(b) Simulate the Ising model with $L = 2$ and estimate E, M, C, and χ for $T = 0.5$ and 0.25. Use the relations (15.19) to compute C. 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 to within 1%?

(c) Choose $L = 4$ and the direction of each spin at random and equilibrate the system at $T = 3$. 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 $L = 32$ (and $T = 3$)? Although the direction of the spins is initially chosen at random, it is likely that the number of up spins will not exactly cancel the number of down spins. Is that statement consistent with your observations? If the net number of spins is up, how long does the net magnetization remain positive for a given value of L?

(d) The calculation of χ is more complicated because the sign of M can change during the simulation for smaller values of L. Compare your results for χ from using (15.21) and from using (15.21) with $\langle M \rangle$ replaced by $\langle |M| \rangle$. Which way of computing χ gives more accurate results? ■

Now that you have checked your program and obtained typical equilibrium configurations, we consider in more detail 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 some cases, the calculation of A for a given configuration 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 your preliminary calculations.

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

$$C_A(t) = \frac{\langle A(t+t_0)A(t_0)\rangle - \langle A\rangle^2}{\langle A^2\rangle - \langle A\rangle^2}, \tag{15.23}$$

where $A(t)$ is the value of the quantity A at time t. The averages in (15.23) are over all possible time origins t_0. 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 $\langle A(t+t_0)A(t_0)\rangle \to \langle A(t+t_0)\rangle\langle A(t_0)\rangle = \langle A\rangle^2$. Hence, $C_A(t) \to 0$ as $t \to \infty$. Also, $C_A(t=0)$ is normalized to unity. 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.

The time dependence of the two most common correlation functions $C_M(t)$ and $C_E(t)$ is investigated in Problem 15.14. As an example of the calculation of $C_E(t)$, consider the equilibrium time series for E for the $L = 4$ Ising model on the square lattice 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, $E(4)E(0)$ is given by

$$\begin{aligned}\langle E(4)E(0)\rangle = \frac{1}{12}[&(-20\times -4)+(-4\times -8)+(0\times 0)\\ &+(0\times -8)+(-24\times -20)+(-32\times -4)\\ &+(-24\times 0)+(-24\times 0)+(-8\times -24)\\ &+(-8\times -32)+(-16\times -24)+(-12\times -24)].\end{aligned} \tag{15.24}$$

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

To implement this procedure on a computer, we could store the time series in memory, if it is not too long, or save it in a data file. You can save the data for $M(t)$ and $E(t)$ by pressing the `Save XML` menu item under the `File` menu on the frame containing the plots for $M(t)$ and $E(t)$. The class `IsingAutoCorrelatorApp` in Listing 15.6 reads in data created by the `IsingApp` class. Method `computeCorrelation` computes the mean and mean square of the magnetization and the energy, which are needed to compute C_M and C_E as defined in (15.23). Then it computes the time displaced autocorrelation for all possible choices of t_0.

Listing 15.6 Listing of class for computing autocorrelation function of M and E.

```
package org.opensourcephysics.sip.ch15;
import java.util.*;
import javax.swing.*;
import org.opensourcephysics.controls.*;
import org.opensourcephysics.display.*;
import org.opensourcephysics.frames.*;

public class IsingAutoCorrelatorApp extends AbstractCalculation {
   PlotFrame plotFrame = new PlotFrame("tau",
        "<E(t+tau)E(t)> and <M(t+tau)M(t)>", "Time correlations");
   double[] energy = new double[0], magnetization = new double[0];
   int numberOfPoints;

   public void calculate() {
      computeCorrelation(control.getInt("Maximum time interval, tau"));
   }

   public void readXMLData() {
      energy = new double[0];
      magnetization = new double[0];
      numberOfPoints = 0;
      String filename = "ising_data.xml";
      JFileChooser chooser = OSPFrame.getChooser();
      int result = chooser.showOpenDialog(null);
      if(result==JFileChooser.APPROVE_OPTION) {
         filename = chooser.getSelectedFile().getAbsolutePath();
      } else {
         return;
      }
      XMLControlElement xmlControl = new XMLControlElement(filename);
```