Project I: Compulsory (grade 3)

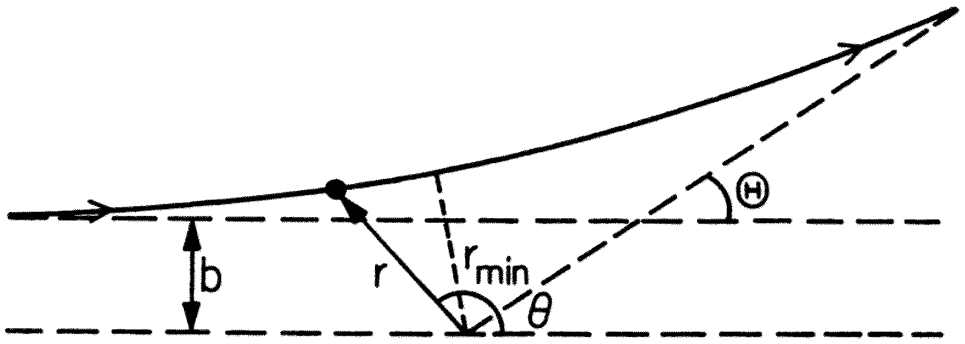

Figure I.1 Quantities involved in the scattering of a particle by a central potential.

vibrational state. Find the value of β appropriate for the H_2 molecule, modify the program above to use the Morse potential, and calculate the spectrum of vibrational states. Show that a much more reasonable number of levels is now obtained. Compare the energies with experiment and with those of the Lennard-Jones potential and interpret the latter differences.

Project I: Scattering by a central potential

In this project, we will investigate the classical scattering of a particle of mass m by a central potential, in particular the Lennard-Jones potential considered in Section 1.4 above. In a scattering event, the particle, with initial kinetic energy E and impact parameter b, approaches the potential from a large distance. It is deflected during its passage near the force center and eventually emerges with the same energy, but moving at an angle Θ with respect to its original direction. Since the potential depends upon only the distance of the particle from the force center, the angular momentum is conserved and the trajectory lies in a plane. The polar coordinates of the particle, (r, θ), are a convenient way to describe its motion, as shown in Figure I.1. (For details, see any textbook on classical mechanics, such as [Go80].)

Of basic interest is the deflection function, $\Theta(b)$, giving the final scattering angle, Θ, as a function of the impact parameter; this function also depends upon the incident energy. The differential cross section for scattering at an angle Θ, $d\sigma/d\Omega$, is an experimental observable that is

related to the deflection function by

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\Theta}\left|\frac{db}{d\Theta}\right| . \qquad (I.1)$$

Thus, if $d\Theta/db = (db/d\Theta)^{-1}$ can be computed, then the cross section is known.

Expressions for the deflection function can be found analytically for only a very few potentials, so that numerical methods usually must be employed. One way to solve the problem would be to integrate the equations of motion in time (i.e., Newton's law relating the acceleration to the force) to find the trajectories corresponding to various impact parameters and then to tabulate the final directions of the motion (scattering angles). This would involve integrating four coupled first-order differential equations for two coordinates and their velocities in the scattering plane, as discussed in Section 2.5 below. However, since angular momentum is conserved, the evolution of θ is related directly to the radial motion, and the problem can be reduced to a one-dimensional one, which can be solved by quadrature. This latter approach, which is simpler and more accurate, is the one we will pursue here.

To derive an appropriate expression for Θ, we begin with the conservation of angular momentum, which implies that

$$L = mvb = mr^2\frac{d\theta}{dt} , \qquad (I.2)$$

is a constant of the motion. Here, $d\theta/dt$ is the angular velocity and v is the asymptotic velocity, related to the bombarding energy by $E = \frac{1}{2}mv^2$. The radial motion occurs in an effective potential that is the sum of V and the centrifugal potential, so that energy conservation implies

$$\frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{L^2}{2mr^2} + V = E . \qquad (I.3)$$

If we use r as the independent variable in (I.2), rather than the time, we can write

$$\frac{d\theta}{dr} = \frac{d\theta}{dt}\left(\frac{dr}{dt}\right)^{-1} = \frac{bv}{r^2}\left(\frac{dr}{dt}\right)^{-1} , \qquad (I.4)$$

and solving (I.3) for dr/dt then yields

$$\frac{d\theta}{dr} = \pm\frac{b}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2} . \qquad (I.5)$$

Recalling that $\theta = \pi$ when $r = \infty$ on the incoming branch of the trajectory and that θ is always decreasing, this equation can be integrated immediately to give the scattering angle,

$$\Theta = \pi - 2\int_{r_{\min}}^{\infty} \frac{b\,dr}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2} , \qquad (I.6)$$

where $r_{\min}$ is the distance of closest approach (the turning point, determined by the outermost zero of the argument of the square root) and the factor of 2 in front of the integral accounts for the incoming and outgoing branches of the trajectory, which give equal contributions to the scattering angle.

