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A new efficient Monte Carlo technique

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Abstract. A new efficient Monte Carlo technique is developed and tested using the 2D Ising model for which exact solutions are known. The new technique calculates continuous thermodynamic functions of continuous thermodynamic variables from independent samples taken within an interval of typically a few hundredths of a Monte Carlo step per spin. The new technique is not only efficient and accurate but also furnishes some new information concerning the relationship between canonical and microcanonical averages for finite systems. It also furnishes primary thermodynamic functions such as free energy directly from the Monte Carlo data, a feature not available in the conventional Monte Carlo method.

1. Introduction

Thanks to the recent development of enormous computing power together with the well established finite-size scaling theory, numerical methods, especially the Monte Carlo technique (which will be abbreviated as MCT hereafter), have become popular tools for the investigation of various statistical mechanical problems. While efforts are being made to take advantage of top of the line supercomputers or to develop special purpose processors (Pearson *et al* 1983, Hoogland *et al* 1983) to deal with specific statistical mechanical problems, some slow progress and changes have also been made (Creutz 1983, Swendsen and Wang 1987, Bhanot *et al* 1987a, b, Ferrenberg and Swendsen 1988) in the fundamental aspect of MCT since the first time when Metropolis *et al* (1953) introduced the technique based on the idea of 'importance sampling'.

Is the conventional MCT the most efficient to calculate thermodynamic quantities of finite-sized systems? Suppose we wish to calculate thermodynamic quantities of a given system at two nearby temperatures. In the conventional MCT one has to generate equilibrium configurations for sampling for each temperature independently. The underlying assumption of the conventional MCT is that microscopic configurations, which predominantly contribute to canonical averages, are quite different so that at each temperature a new set of equilibrium configurations needs to be generated. If we wish to calculate a thermodynamic quantity as a continuous function of a continuous temperature variable, we have to generate an infinite set of equilibrium configurations corresponding to the temperature variable. However there cannot be an infinite set of different configurations in a finite-sized system with a finite number of energy levels for each degree of freedom. For example, if our system is a spin-$\frac{1}{2}$ Ising model with N spins there are a total of only 2^N microscopic configurations, which is not infinite, although it is extremely large even for moderate N. Therefore there must be some

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way to calculate continuous thermodynamic functions without generating an infinite number of sets of microscopic configurations.

The new method proposed in this paper is based on this observation and eliminates the repetitive realisation of the same microscopic configuration to make the method efficient. To accomplish this objective we generate microscopic configurations of fixed energy for the purpose of data taking, although we eventually take canonical averages. The method is similar to that developed recently by Bhanot *et al* (1987a). However, in the present method, a finely tuned sampling algorithm allows us to take samples from freshly generated configurations with the shortest time interval, typically of a few hundredths of an MC step, thereby enhancing the efficiency of the MC simulation tremendously. Sampling from configurations constrained by some constant energies has been attempted by Cruetz (1983). However in his attempt, he calculates microcanonical averages instead of canonical averages which the conventional MCT calculates. In the new method we calculate canonical averages although we calculate microcanonical averages as a preliminary procedure. Temperatures come in as an input as in the conventional MCT, which is to be contrasted with the microcanonical MCT of Creutz (1983).

As will be shown later in this paper the canonical averaging yields smooth results for a typical finite-sized system because they are averaged over quite *large* energy intervals especially near the critical temperature! (The system susceptible to MCT is too small to apply the central-limit theorem yet.) Bhanot *et al* (1987a, b) proposed a similar idea and calculated the critical exponent ν for the three-dimensional Ising model. However, their simulations are limited to the calculation of $\Omega(E)$, the total number of configurations with fixed energy E and the calculation of microcanonical averages of thermodynamic functions such as magnetisation was not attempted. Our method in this paper has a subtle but crucial difference from that of Bhanot *et al* (1987a) in that it furnishes independent samples within a very short time interval, which is crucial for the accurate calculation of microcanonical averages such as magnetisation. Recently Ferrenberg and Swendsen (1988) also proposed a closely related approach. However they used the conventional MCT for data taking in order to extract extra information contained in the simulation data for the single temperature point.

