In general we don't know this value, which makes it difficult to perform the fit. It is possible to guess T_c and then vary the guess to make the line in Figure 8.5 as close to straight as possible. However, this process is highly susceptible to error. The curvature which is already present in the line as we move away from T_c can be particularly misleading when we are trying to gauge the straightness of the line, and it also turns out that rather small miscalculations in the value of T_c can lead to large errors in the measured critical exponent.

There are also other reasons for avoiding the direct method of measuring exponents. It requires simulations of rather high accuracy to give reasonable results, and it requires us to work with large systems to avoid problems with "finite size effects" (see below). In short, the method is to be avoided. In its place another technique has been developed which circumvents all of these problems: finite size scaling.

8.3.2 The finite size scaling method

The finite size scaling method is a way of extracting values for critical exponents by observing how measured quantities vary as the size L of the system studied changes. In fact, we saw a simple version of finite size scaling in action in Chapter 4, where we used it to calculate the dynamic exponent of a number of different algorithms for simulating the Ising model by measuring the correlation time τ for systems of a variety of different sizes. However, the techniques we used for those calculations required that we perform simulations exactly at the critical temperature of the model, which in turn requires us to know T_c. In the case of the Ising model we know T_c in two dimensions from the exact solution of the model. In some other cases we may be able to apply a method such as the invaded cluster algorithm of Section 4.4.4 to calculate T_c. However, in most cases we do not know T_c, which means that the simple method of Chapter 4 will not work. We now describe a more sophisticated version of the finite size scaling technique which not only does not require us to know T_c, but in fact returns a value of T_c itself, as well as giving us estimates of the critical exponents. We illustrate the technique for the case of the susceptibility exponent γ.

We begin, as we did in Section 4.1, by expressing the quantity of interest in terms of the correlation length ξ of the system. In this case the quantity of interest is the magnetic susceptibility. Eliminating $|t|$ from Equations (8.41) and (8.42) we get

$$\chi \sim \xi^{\gamma/\nu} \tag{8.45}$$

in the vicinity of the phase transition. Now, consider what happens in a system of finite size L, such as we use in our Monte Carlo simulations. In finite systems, as depicted in Figure 4.1, the correlation length is cut off as it approaches the system size, so that the susceptibility χ will also be cut

off; in systems of finite size the susceptibility never actually diverges. We can express this cut-off mathematically as follows. If we continue to denote by ξ the value which the correlation length *would* have in an infinite system at temperature t, then the cut-off takes place when $\xi > L$. As long as $\xi \ll L$ the value of χ should be the same as that for the infinite system. We can express this by writing

$$\chi = \xi^{\gamma/\nu}\chi_0(L/\xi), \tag{8.46}$$

where χ_0 is a dimensionless function of a single variable which has the properties

$$\chi_0(x) = \text{constant} \qquad \text{for } x \gg 1 \tag{8.47}$$

and

$$\chi_0(x) \sim x^{\gamma/\nu} \qquad \text{as } x \to 0. \tag{8.48}$$

The precise way in which the susceptibility gets cut off close to T_c is contained in the functional form of χ_0. It is this function which we will measure in our Monte Carlo simulations.

Equation (8.46) in fact contains all the information we need about the behaviour of our system with varying system size. However, it is not in a very useful form, since it still contains the variable ξ, the correlation length at temperature t in the infinite system, which we don't know. For this reason it is both conventional and convenient to reorganize the equation a little. Defining a new dimensionless function $\tilde{\chi}$ thus:

$$\tilde{\chi}(x) = x^{-\gamma}\chi_0(x^{\nu}). \tag{8.49}$$

and making use of Equation (8.41), we get

$$\chi = L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}|t|). \tag{8.50}$$

In fact, to be strictly correct, we should have two equations such as this, one for positive and one for negative values of t with different functions $\tilde{\chi}$, since the behaviour of χ is not symmetric on the two sides of the phase transition. However, we can easily combine these two equations into one by extending the definition of $\tilde{\chi}(x)$ to negative values of x. Then we can write

$$\chi = L^{\gamma/\nu}\tilde{\chi}(L^{1/\nu}t). \tag{8.51}$$

This is the basic equation for the finite size behaviour of the magnetic susceptibility. It tells us how the susceptibility should vary with system size L for finite systems close to the critical temperature. Note that we have derived this equation for the susceptibility *per spin* as defined in Section 1.2.2. If we were to use the extensive susceptibility, the leading power of L would be $L^{\gamma/\nu+d}$ instead of just $L^{\gamma/\nu}$, where d is the dimensionality of the system. It is very important to recognize this distinction if you want to get the

correct answers for exponents using the finite size scaling method. All the equations given in this section are correct for intensive quantities but need to be modified if you are going to use extensive ones.[8]

