3.5 Specific Heat, Reweighting, Error Bars and Jackknife

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

$$C \;=\; \frac{d\,\widehat{E}}{d\,T} \;=\; \beta^2\,\left(\langle E^2\rangle - \langle E\rangle^2\right)\;. \tag{3.126}$$

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 $\left(E - \widehat{E}\right)^2$ and working out the expectation values. Defining

$$\texttt{act2l} = \overline{\left(\frac{\texttt{iact}}{\texttt{mlink}}\right)^2}\,, \tag{3.128}$$

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

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

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

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

When energy histograms are available, (3.130) is calculated by the equations used in `potts_mu2.f` of `ForLib`.

In the limit of infinite statistics specific heat estimates from these equations agree. With finite statistics a number of problems emerge. In the simple binning approach, where `nrpt` of the production run defines the number of blocks, one may want to use for $\widehat{E}$ 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:

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

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 a bias towards too small $\overline{C}_i$ values occurs, because E_j and $\overline{E}_i$ come from the same block in the estimate

$$\overline{C}_i = \frac{\beta^2}{N_b} \sum_{j \in \text{block}(i)} \left(E_j^2 - \overline{E}_i^2 \right) = \frac{\beta^2 \sum_E \left(E^2 - \overline{E}_i^2 \right) H_i(E)}{\sum_E H_i(E)} \tag{3.132}$$

$$= \frac{\beta^2}{N_b} \sum_{j \in \text{block}(i)} \left(E_j - \overline{E}_i \right)^2 = \frac{\beta^2 \sum_E (E - \overline{E}_i)^2 H_i(E)}{\sum_E H_i(E)} \ . \tag{3.133}$$

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):

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

Subsequently jackknife histograms (superscript J) are defined by

$$H_i^J(E) = H(E) - H_i(E) \tag{3.135}$$

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 extreme 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

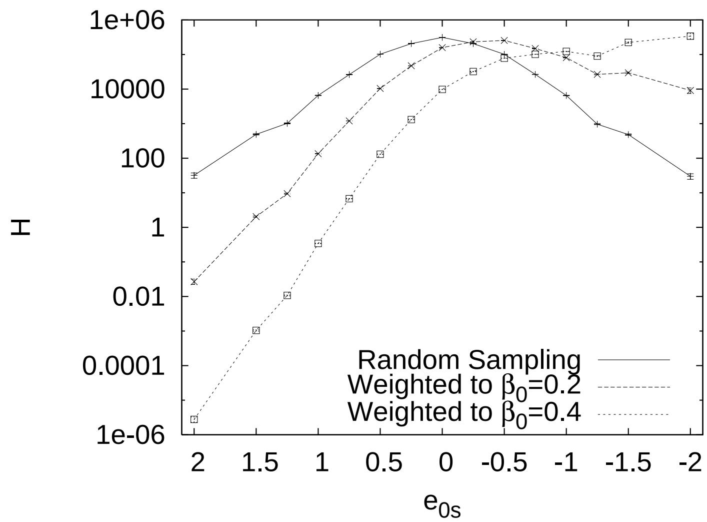

Fig. 3.8 Energy histogram from random sampling of the $2d$ Ising model on a 4×4 lattice together with is reweighting to $\beta_0 = 0.2$ and $\beta_0 = 0.4$ (see assignment 1).

perform a canonical simulations of the 2D Ising model on larger lattices and reweight the specific heat to a small neighborhood 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 4×4 lattice the Ising model has $2^{16} = 65\,536$ 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. Problems are encountered when the statistics covers some states barely.

In assignment 2 we generate the rather small statistics of $32 \times 30\,000$

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

Statistics:	(a) $32 \times 30\,000$		$32 \times 3\,10^8$		$10\,000$ times (a)	
	Estimate	Q	Estimate	Q	Estimate	Q
Simple binning:						
C	$x.xxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx	–	–
with mean from entire statistics:						
C via (3.129)	$x.xx\,(xx)$	x.xx	$x.xxxx\,(xx)$	x.xx	–	–
C via (3.130)	$x.xxxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx
Jackknife binning:						
C	$x.xxxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx
bias corrected	$x.xxxx\,(83)$	x.xx	$x.xxxxx\,(xx)$	x.xx	$x.xxxxx\,(xx)$	x.xx

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 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 no longer identical. From the table the observation is that (3.132) fails entirely, while the estimate from (3.133) is good. The bad estimate comes because the fluctuations of the second moment used in (3.132) 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 single measurements E_j.

