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- (8) Perform the two-parameter fit (3.124) for the  $\beta_c(L)$  values of table 3.16 to obtain the  $L \to \infty$  estimate given in the text.
- (9) Check for assignments 1, 2, 3, 4 and 7 (L = 24), whether the assumption that the binned data are Gaussian distributed passes the upper and lower one-sided Kolmogorov tests (2.142). This is best done by running the program ana\_kol.f of ForProg/MC\_Potts in the folders of assignments 1, 2, 3, 4 and 7, where the parameter and data files ought to be located. For the interpretation compare assignment 3 in section 2.6.4.

# 3.5 Specific Heat, Reweighting, Error Bars and Jackknife

With  $\widehat{E} = \langle E \rangle$  the **specific heat** is defined by

$$C = \frac{d\hat{E}}{dT} = \beta^2 \left( \langle E^2 \rangle - \langle E \rangle^2 \right) . \tag{3.126}$$

The last equal sign follows by working out the temperature derivative in (3.2) and is known as **fluctuation-dissipation theorem**. It is often used to estimate the specific heat from equilibrium simulations without relying on numerical derivatives. An equivalent formulation is

$$C = \beta^2 \left\langle \left( E - \widehat{E} \right)^2 \right\rangle \tag{3.127}$$

as is easily shown by expanding  $\left(E - \hat{E}\right)^2$  and working out the expectation values. Defining

$$act2lm = {\overline{iactm^2} \over mlink}$$
, (3.128)

and using the relation with the energy (3.116), we have instead of (3.126) a notation, which is close to the computer code:

$$C = \frac{\beta^2 N d^2}{n} \sum_{i=1}^{n} \left( \texttt{act2l}_i - \texttt{act1m}^2 \right), \qquad (3.129)$$

where the sum is over all measurements in the times series. Translating (3.127) similarly gives

$$C = \frac{\beta^2 N d^2}{n} \sum_{i=1}^{n} (\text{actl}_i - \text{actlm})^2.$$
 (3.130)

When energy histograms are available, (3.130) is calculated by the equations used in potts\_mu2.f of ForLib.

In the limit of an infinite statistics specific heat estimates from all these equation agree. But with a finite statistics a number of problems emerge. In the simple binning approach (1.133), where **nrpt** of the production run defines the number of blocks, one may want to use for  $\hat{E}$  estimators  $\overline{E}_i$  which are constructed from the histograms of the blocks. With  $N_b$  the number of data in each bin and  $H_i$  the energy histogram of block *i*:

$$\overline{E}_i = \frac{1}{N_b} \sum_{j \in \text{block}(i)} E_j = \frac{\sum_E E H_i(E)}{\sum_E H_i(E)} .$$
(3.131)

Estimates of  $\overline{C}_i$  from either equation (3.126) or (3.127) agree then and Gaussian error bars are expected due to the binning. However, for a not so good statistics as bias towards too small  $\overline{C}_i$  values is occurs, because  $E_j$ and  $\overline{E}_i$  come from the same block in the estimate

$$\overline{C}_{i} = \frac{\beta^{2}}{N_{b}} \sum_{j \in \text{block}(i)} \left( E_{j}^{2} - \overline{E}_{i}^{2} \right) = \frac{\beta^{2} \sum_{E} \left( E^{2} - \overline{E}_{i}^{2} \right) H_{i}(E)}{\sum_{E} H_{i}(E)} (3.132)$$
$$= \frac{\beta^{2}}{N_{b}} \sum_{j \in \text{block}(i)} \left( E_{j} - \overline{E}_{i} \right)^{2} = \frac{\beta^{2} \sum_{E} (E - \overline{E}_{i})^{2} H_{i}(E)}{\sum_{E} H_{i}(E)} . \quad (3.133)$$

The  $\overline{E}_i$  estimators are certainly inferior to the estimate  $\overline{E}$ , which relies on the entire statistics. Therefore, one may consider to use  $\overline{E}$  instead of  $\overline{E}_i$  in equations (3.132) and (3.133). However, then one does not know anymore how to calculate the error bar of  $\overline{C}$  as the  $\overline{C}_i$  estimates would rely on overlapping data. The situation gets even worse when we include reweighting (3.33), as this non-linear procedure implies that the estimators (3.132) and (3.133) will in general differ. These difficulties are overcome by the jackknife method of chapter 2.7. When histograms can be used the fast way to create jackknife bins is to sum first the entire statistics (HSUM in the code):

$$H(E) = \sum_{i=1}^{N_b} H_i(E) . \qquad (3.134)$$

Subsequently jackknife histograms (superscript J) are defined by

$$H_i^J(E) = H(E) - H_i(E)$$
(3.135)

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Fig. 3.8 Energy histogram from random sampling of the 2d Ising model on a  $4 \times 4$  lattice together with is reweighting to  $\beta_0 = 0.2$  and  $\beta_0 = 0.4$  (see assignment 1).

and jackknife estimates  $\overline{C}_i^J$  are obtained by using  $H_i^J(E)$  instead of  $H_i(E)$  in equations (3.131), (3.132) and (3.133).