One final transformation is useful before beginning a numerical calculation. Suppose that there exists a distance $r_{\max}$ beyond which we can safely neglect V. In this case, the integrand in (I.6) vanishes as r^{-2} for large r, so that numerical quadrature could be very inefficient. In fact, since the potential has no effect for $r > r_{\max}$, we would just be "wasting time" describing straight-line motion. To handle this situation efficiently, note that since $\Theta = 0$ when $V = 0$, Eq. (I.6) implies that

$$\pi = 2\int_{b}^{\infty} \frac{b\,dr}{r^2}\left(1 - \frac{b^2}{r^2}\right)^{-1/2} , \qquad (I.7)$$

which, when substituted into (I.6), results in

$$\Theta = 2b\left[\int_{b}^{r_{\max}} \frac{dr}{r^2}\left(1 - \frac{b^2}{r^2}\right)^{-1/2} - \int_{r_{\min}}^{r_{\max}} \frac{dr}{r^2}\left(1 - \frac{b^2}{r^2} - \frac{V}{E}\right)^{-1/2}\right] . \qquad (I.8)$$

The integrals here extend only to $r_{\max}$ since the integrands become equal when $r > r_{\max}$.

Our goal will be to study scattering by the Lennard-Jones potential (1.16), which we can safely set to zero beyond $r_{\max} = 3a$ if we are not interested in energies smaller than about

$$V(r = 3a) \approx 5 \times 10^{-3} V_0 .$$

The study is best done in the following sequence of steps:

Step 1 Before beginning *any* numerical computation, it is important to have some idea of what the results should look like. Sketch what you think the deflection function is at relatively low energies, $E \lesssim V_0$, where the peripheral collisions at large $b \leq r_{\max}$ will take place in a predominantly attractive potential and the more central collisions will "bounce" against the repulsive core. What happens at much higher energies, $E \gg V_0$, where

the attractive pocket in V can be neglected? Note that for values of b where the deflection function has a maximum or a minimum, Eq. (I.1) shows that the cross section will be infinite, as occurs in the rainbow formed when light scatters from water drops.

Step 2 To have analytically soluble cases against which to test your program, calculate the deflection function for a square potential, where $V(r) = U_0$ for $r < r_{\max}$ and vanishes for $r > r_{\max}$. What happens when U_0 is negative? What happens when U_0 is positive and $E < U_0$? when $E > U_0$?

Step 3 Write a program that calculates, for a specified energy E, the deflection function by a numerical quadrature to evaluate both integrals in Eq. (I.8) at a number of equally spaced b values between 0 and $r_{\max}$. (Note that the singularities in the integrands require some special treatment.) Check that the program is working properly and is accurate by calculating deflection functions for the square-well potential discussed in Step 2. Compare the accuracy with that of an alternative procedure in which the first integral in (I.8) is evaluated analytically, rather than numerically.

Step 4 Use your program to calculate the deflection function for scattering from the Lennard-Jones potential at selected values of E ranging from $0.1\,V_0$ to $100\,V_0$. Reconcile your answers in Step 1 with the results you obtain. Calculate the differential cross section as a function of Θ at these energies.

