the analysis of data, are similar to those encountered in simulations. However, the tasks involved in *real-time control* and interactive data analysis are qualitatively different and involve the interfacing of computer hardware to various types of instrumentation. We will not discuss this use of the computer.

1.2 ■ THE IMPORTANCE OF COMPUTER SIMULATION

Why is computation becoming so important in physics? One reason is that most of our analytical tools such as differential calculus are best suited to the analysis of *linear* problems. For example, you probably have analyzed the motion of a particle attached to a spring by assuming a linear restoring force and solving Newton's second law of motion. In this case a small change in the displacement of the particle leads to a small change in the force. However, many natural phenomena are *nonlinear*, and a small change in a variable might produce a large change in another. Because relatively few nonlinear problems can be solved by analytical methods, the computer gives us a new tool to explore nonlinear phenomena.

Another reason for the importance of computation is the growing interest in systems with many variables or with many degrees of freedom. The money exchange model described in Section 1.1 is a simple example of a system with many variables. A similar problem is given at the end of this chapter.

Computer simulations are sometimes referred to as *computer experiments* because they share much in common with laboratory experiments. Some of the analogies are shown in Table 1.1. The starting point of a computer simulation is the development of an idealized model of a physical system of interest. We then need to specify a procedure or *algorithm* for implementing the model on a computer and decide what quantities to measure. The results of a computer simulation can serve as a bridge between laboratory experiments and theoretical calculations. In some cases we can obtain essentially exact results by simulating an idealized model that has no laboratory counterpart. The results of the idealized model can serve as a stimulus to the development of the theory. On the other hand, we sometimes can do simulations of a more realistic model than can be done theoretically, and hence make