In this paper we present our own version of the new MCT, which allows us to take independent samples within a very short time interval, typically a few hundredths of a MC step, together with the results of the efficiency and accuracy tests of the technique using the two-dimensional Ising model for which exact solutions are known. The new method not only is efficient and accurate but also furnishes some new information concerning the relationship between the canonical and microcanonical averages for finite systems.

We begin by reviewing the new MCT in the next section and present the results of the calculation done on the 2D Ising model in section 3. The accuracy is shown by comparing the results with the exact solutions wherever available. In section 4 we will discuss the efficiency of the new MCT together with its advantage over the conventional MCT. The final section is devoted to a summary and further remarks concerning the new method.

2. New Monte Carlo technique

In order to illustrate the new method let us take as an example a spin-$\frac{1}{2}$ Ising model of

N spins in the absence of an external field. The energy of the system can be written as

$$E(\{S_i\}) = -J \sum_{\langle i,j \rangle} S_i S_j \tag{1}$$

where S_i is the spin variable assuming ± 1 values, J is the exchange energy and $\langle i, j \rangle$ runs over interacting nearest-neighbour pairs i, j. The canonical average $\langle A \rangle$ of any thermodynamic quantity $A(\{S_i\})$ is defined by

$$\langle A \rangle = \sum_{\{S_i\}}^{2^N} A(\{S_i\}) \exp(-\beta E(\{S_i\}))/Q \tag{2}$$

where β is the inverse temperature $1/kT$ with Boltzmann's constant k and Q is the partition function defined by

$$Q = \sum_{\{S_i\}}^{2^N} \exp(-\beta E(\{S_i\})). \tag{3}$$

We can rewrite (2) and (3) in slightly different forms as

$$\langle A \rangle = \sum_{E=E_0}^{E_m} \Omega(E) \exp(-\beta E) \overline{A}(E)/Q \tag{4}$$

and

$$Q = \sum_{E=E_0}^{E_m} \Omega(E) \exp(-\beta E) \tag{5}$$

where $\overline{A}(E)$ is the microcanonical average of the variable A defined by

$$\overline{A}(E) = \sum_{\{S_i\}}^{\Omega(E)\prime} A(\{S_i\})/\Omega(E) \tag{6}$$

and $\Omega(E)$ is the total number of configurations with a fixed E. The prime in (6) indicates that the summation is over microscopic configurations with fixed E. From this point of view, the calculation of $\langle A \rangle$ is reduced to the calculations of $\Omega(E)$ and microcanonical average $\overline{A}(E)$.

Let q, N^+ and N^{++} be the coordination number, the total number of up-spins, and the total number of interacting up-spin pairs respectively. Then the energy of the system can be written as

$$E = -4J(N^{++} - \tfrac{1}{2}qN^+) \tag{7}$$

where the constant term $\frac{1}{2}JqN$ has been dropped. Therefore configurations with constant E can be generated by keeping $N^{++} - \frac{1}{2}qN^+$ constant. In this description, the lowest energy, $E_0 = E(N^{++} = 0, N^+ = 0) = 0$ and highest energy, $E_{\max} = E(T = \infty) = \frac{1}{2}JqN$ so that there are only $qN/8$ discrete energies separated by $\Delta E \equiv 4J$. Therefore

we only need to generate $qN/8$ independent sets of configurations to evaluate $\Omega(E)$ and $\overline{A}(E)$. The crux of the new technique is how to evaluate $\overline{A}(E_j)$ and $\Omega(E_j)$ efficiently. The subtle but crucial difference of our method from that of Bhanot *et al* (1987a, b) is that we set up a random walk through a configuration space restricted to a narrow energy band given by

$$E_j - \tfrac{1}{2}q\Delta E \leq E(\{S_i\}) \leq E_j + (\tfrac{1}{2}q + 1)\Delta E \tag{8}$$

and use, for data taking, configurations which satisfy

$$E(\{S_i\}) = E_j \qquad \text{and} \qquad E(\{S_i\}) = E_j + \Delta E. \tag{9}$$