Step 5 If your program is working correctly, you should observe, for energies $E \lesssim V_0$, a singularity in the deflection function where Θ appears to approach $-\infty$ at some critical value of b, b_{crit}, that depends on E. This singularity, which disappears when E becomes larger than about V_0, is characteristic of "orbiting." In this phenomenon, the integrand in Eq. (I.6) has a linear, rather than a square root, singularity at the turning point, so that the scattering angle becomes logarithmically infinite. That is, the effective potential,

$$V + E\left(\frac{b}{r}\right)^2,$$

has a parabolic maximum and, when $b = b_{\text{crit}}$, the peak of this parabola is equal to the incident energy. The trajectory thus spends a very long time at the radius where this parabola peaks and the particle spirals many times around the force center. By tracing b_{crit} as a function of energy

and by plotting a few of the effective potentials involved, convince yourself that this is indeed what's happening. Determine the maximum energy for which the Lennard-Jones potential exhibits orbiting, either by a solution of an appropriate set of equations involving V and its derivatives or by a systematic numerical investigation of the deflection function. If you pursue the latter approach, you might have to reconsider the treatment of the singularities in the numerical quadratures.

Attempt all the questions.

Project: II (grade 4 & 5)

and estimate the uncertainty in your answer. Study how your results depend upon where the random walker is started and on how many thermalization steps you take before beginning the sampling. Compare the efficiency of the Metropolis algorithm with that of a calculation that uses one of the methods discussed in Section 8.2 to generate the normal distribution directly.

8.4 The Ising model in two dimensions

Models in which the degrees of freedom reside on a lattice and interact locally arise in several areas of condensed matter physics and field theory. The simplest of these is the Ising model [Hu63], which can be taken as a crude description of a magnetic material or a binary alloy. In this example, we will use Monte Carlo methods to calculate the thermodynamic properties of this model.

If we speak in the magnetic language, the Ising model consists of a set of spin degrees of freedom interacting with each other and with an external magnetic field. These might represent the magnetic moments of the atoms in a solid. We will consider in particular a model in two spatial dimensions, where the spin variables are located on the sites of an $N_x \times N_y$ square lattice. The spins can therefore be labeled as S_{ij}, where i, j are the indices for the two spatial directions, or as S_α, where α is a generic site label. Each of these spin variables can be either "up" ($S_\alpha = +1$) or "down" ($S_\alpha = -1$). This mimics the spin-1/2 situation, although note that we take the spins to be classical degrees of freedom and do not impose the angular momentum commutation rules characteristic of a quantum description. (Doing so would correspond to the Heisenberg model.)

The Hamiltonian for the system is conventionally written as

$$H = -J \sum_{\langle \alpha\beta \rangle} S_\alpha S_\beta - B \sum_\alpha S_\alpha. \tag{8.18}$$

Here, the notation $\langle \alpha\beta \rangle$ means that the sum is over nearest-neighbor *pairs* of spins; these interact with a strength J (see Figure 8.2). Thus, the spin at site ij interacts with the spins at $i \pm 1j$ and $ij \pm 1$. (We assume periodic boundary conditions on the lattice, so that, for example, the lower neighbors of the spins with $i = N_x$ are those with $i = 1$ and the left-hand neighbors of those with $j = 1$ are those with $j = N_y$; the lattice therefore has the topology of a torus.) When J is positive, the energy is lower if a spin is in the same direction as its neighbors (ferromagnetism), while when J is negative, a spin will tend to be anti-aligned with its

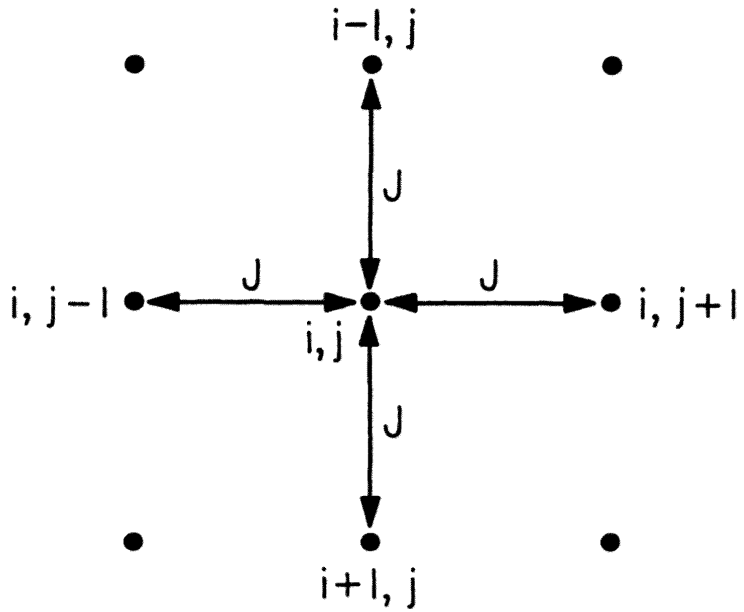

Figure 8.2 Schematic illustration of the two-dimensional Ising model.

neighbors (anti-ferromagnetism). The term involving B represents the interaction of the spins with an external magnetic field, which tends to align all spins in the same direction.