Equation (8.51) contains the unknown function $\tilde{\chi}(x)$ which we call the **scaling function** for the susceptibility. Although the scaling function is unknown, there are certain things we do know about it. Equation (8.48) tells us that

$$\tilde{\chi}(x) \to x^{-\gamma}(x^{\nu})^{\gamma/\nu} = \text{constant} \qquad \text{as } x \to 0. \tag{8.52}$$

In other words, $\tilde{\chi}$ is finite at the origin, which in this case means close to the critical temperature. Another important point is that, by design, all the L-dependence of χ is displayed explicitly in Equation (8.51); the scaling function does not contain any extra hidden dependence on L which is not accounted for. In other words, if we measure $\tilde{\chi}(x)$ we should get the same result regardless of the size of the system. It is this last fact that allows us to use Equation (8.51) to calculate the exponents γ and ν and the value of the critical temperature.

Suppose we perform a set of Monte Carlo calculations of the system of interest for a variety of different system sizes L over a range of temperatures close to where we believe the critical temperature to be. (With this method we do not need to be exactly at the critical temperature, only in the rough vicinity. We can estimate where this region is by, for example, looking for the tell-tale peak in the magnetic susceptibility or the specific heat—see Figure 3.10.) For each system size, we measure the magnetic susceptibility $\chi_L(t)$ at a set of temperatures t. We can now rearrange Equation (8.51) thus

$$\tilde{\chi}(L^{1/\nu}t) = L^{-\gamma/\nu}\chi_L(t), \tag{8.53}$$

to get an estimate of the scaling function $\tilde{\chi}$ for several different values of the scaling variable

$$x = L^{1/\nu}t \tag{8.54}$$

for each system size. Since the scaling function is supposed to be the same for all system sizes, these estimates should coincide with one another—they should all fall on the same curve if we plot them together on one graph. However—and this is the crucial point—this will only happen if we use *the correct values* of the exponents γ and ν in Equation (8.53). Also, although it's not immediately obvious from the equation, we must use the correct value of the critical temperature T_c, which enters in the calculation of the reduced temperature t through Equation (8.40). The idea behind finite size scaling therefore is to calculate $\tilde{\chi}(x)$ for each of our different system sizes,

[8]The reader might be interested to work out where in the preceding derivation the extra powers of L would come in if we were to use the extensive susceptibility.

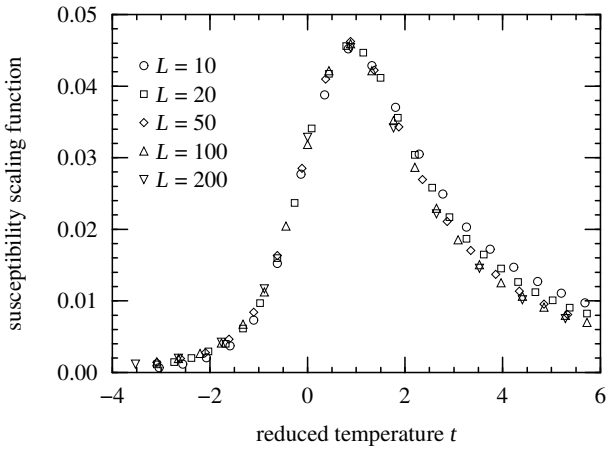

FIGURE 8.6 Data collapse of magnetic susceptibility data for the two dimensional Ising model. The points are taken from Monte Carlo measurements of the susceptibility for five different sizes of system as indicated. From this collapse we find $\gamma = 1.76$, $\nu = 1.00$ and $T_c = 2.27J$. Notice that the collapse fails once we get sufficiently far away from the critical temperature ($t = 0$).

and then vary the exponents γ and ν and the critical temperature until the resulting curves all fall or **collapse** on top of one another. An example of such a calculation is shown for the two-dimensional Ising model in Figure 8.6. Here we performed simulations around the critical temperature for square systems of size $L = 10$, 20, 50, 100 and 200. The best data collapse is obtained when $\gamma = 1.76 \pm 0.01$, $\nu = 1.00 \pm 0.05$ and $T_c/J = 2.27 \pm 0.01$. These values are in good agreement with the exact known values of $\gamma = \frac{7}{4}$, $\nu = 1$ and $T_c = 2.269J$. (The error bars are quite rough here, calculated by estimating the region over which the collapse appears optimal. Error estimation is discussed in more detail in the following section.)