In the following we compare results obtained by several variants of simple binning to those of the jackknife method. To pin down the subtleties of the statistical analysis we first consider the rather extrem case of reweighting of random sampling on a lattice which is small enough to allow for the calculation of its partition function at all temperatures. Afterwards we perform a canonical simulations of the 2D Ising model on larger lattices and reweight the specific heat to a small neighbourhood of the simulation temperature.

# 3.5.1 Reweighting of random sampling

To illustrate the jackknife method, we consider again reweighting of random sampling. On a  $4 \times 4$  lattice the Ising model has  $2^{16} = 65536$  states. This

is small enough to generate them all by random sampling. For the large statistics of assignment 1 figure 3.8 depicts on a log scale the histogram of random sampling together with its reweighting to  $\beta_0 = 0.2$  and  $\beta_0 = 0.4$ . As all energies are covered we are able to calculate the specific heat at all temperatures. If the statistics is very large, simple binning gives reliable results. However, problems are encountered when the statistics covers some states barely.

Table 3.17 Calculation of the specific heat by reweighting of random sampling for the Ising model on a  $4 \times 4$  lattice (assignments 2 to 4).

Statistics:	(a) $32 \times 30000$		$32 \times 310^8$		10000  times (a)	
	Estimate	Q	Estimate	Q	Estimate	Q
Simple binning:						
C	$x.xxx\left( xx ight)$	x.xx	x.xxxxx(xx)	x.xx	-	_
with mean from entire statistics:						
C via (3.129)	$x.xx\left(xx ight)$	x.xx	$x.xxxx\left( xx ight)$	x.xx	-	_
C via (3.130)	x.xxxx(xx)	x.xx	x.xxxxx(xx)	x.xx	x.xxxxx(xx)	0.00
Jacknife binning:						
C	x.xxxx(xx)	x.xx	x.xxxxx(xx)	x.xx	x.xxxxx(xx)	x.xx
bias corrected	x.xxxxx(xx)	x.xx	x.xxxxxx(xx)	x.xx	x.xxxxxx(xx)	x.xx

In assignment 2 we generate the rather small statistics of  $32 \times 30\,000$  sweeps. Resulting estimates of the specific heat are shown in column two of table 3.17. First simple binning is used as in equations (3.132) and (3.133), which are identical as the  $E_j$  and  $\overline{E}_i$  rely on the same measurement for each bin. The estimate is unsatisfactory, because comparison with the exact result

# C = 0.812515

from ferdinand.f (3.16) gives Q = 0.00 for the Gaussian difference test (2.33). We try to improve on this by using the average energy  $\overline{E}$  of the entire statistics in equations (3.132) and (3.133), which are then non longer identical. In the table the computer notation of these equation, (3.129) and (3.130), is quoted. The observation is that (3.129) fails entirely, while the estimate from (3.130) is good. The bad estimate comes because the error of the fluctuations of the second moment used in (3.129) are large, whereas the reduced second moment used in (3.130) enforces a positive result with smaller fluctuations. In either case  $\overline{E}$  is entered without statistical error, because its fluctuations are small compared to those of  $E_i$ .

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Fig. 3.9 Empirical peaked distribution function of three estimators of the specific heat of the Ising model as discussed in the text.

To demonstrate that the bad estimator does still converge towards the exact result we increase in assignment 3 our statistics by a factor of 1 000. As shown in column 4 of the table, the value has become reasonable when compared with the exact result, but the error bar is five times larger than for the other estimators, which agree very well with one another. Independently of any increase of the statistics the fluctuations of the bad estimator stay to large, because they are calculated with respect to zero instead of  $\overline{E}$ .

Using jackknife bins, the estimates (3.129) and (3.130) ar identical again, and the goodness of fit is satisfactory. However, it remains inconclusive whether there is an advantage compared to the simple binning estimates (3.130) in column two. Also, there is no improvement when we use equation (2.168) to correct for the bias (we keep the error bars of the jackknife estimators as the bias turns out to be small compared to them, so that a next level jackknife analysis is not necessary). The results are so close to one another that we cannot draw conclusions about the quality of the

estimators from a single low statistics run. To get to the bottom of this we repeat 10 000 times in assignment 4 the low statistics simulation of assignment 2. From these simulation averages and error bars with respect to the 10 000 repetitions are given in column 6 of table 3.17. Only the bias corrected jackknife estimator averages to an acceptable value. The uncorrected jackknife estimator comes in second and the good simple binning estimate third. Figure 3.9 depicts the empirical peaked distribution functions (1.46) of these estimates. As there is no disadvantage in applying jackknife instead of simple binning: The jackknife method should in essence always be used.