We will be interested in the thermodynamics of this system. In this case, it is convenient to measure the coupling energies J and B in units of the temperature, so that heating the system corresponds to decreasing these couplings. Configurations of the system are specified by giving the values of all $N_x \times N_y \equiv N_s$ spin variables and the weighting of any one of the 2^{N_s} spin configurations, $\mathbf{S}$, in the canonical ensemble is

$$w(\mathbf{S}) = \frac{e^{-H(\mathbf{S})}}{Z} , \tag{8.19}$$

where the partition function is

$$Z(J,B) = \sum_{\mathbf{S}} e^{-H(\mathbf{S})} . \tag{8.20}$$

The thermodynamic quantities we will be interested are the magnetization

$$M = \frac{\partial \log Z}{\partial B} = \sum_{\mathbf{S}} w(\mathbf{S}) \Big(\sum_{\alpha} S_\alpha \Big) , \tag{8.21a}$$

the susceptibility

$$\chi = \frac{\partial M}{\partial B} = \sum_{\mathbf{S}} w(\mathbf{S}) \Big(\sum_{\alpha} S_\alpha \Big)^2 - M^2 , \tag{8.21b}$$

the energy

$$E = \sum_{\mathbf{S}} w(\mathbf{S}) H(\mathbf{S}) , \tag{8.21c}$$

and the specific heat at constant field,

$$C_B = \sum_{\mathbf{S}} w(\mathbf{S}) H^2(\mathbf{S}) - E^2 . \tag{8.21d}$$

In the limit of an infinitely large lattice ($N_{x,y} \to \infty$), it is possible to solve the Ising model exactly; discussions of the solution, originally due to Onsager, can be found in [Hu63] and [Mc73]. The expressions are simplest at $B = 0$. In this limit, the energy is given by

$$E = -N_s J (\coth 2J) \left[1 + \frac{2}{\pi} \kappa' K_1(\kappa) \right] , \tag{8.22a}$$

and the specific heat is

$$C_B = N_s \frac{2}{\pi} (J \coth 2J)^2 \left(2K_1(\kappa) - 2E_1(\kappa) - (1 - \kappa') \left[\frac{\pi}{2} + \kappa' K_1(\kappa) \right] \right) , \tag{8.22b}$$

while the magnetization is given by

$$M = \pm N_s \frac{(1 + z^2)^{1/4} (1 - 6z^2 + z^4)^{1/8}}{(1 - z^2)^{1/2}} \tag{8.22c}$$

for $J > J_c$ and vanishes for $J < J_c$. In these expressions,

$$\kappa = 2 \frac{\sinh 2J}{\cosh^2 2J} \leq 1 , \quad \kappa' = 2 \tanh^2 2J - 1 ,$$

the complete elliptic integrals of the first and second kinds are

$$K_1(\kappa) \equiv \int_0^{\pi/2} \frac{d\phi}{(1 - \kappa^2 \sin^2 \phi)^{1/2}} , \quad E_1(\kappa) \equiv \int_0^{\pi/2} d\phi \, (1 - \kappa^2 \sin^2 \phi)^{1/2} ,$$

$z = e^{-2J}$, and $J_c = 0.4406868$ is the critical value of J for which $\kappa = 1$, where K_1 has a logarithmic singularity. Thus, all thermodynamic functions are singular at this coupling, strongly suggesting a phase transition. This is confirmed by the behavior of the magnetization, which vanishes below the critical coupling (or above the critical temperature), and can take on one of two equal and opposite values above this coupling.

