```
    PRINT "temperature = "; T
    PRINT "acceptance probability = "; accept
    PRINT "mean energy per spin = "; eave
    PRINT "mean squared energy per spin = "; e2ave
    PRINT "mean magnetization per spin = "; mave
    PRINT "mean of absolute magnetization per spin = "; abs_mave
    PRINT "mean squared magnetization per spin = "; m2ave
END SUB
```

Achieving thermal equilibrium can account for a substantial fraction of the total run time. The most practical choice of initial conditions is a configuration from a previous run that is at a temperature close to the desired temperature. The following subroutine saves the last configuration of a run and can be included at the end of the main loop in `Program ising`.

```
SUB save_config(N,L,T,spin(,))
    INPUT prompt "name of file for last configuration = ": file$
    OPEN #2: name file$, access output, create new
    PRINT #2: T
    FOR y = 1 to L
        FOR x = 1 to L
            PRINT #2: spin(x,y)
        NEXT x
    NEXT y
    CLOSE #2
END SUB
```

A previous configuration can be used in a later run by adding a few statements to `SUB initial` to allow the user to choose a previous configuration or a random configuration. A previous configuration can be read by calling the following subroutine:

```
SUB read_config(N,L,T,spin(,))
    INPUT prompt "filename?": file$
    OPEN #1: name file$, access input
    INPUT #1: T
    FOR y = 1 to L
        FOR x = 1 to L
            INPUT #1: spin(x,y)
        NEXT x
    NEXT y
    CLOSE #1
END SUB
```

from Gould-Tobochnik. Solve problems 17.5 (similar to the exercise done during the course) + 17.7 (BOTH!)

Problem 17.5. Equilibration of the two-dimensional Ising model

a. Run `Program ising` with the linear dimension of the lattice $L = 16$ and the heat bath temperature $T = 2$. Determine the time, `nequil`, needed to equilibrate the system, if the directions of the spins are initially chosen at random. Plot the values of E and M after each Monte Carlo

step per spin. Estimate how many Monte Carlo steps per spin are necessary for the system to reach equilibrium.

b. Write a subroutine that shows the spin configurations on the screen. One simple way to do so is to draw a solid square about each spin site and color code the orientation of the spins. Is the system "ordered" or "disordered" at $T = 2$ after equilibrium has been established?

c. Repeat part (a) with all spins initially up. Does the equilibration time increase or decrease?

d. Repeat parts (a)–(c) for $T = 2.5$.

Problem 17.6. Comparison with exact results

In general, a Monte Carlo simulation yields exact answers only after an infinite number of configurations have been sampled. How then can we be sure our program works correctly, and our results are statistically meaningful? One check is to ensure that our program can reproduce exact results in known limits. In the following, we test `Program ising` by considering a small system for which the mean energy and magnetization can be calculated analytically.

a. Calculate analytically the T dependence of E, M, C and χ for the two-dimensional Ising model with $L = 2$ and periodic boundary conditions. (A summary of the calculation is given in Appendix 17.31.)

b. Use `Program ising` with $L = 2$ and estimate E, M, C, and χ for $T = 0.5$ and 0.25. Use the relations (17.12) and (17.14) to compute C and χ, respectively. Compare your estimated values to the exact results found in part (a). Approximately how many Monte Carlo steps per spin are necessary to obtain E and M to within 1%? How many Monte Carlo steps per spin are necessary to obtain C and χ to within 1%?

Now that we have checked our program and obtained typical equilibrium configurations, we consider the calculation of the mean values of the physical quantities of interest. Suppose we wish to compute the mean value of the physical quantity A. In general, the calculation of A is time consuming, and we do not want to compute its value more often than necessary. For example, we would not compute A after the flip of only one spin, because the values of A in the two configurations would almost be the same. Ideally, we wish to compute A for configurations that are statistically independent. Because we do not know *a priori* the mean number of spin flips needed to obtain configurations that are statistically independent, it is a good idea to estimate this time in our preliminary calculations.