## 3.5.2 Reweighting of a canonical simulation

In real applications reweighting is mostly of importance when one wants to locate maxima of observables such as the specific heat. In assignment 5 canomnical MC simulations are performed at for the 2*d* Ising model at  $\beta = 0.43$ , which is relatively close to  $\beta_c$ . After reweighting bias corrected jackknife estimates of the specific heat are calculated and plotted in figure 3.10.

Maxima of the specific heat are clearly within the reweighting range and the peak is more pronounced on the larger lattice. On the other hand the reweighted values start to deviate on the larger lattice from the exact curve at the boundary of the chosen  $\beta$  range. That reflects the shrinking of the reweighting range with increasing lattice size. A fit of the *L* depence of the location of the peak allows, however, to determine a good value for the simulation temperature on the next larger lattice and so one. FSS investigation can be performed by iterating such a process. After introducing more advanced simulation algorithms FSS techniques are discussed in chapter 7.4.

## 3.5.3 Assignments for section 3.5

As in the previous assignment sections we use always Marsaglia random number with their default seed.

(1) Repeat the reweighting to  $\beta_0 = 0.2$  of assignment 2 of section 3.1 on a  $4 \times 4$  lattice. Reweight also to  $\beta_0 = 0.4$ . Increase the statistics by a factor of ten. Markov Chain Monte Carlo

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Fig. 3.10 Specific heat of the Ising model on  $L \times L$  lattices. Exact result produced by the program ferdinand.f (3.16) versus reweighting of simulations from  $\beta = 0.43$ .

- (2) Use random sampling to create a statistics of 32 × 30 000 sweeps for the 2d Ising model on on a 4 × 4 lattice. Reweight to β<sub>0</sub> = 0.4 and perform the following estimates: actlm using simple binning, actlm from all data, C using simple binning, C using (3.129) with simple binning and actlm from all data, C using (3.130) with simple binning and actlm from all data, C from jackknife binning, and the bias corrected C.
- (3) Increase the statistics of the previous assignment to  $32 \times 310^8$  and show that all estimators give now reasonable results. But are their error bars consistent in the sense of the F-test. If not, which of the error bars should one trust?
- (4) Repeat 10 000 times the analysis of assignment 2 for the good estimator of simple binning, the jacknife and the biased improved jackknife estimator. Compute mean values and their standard deviations with respect to the 10 000 events in each case.

(5) Use the Metropolis algorithm to simulate the Ising model on  $10 \times 10$ and  $20 \times 20$  lattices at  $\beta = 0.43$ . Reweight to the  $\beta_0$  range [0.38:0.48]and plot bias corrected jackknife estimates of the specific heat together with the exact result for  $C(\beta)$ . For the  $20 \times 20$  lattice: Compare the estimates of actlm from simple binning and from jackknife binning (a) at  $\beta = 0.43$  (no reweighting) and (b) at  $\beta = 0.40$  (reweighting).

#### 3.6 Continuous Systems

MC simulations of systems with continuous variables face additional difficulties. Histogramming of the observables leads to discretization errors and it is better to keep the time series. However, keeping too many data can slow down the code and exhaust available storage facilities. One may also become concerned that the discretization of the Marsaglia random numbers will matter. Any resolution smaller than  $\epsilon_{\text{Marsaglia}} = 2^{-24} = 1/16,777,216$ needs special attention and one may want to employ ranmar2.f (1.22). Another complication is that rounding errors may limit the bit by bit reproducibility of our numerical results, see below.

To give an impression about dealing with continuous systems, we consider simulations of O(n),  $n \ge 2$  spin systems in  $d \ge 1$  dimensions. The systems are defined by equations (3.64) to (3.67), only that we allow now for **n-component spins**, instead of just for n = 3 (n = 1 is the Ising model). Of particular physical interest are the cases n = 3, which we introduced in section 3.2.2, and the n = 2 planar rotator, also called XY model. According to Kosterlitz and Thouless (1973); Kosterlitz (1974) there exists a low temperature phase of the d = 2 planar rotator which is characterized by a power law decay in the pair correlation function, modified by the presence of pairs of vortices. The vortex pairs unbind at the critical temperature to create a high temperature phase where the correlations decay exponentially. In this way the transition does not violate the *theorem* by Mermin and Wagner (1966), which forbids spontaneous breaking of a continuous symmetry in two dimensions. Coleman (1973)] explains the rationale behind the Mermin-Wagner theorem as follows: The breaking of a continuous symmetry leads to massless Goldstone bosons, but this is not possible in two dimensions where the massless scalar field fails to exist.

It is straightforward to write an O(n) Metropolis code for generic  $n \ge 2$  values, see the next subsection. The code illustrates the simplicity of