This method can easily be extended to quantities other than the susceptibility. For the Ising model for example, we can derive scaling equations similar to (8.51) for the specific heat and the magnetization by arguments closely similar to the ones given above. The results are:

$$c = L^{\alpha/\nu}\tilde{c}(L^{1/\nu}t), \tag{8.55}$$

$$m = L^{-\beta/\nu}\widetilde{m}(L^{1/\nu}t). \tag{8.56}$$

Performing data collapses using these equations yields values for α and β, as well as values for ν and T_c again. (If we perform collapses for a number of different quantities, we can use the several values of ν and T_c which

we get as a consistency check on the different calculations.) Note the different sign in (8.56), which arises from the definition of the exponent β in Equation (8.44).

8.3.3 Difficulties with the finite size scaling method

Although the basic finite size scaling method outlined in the last section often works extremely well, there are nonetheless a number of problems with the method as described. How, for instance, are we to assess the errors on our critical exponents? In the example above, we gauged by eye when the various curves best fit one another and took our values for the critical exponents and critical temperature at that point. The errors were estimated by judging (again by eye) the range of values of the exponents over which the collapse appears equally good. When the collapse begins to look significantly poorer, we have reached the limits of the acceptable values of the exponents. A more thorough method of error estimation is to use one of the techniques discussed in Section 3.4, such as bootstrap resampling. By resampling our data a number of times and repeating the data collapse for each resampled data set, we can estimate the errors from the variation in the values of the exponent from one set to another. In order to do this however, it helps greatly if we have a quicker way of performing the data collapse than simply fiddling with values of the exponents until it looks good. This brings us on to another problem. Performing the collapse by eye is, after all, hardly a very scientific way to proceed. It is much better if we can construct a quantitative measure of the quality of our data collapse. One such measure is the variance of the set of curves, integrated over a range of values of x close to criticality. In the case of the susceptibility for instance, we could calculate

$$\sigma^2 = \frac{1}{x_{\max} - x_{\min}} \int_{x_{\min}}^{x_{\max}} \sum_L \tilde{\chi}_L^2(x) - \Big[\sum_L \tilde{\chi}_L(x)\Big]^2 \mathrm{d}x. \tag{8.57}$$

This however is a little difficult to estimate, since the points at which the scaling function is evaluated are different for each system size. What we need is some way of interpolating between these points, and the perfect technique is provided by the multiple histogram method of Section 8.2. If we use this method, then we can directly evaluate (8.57) by using for example a simple trapezium rule integration (or any other form of numerical integration that we happen to favour) and then minimize it to give an estimate of the critical exponents and T_c. Bootstrapping then gives an estimate of our statistical errors.

There is still a problem however, which is evident in Figure 8.6: if we stray too far from the critical temperature, our scaling equation (8.51) is no longer correct, simply because we are no longer in the critical region.

Furthermore, the range of values of the scaling variable, Equation (8.54), over which the critical region extends varies as a function of L, so that the region over which it is safe to perform our data collapse depends on the size of the systems studied. How are we to estimate the extent of this region? There are a couple of commonly used methods. One is to perform a series of collapses over smaller and smaller ranges Δx and extrapolate the results to the limit $\Delta x \to 0$. In order to use this method, we need to choose a point x_0 about which to centre our data collapse. The standard choice is to set x_0 to be the point at which the scaling function (or equivalently the susceptibility or other quantity of interest) is a maximum. (For scaling functions such as $\widetilde{m}$ which are monotonic and therefore do not have a maximum, we choose x_0 to be the point at which the scaling function has its steepest gradient.) Note that the maximum in the scaling function is not at the critical temperature $t = 0$ (see Figure 8.6). This is a reflection of the fact that the maximum of the susceptibility (or specific heat, or whatever) is also not precisely at the critical temperature, except in an infinite system. However, the maximum of the susceptibility (and hence the scaling function) does correspond approximately to the maximum value of the correlation length in the finite system and hence marks roughly the centre point of the critical region, which makes it a good choice for x_0.