One way to estimate the time interval over which configurations are correlated is to compute the time displaced *autocorrelation* function $C_A(t)$ defined as

$$C_A(t) = \frac{\langle A(t+t_0)A(t_0)\rangle - \langle A\rangle^2}{\langle A^2\rangle - \langle A\rangle^2}. \tag{17.16}$$

$A(t)$ is the value of the quantity A at time t. The averages in (17.16) are over all possible time origins t_0 for an equilibrium system. Because the choice of the time origin is arbitrary for an equilibrium system, C_A depends only on the time difference t rather than t and t_0 separately. For sufficiently large t, $A(t)$ and $A(0)$ will become uncorrelated, and hence $\langle A(t+t_0)A(t_0)\rangle \rightarrow$

$\langle A(t+t_0)\rangle\langle A(t_0)\rangle = \langle A\rangle^2$. Hence $C_A(t) \to 0$ as $t \to \infty$. In general, $C_A(t)$ will decay exponentially with t with a decay or correlation time τ_A whose magnitude depends on the choice of the physical quantity A as well as the physical parameters of the system, for example, the temperature. Note that $C_A(t = 0)$ is normalized to unity.

The time dependence of the two most common correlation functions, $C_M(t)$ and $C_E(t)$ is investigated in Problem 17.7. As an example of the calculation of $C_E(t)$, consider the equilibrium time series for E for the $L = 4$ Ising model at $T = 4$: -4, -8, 0, -8, -20, -4, 0, 0, -24, -32, -24, -24, -8, -8, -16, -12. The averages of E and E^2 over these sixteen values are $\langle E\rangle = -12$, $\langle E^2\rangle = 240$, and $\langle E^2\rangle - \langle E\rangle^2 = 96$. We wish to compute $E(t)E(0)$ for all possible choices of the time origin. For example, $E(t = 4)E(0)$ is given by

$$\begin{aligned}\langle E(t=4)E(0)\rangle = \frac{1}{12}\big[&(-20\times -4)+(-4\times -8)+(0\times 0)\\ &+(0\times -8)+(-24\times -20)+(-32\times -4)\\ &+(-24\times 0)+(-24\times 0)+(-8\times -24)\\ &+(-8\times -32)+(-16\times -24)+(-12\times -24)\big].\end{aligned} \tag{17.17}$$

We averaged over the twelve possible choices of the origin for the time difference $t = 4$. Verify that $\langle E(t = 4)E(0)\rangle = 460/3$ and $C_E(t = 4) = 7/72$.

In the above calculation of $\langle E(t)E(0)\rangle$, we included all possible combinations of $E(t)E(0)$ for a given time series. To implement this procedure on a computer, we would need to store the time series in memory or in a data file. An alternative procedure is to save the last `nsave` values of the time series in memory and to average over fewer combinations. This procedure is implemented in `SUB correl`; the correlation functions are computed and printed in `SUB c_output`. `SUB correl` uses two arrays, `Esave` and `Msave`, to store the last `nsave` values of the energy and the magnetization at each Monte Carlo step per spin. These arrays and the arrays `Ce` and `Cm` may be initialized in a separate subroutine.

```
SUB correl(Ce(),Cm(),E,M,esave(),msave(),pass,nsave)
    ! accumulate data for time correlation functions
    ! save last nsave values of M and E
    ! index0 = array index for earliest saved time
    IF pass > nsave then
       ! compute Ce and Cm after nsave values are saved
       LET index0 = mod(pass-1,nsave) + 1
       LET index = index0
       FOR tdiff = nsave to 1 step -1
           LET Ce(tdiff) = Ce(tdiff) + E*esave(index)
           LET Cm(tdiff) = Cm(tdiff) + M*msave(index)
           LET index = index + 1
           IF index > nsave then LET index = 1
       NEXT tdiff
    END IF
    ! save latest value in array position of earliest value
    LET esave(index0) = E
    LET msave(index0) = M
```

```
END SUB

SUB c_output(N,Ce(),Cm(),accum(),mcs,nsave)
    ! compute time correlation functions
    LET ebar = accum(1)/mcs
    LET e2bar = accum(2)/mcs
    LET Ce(0) = e2bar - ebar*ebar
    LET mbar = accum(3)/mcs
    LET m2bar = accum(4)/mcs
    LET Cm(0) = m2bar - mbar*mbar
    LET norm = 1/(mcs - nsave)
    PRINT
    PRINT "t","Ce(t)","Cm(t)"
    PRINT
    FOR tdiff = 1 to nsave
        ! correlation functions defined so that C(t=0) = 1
        ! and C(infinity) = 0
        LET Ce(tdiff) = (Ce(tdiff)*norm - ebar*ebar)/Ce(0)
        LET Cm(tdiff) = (Cm(tdiff)*norm - mbar*mbar)/Cm(0)
        PRINT tdiff,Ce(tdiff),Cm(tdiff)
    NEXT tdiff
END SUB
```