A numerical solution of the Ising model is useful both as an illustration of the techniques we have been discussing and because it can be generalized readily to more complicated Hamiltonians [Fo63]. Because of the large number of terms involved, a direct evaluation of the sums in Eqs. (8.21) is out of the question. (For even a modest 16×16 lattice, there are $2^{256} \approx 10^{77}$ different configurations.) Hence, it is most efficient to generate spin configurations $\mathbf{S}$ with probability $w(\mathbf{S})$ using the Metropolis algorithm and then to average the required observables over these configurations. To implement the Metropolis algorithm, we could make our trial step from $\mathbf{S}$ to $\mathbf{S}_t$ by changing all of the spins randomly. This would, however, bring us to a configuration very different from $\mathbf{S}$, and so there would be a high probability of rejection. It is therefore better to take smaller steps, and so we consider trial configurations that differ from the previous one only by the flipping of one spin. This is done by sweeping systematically through the lattice and considering whether or not to flip each spin, one at a time. Hence, we consider two configurations, $\mathbf{S}$ and $\mathbf{S}_t$, differing only by the flipping of one spin, $S_\alpha \equiv S_{ij}$. Acceptance of this trial step depends upon the ratio of the weight functions,

$$r = \frac{w(\mathbf{S}_t)}{w(\mathbf{S})} = e^{-H(\mathbf{S}_t)+H(\mathbf{S})} .$$

Specifically, if $r > 1$ or if $r < 1$ but larger than a uniformly distributed random number between 0 and 1, then the spin S_α is flipped; otherwise, it is not. From (8.18), it is clear that only terms involving S_{ij} will contribute to r, so that after some algebra, we have

$$r = e^{-2S_\alpha(Jf+B)} \; ; \; f = S_{i+1j} + S_{i-1j} + S_{ij+1} + S_{ij-1} \, .$$

Here, f is the sum of the four spins neighboring the one being flipped. Because f can take on only 5 different values, 0, ± 2, ± 4, only 10 different values of r can ever arise (there are two possible values of S_α); these can be conveniently calculated and stored in a table before the calculation begins so that exponentials need not be calculated repeatedly. Note that if we had used trial configurations that involved flipping several spins, the calculation of r would have been much more complicated.

Write a Monte Carlo code with Metropolis algorithm for a 2D Ising model (eqn. 8.18)

Grade: 4

■ **Exercise 8.8** Modify the code to compute the sweep-to-sweep correlation functions for the energy and the magnetization using (8.17). Using runs for a 16×16 lattice for $B = 0$ and for several values of J between 0.1 and 0.6, estimate the proper sampling frequency at each coupling strength. Show that the two estimates of the uncertainties in the energy and magnetization agree when a proper sampling frequency is used and that they disagree when the samples are taken too often (a reasonable group size is 10). Also show that the sweep-to-sweep correlations become stronger when the system is close to the phase transition (critical slowing down).

■ **Exercise 8.9** Run the code to obtain results for 8×8, 16×16, and 32×32 lattices at $B = 0$ for a sequence of ferromagnetic couplings from 0.1 to 0.6; pay particular attention to the region near the expected phase transition. Compare your results with the exact behavior of the infinite lattice and show that the finite size smooths out the singularities in the thermodynamic observables. Notice that the size of the magnetic domains becomes very large near the critical coupling.

Plot the equilibrium magnetic configurations for different temperatures.

Grade: 5

■ **Exercise 8.10** Use the code to explore the thermodynamics of the model for finite B and for anti-ferromagnetic couplings ($J < 0$). Also consider simulations of a model in which a given spin S_{ij} interacts with its neighbors ferromagnetically and with its diagonal neighbors S_{i-1j-1}, S_{i+1j-1}, S_{i-1j+1}, S_{i+1j+1} anti-ferromagnetically.

■ **Exercise 8.11** The "heat bath" algorithm is an alternative to the Metropolis algorithm for sampling the canonical ensemble. In this method, the particular spin being considered is set to -1 with probability $1/(1+g)$ and to $+1$ with probability $g/(1+g)$, where $g = \exp[2(Jf + B)]$. This can be interpreted as placing the spin in equilibrium with a heat bath at the specified temperature. Verify that this algorithm corresponds to putting $A = 1$ and taking

$$T(\mathbf{S} \to \mathbf{S}') = \frac{w(\mathbf{S}')}{w(\mathbf{S}') + w(\mathbf{S})}$$

in Eq. (8.16) and so leads to a correct sampling of spin configurations. Modify the code to use the heat-bath algorithm and compare its efficiency with that of the conventional Metropolis algorithm.

Deadline: April 30, 2016

Write a nice report showing all exercise steps. Define the problem, solve, plot, analyze, and conclude. Attach the codes.