Now if we perform our data collapse, Equation (8.57), over a range from $x_{\min} = x_0 - \Delta x$ to $x_{\max} = x_0 + \Delta x$, make an estimate with errors of the critical exponents, and then repeat the calculation for successively smaller values of Δx, we can extrapolate the result to the limit $\Delta x \to 0$ by making a weighted fit through the resulting data points. The authors used this technique, for example, in a calculation of the critical exponents for the random-field Ising model of Section 6.1.1 (Newman and Barkema 1996). In Figure 8.7 we have reproduced the results for the exponents ν and γ. The quantities measured directly by the data collapse are $1/\nu$ and γ/ν. The extrapolation to $\Delta x = 0$ was done in this case by the weighted fit of a quadratic to the data points, giving $1/\nu = 0.98 \pm 0.06$ and $\gamma/\nu = 1.85 \pm 0.07$. This in turn gives us values of $\nu = 1.02 \pm 0.06$ and $\gamma = 1.89 \pm 0.13$ for the exponents themselves.

Another common method for circumventing the question of the size of the critical region is to perform the data collapse at only one point, the point x_0 at which the scaling function is a maximum (or has maximum gradient in the case of the magnetization). This is clearly less accurate than the method described above, but in many cases, especially when the accuracy of our Monte Carlo data is good, it gives perfectly adequate results. With this method we can use either the single or multiple histogram method to calculate the temperature T_0 at which the quantity of interest (susceptibility for example) is greatest, which is also the point at which the corresponding scaling function is greatest. We repeat this for each system size L. Since

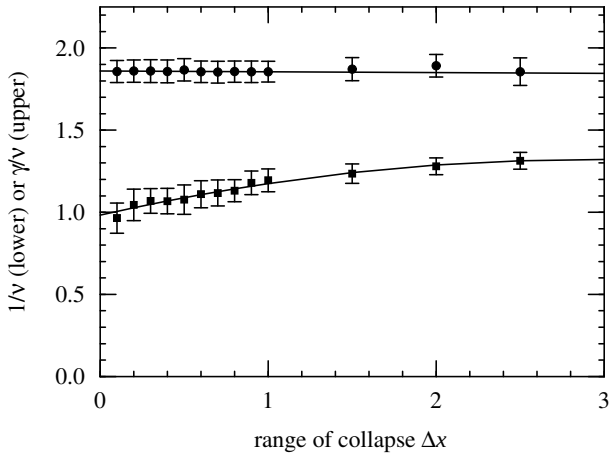

FIGURE 8.7 Calculation of critical exponents for the random-field Ising model by collapsing data over successively smaller ranges Δx. The limit as $\Delta x \to 0$ gives us the values of the exponents. In this case the method measures the quantities $1/\nu$ and γ/ν. The end result is $\nu = 1.02 \pm 0.06$ and $\gamma = 1.89 \pm 0.13$. After Newman and Barkema (1996).

the scaling function is the same for each system size, the values x_0 of the scaling variable at which we find these maxima should be the same for all system sizes. From Equations (8.40) and (8.54) we see that the temperature T_0 corresponding to x_0 is given by

$$T_0 = T_c(1 + x_0 L^{-1/\nu}). \tag{8.58}$$

Thus, if we plot T_0 against $L^{-1/\nu}$, the resulting points should lie on a straight line, provided we use the correct value of ν. And the intercept of this line with the vertical axis gives us an estimate of T_c. So, for example, we can fit our data points to a straight line using a least-squares fit, and minimize the variance on the fit to give the best straight line. The result is an estimate of both ν and the critical temperature. As before, we can use any of our standard methods of error estimation to calculate the errors on these values.