Problem 17.7. Correlation times

a. Choose $L = 4$ and $T = 3$ and equilibrate the system. Then look at the time series of M and E after every Monte Carlo step per spin and estimate how often M changes sign. Does E change sign when M changes sign? How often does M change sign for $L = 8$ (and $T = 3$)? In equilibrium, positive and negative values of M are equally likely in the absence of an external magnetic field. Is your time series consistent with this equilibrium property? Why is it more meaningful to compute the time displaced correlation function of the absolute value of the magnetization rather than the magnetization itself if L is relatively small?

b. Choose $L = 16$ and $T = 1$ and equilibrate the system. Then look at the time series of M. Do you find that positive and negative values of M are equally likely? Explain your results.

c. Modify `Program ising` so that the equilibrium averaged values of $C_M(t)$ and $C_E(t)$ are computed. As a check on your program, use the time series for E given in the text to do a hand calculation of $C_E(t)$ in the way that it is computed in `SUB correl` and `SUB c_output`. Choose `nsave` $= 10$.

d. Estimate the correlation times from the energy and the magnetization correlation functions for $L = 8$, and $T = 3$, $T = 2.3$, and $T = 2$. Save the last `nsave` $= 100$ values of the magnetization and energy only after the system is equilibrated. Are the correlation times τ_M and τ_E comparable? One way to determine τ is to fit $C(t)$ to an assumed exponential form $C(t) \sim e^{-t/\tau}$. Another way is to define the integrated correlation time as

$$\tau = \sum_{t=1} C(t). \tag{17.18}$$

The sum is cut off at the first negative value of $C(t)$. Are the negative values of $C(t)$ physically meaningful? How does the behavior of $C(t)$ change if you average your results over longer runs? How do your estimates for the correlation times compare with your estimates of the relaxation time found in Problem 17.5? Why would the term "decorrelation time" be more appropriate than "correlation time?"

e. To describe the relaxation towards equilibrium as realistically as possible, we have randomly selected the spins to be flipped. However, if we are interested only in equilibrium properties, it might be possible to save computer time by selecting the spins sequentially. Determine if the correlation time is greater, smaller, or approximately the same if the spins are chosen sequentially rather than randomly. If the correlation time is greater, does it still save CPU time to choose spins sequentially? Why is it not desirable to choose spins sequentially in the one-dimensional Ising model?

Problem 17.8. Estimate of errors

How can we quantify the accuracy of our measurements, for example, the accuracy of the mean energy $\langle E\rangle$? As discussed in Chapter 11, the usual measure of the accuracy is the standard deviation of the mean. If we make n independent measurements of E, then the most probable error is given by

$$\sigma_m = \frac{\sigma}{\sqrt{n-1}}, \tag{17.19}$$

where the standard deviation σ is defined as

$$\sigma^2 = \langle E^2\rangle - \langle E\rangle^2. \tag{17.20}$$

The difficulty is that, in general, our measurements of the time series E_i are not independent, but are correlated. Hence, σ_m as given by (17.19) is an underestimate of the actual error.

How can we determine whether the measurements are independent without computing the correlation time? One way is based on the idea that the magnitude of the error should not depend on how we group the data. For example, suppose that we group every two data points to form $n/2$ new data points $E_i^{(2)}$ given by $E_i^{(g=2)} = (1/2)[E_{2i-1} + E_{2i}]$. If we replace n by $n/2$ and E by $E^{(2)}$ in (17.19) and (17.20), we would find the same value of σ_m as before provided that the original E_i are independent. If the computed σ_m is not the same, we continue this averaging process until σ_m calculated from

$$E_i^{(g)} = \frac{1}{2}[E_{2i-1}^{(g/2)} + E_{2i}^{(g/2)}] \qquad (g = 2, 4, 8, \dots) \tag{17.21}$$

is approximately the same as that calculated from $E^{(g/2)}$.

a. Use the above averaging method to estimate the errors in your measurements of $\langle E\rangle$ and $\langle M\rangle$ for the two-dimensional Ising model. Let $L = 8$, $T = 2.269$, and `mcs` ≥ 16384, and calculate averages after every Monte Carlo step per spin after the system has equilibrated. If necessary, increase the number of Monte Carlo steps for averaging. A rough measure of the correlation time is the number of terms in the time series that need to be averaged for σ_m to be approximately unchanged. What is the qualitative dependence of the correlation time on $T - T_c$?