To demonstrate that the bad estimator does also 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) are identical again, and the goodness of fit is satisfactory. However, it remains inconclusive whether there is an advantage compared to the simple binning es-

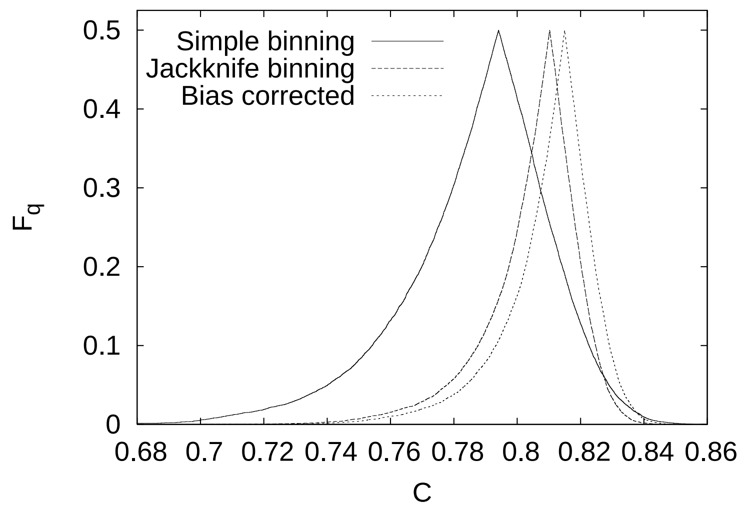

Fig. 3.9 Empirical peaked distribution function of three estimators of the specific heat of the Ising model as discussed in the text (assignment 4).

timates (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 of the two methods 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 simple binning estimate third. Figure 3.9 depicts the empirical peaked distribution functions (1.47) of these estimates. As there is no disadvantage in applying jackknife instead of simple binning: **The jackknife method should in essence always be used.**

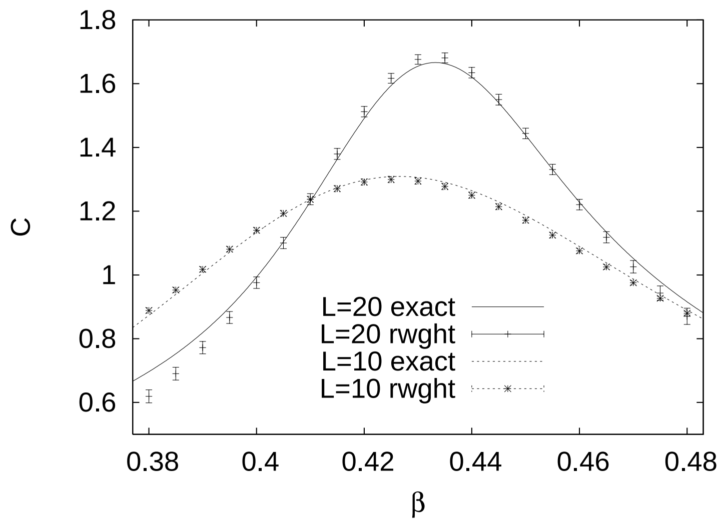

Fig. 3.10 Specific heat of the Ising model on $L \times L$ lattices. Exact results produced by the program `ferdinand.f` versus reweighting of simulations from $\beta = 0.43$ (assignment 5).

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 canonical MC simulations are performed for the $2d$ Ising model at $\beta = 0.43$, which is relatively close to β_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 β range. That reflects the shrinking of the reweighting range with increasing lattice size. A fit of the L dependence of the location of the peak allows, however, to determine a good value for the simulation temperature on the next larger lattice, and so on. Finite size scaling investigations can be performed by iterating such a process.

3.5.3 *Assignments for section 3.5*

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

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

(2) Use random sampling to create a statistics of $32 \times 30\,000$ sweeps for the $2d$ Ising model on a 4×4 lattice. Reweight to $\beta_0 = 0.4$ 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 $32 \times 3\,10^8$ 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 using the `actlm` from all data, for the jackknife 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 10×10 and 20×20 lattices at $\beta = 0.43$. Reweight to the β_0 range $[0.38 : 0.48]$ and plot bias corrected jackknife estimates of the specific heat together with the exact result for $C(\beta)$.