Once we have estimated ν and T_c in this fashion, we can use them to make estimates of the values of the other exponents. Since the scaling function is the same for all system sizes, its value $\tilde{\chi}(x_0)$ at x_0 should be independent of L. The value of the susceptibility at its maximum should therefore take the particularly simple form

$$\chi_L(T_0) \propto L^{\gamma/\nu}, \tag{8.59}$$

with $\tilde{\chi}(x_0)$ being the constant of proportionality. Thus if we plot the maximum value of χ as a function of L on logarithmic scales we should again get

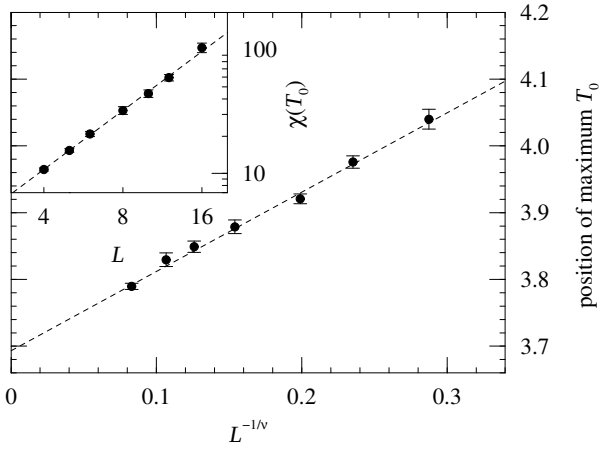

FIGURE 8.8 An illustration of finite size scaling in the random-field Ising model using only one point on the scaling function. The main figure shows the calculation of the exponent ν. The inset shows the calculation of γ. The results in this case were $\nu = 1.1 \pm 0.2$, $\gamma = 1.7 \pm 0.2$. After Rieger (1995).

a straight line. The slope of this line gives us a measure of γ/ν, and hence γ, since we already know ν. We can calculate an error on our figure just as before.

In Figure 8.8 we show an example of the application of this method, again to the random-field Ising model, taken from Rieger (1995). The main figure shows the calculation of ν and T_c from Equation (8.58) and the inset shows the calculation of γ. The results for the exponents, $\nu = 1.1 \pm 0.2$ and $\gamma = 1.7 \pm 0.2$, are in respectable agreement with those from the other method.

A third problem with the finite size scaling method as we have described it here is that scaling equations such as Equation (8.51) are only approximate, even close to the critical point. In particular, the arguments leading to the scaling equations are only valid for sufficiently large system sizes. If the system size L becomes small—how small depends on the particular model being studied—there are correction terms in the equations which become important. These terms can lead to systematic errors in the values of our exponents if they are not taken into account in the analysis. In fact, except for very high-resolution studies, such corrections are usually not important. Furthermore, a detailed discussion of them would take us some way away from the Monte Carlo simulations which are the principal topic of this book. For more information on corrections to the scaling forms discussed here, we therefore refer the reader to other sources. For the case of the normal Ising

model a good discussion has been given by Ferrenberg and Landau (1991). Binder and Heermann (1992) also cover the subject in some detail.

8.4 Monte Carlo renormalization group

A completely different approach to the calculation of critical exponents and critical temperatures is the **Monte Carlo renormalization group** method pioneered by Swendsen (1979, 1982) and others, based on the renormalization group ideas introduced in the early 1970s by Wilson and Fisher (1972, Wilson and Kogut 1974, Fisher 1974). This method is often more accurate than the finite size scaling method of the last section for the same expenditure of computational effort, and furthermore it only requires us to perform simulations for one system size, or at most two. Its main disadvantage is that it contains some rather poorly controlled approximations which make it difficult to estimate accurately the errors in our values for the critical exponents. Nevertheless, for many problems it is sufficiently superior to the finite size scaling method that we would recommend it as the method of choice for the calculation of critical properties.

The developments of this section will require us to learn a little about the ideas behind the renormalization group. We will not go into the subject in great depth however, and we would encourage those interested in learning more to consult one of the many books devoted to the topic.

8.4.1 Real-space renormalization

Despite its formidable-sounding name, real-space renormalization is really quite simple. Here we first describe how it can be used to calculate the critical temperature of a system. In Section 8.4.2 we describe the calculation of critical exponents.

The fundamental concept behind the real-space renormalization method is that of **blocking**,[9] whereby the spins or other degrees of freedom on a lattice are grouped into blocks to form a coarser lattice. Consider the configurations of the ordinary two-dimensional Ising model shown in Figure 8.9. In the first frame we show a state of the model on a 16×16 square lattice, with the black and white squares representing up- and down-spins respectively. The frame next to it shows the result of performing a blocking procedure on this state: we group the spins into blocks of four and in the blocked system we represent each such block by just one bigger **block spin**. In this case the value of this spin is assigned by majority voting amongst the spins making up the block. That is, we set it to point up or down depending on whether

[9] Not to be confused with the error estimation technique of the same name introduced in Section 3.4.2.