As will be explained later, only by this elaboration can it be guaranteed that the samples from which data are taken are independent configurations. In contrast to our sampling technique, Bhanot *et al* set up a random walk on the energy band made of four consecutive energy layers and took data from all four energy layers. Since there is no guarantee that samples are all different from each other in this algorithm, samples must be taken with very large time intervals at a heavy cost to the efficiency in order to get statistically independent samples for the calculation of thermodynamic averages such as magnetisation.

We will sketch briefly the new algorithm. We first generate an initial spin configuration $\{S_i\}$ with given energy $E(\{S_i\})$. We start a random walk by a single spin-flip algorithm as follows. We select a single spin out of N spins either randomly or sequentially and attempt to flip it. Whenever the attempted move takes the walker to a spin configuration $\{S_i\}$ which lies within the energy band (8) the move is allowed; otherwise the move is rejected. Whenever the walker visits points in the configuration space satisfying the energy value given by (9), relevant information such as N^+ is sampled together with the total number of visits. The last information is a vital key to the new method which allows us to evaluate canonical averages.

The random walk we set up by this method is very much like the one used in the microcanonical MCT of Creutz (1983) except for the energy constraint. The allowance of $\frac{1}{2}q\Delta E$ energy width in (8) is crucial for the accurate determination of the distribution of N^+ although it is less so for the estimate of $\Omega(E+\Delta E)/\Omega(E)$ as was done in Bhanot *et al* (1987a, b). The reason is as follows. Since the energy change δE produced by the single spin-flip move from the original configuration is restricted to a range $[-\frac{1}{2}q\Delta E, \frac{1}{2}q\Delta E]$, the allowance of the energy width ensures that the next spin-flip move after sampling always lie within the energy band given by (8). Therefore the walker moves immediately away from the previously sampled configuration thereby eliminating the possibility of repeated sampling of the same configuration. The possibility of such repeated sampling is especially severe at low E values where the rejection rate is very high. This allowance of the energy width also enables the walker to escape trapping in metastable states if any. However an allowance of an energy width larger than $\frac{1}{2}q\Delta E$ rapidly makes the MC process inefficient as will become clear in the efficiency discussion of section 4.

As long as we are interested in macroscopic thermodynamic functions or derivatives such as internal energy or susceptibility we only need to calculate the number of configurations, $\omega(E, N^+)$ of fixed E and N^+ since the $A(\{S_i\})$ corresponding to these quantities depend only on N^+, so that $\Omega(E)$ and $\overline{A}(E)$ are calculable from $\omega(E, N^+)$ by

$$\Omega(E) = \sum_{N^+} \omega(E, N^+)$$

and

$$\overline{A}(E) = \sum_{N^+} A(E,N^+)\omega(E,N^+)/\Omega(E).$$

In order to calculate $\omega(E,N^+)$, we run this random walk starting from the lowest energy E_0 to the highest energy $E_{\max}$. Since we know $\omega(E_0,N^+)$, namely $\omega(E,N^+) = \delta_{N^+,0} + \delta_{N^+,N}$ so that $\Omega(E_0) = 2$ (in practice we can calculate some further $\omega(E,N^+)$ for low-lying E by hand so that we can start the random walk and taking data from some higher E; see the discussion in section 5 and appendix 1), we can estimate $\omega(E,N^+)$ successively in the following way. We count $n(E,N^+)$ and $n(E+\Delta E,N^+)$, the numbers of configurations of two neighbouring energies with given N^+ visited by the random walker in the configuration space given by (9). Let N_d and N_d^+ be the total number of points visited with energy E and $E+\Delta E$, i.e. $N_d = \sum n(E,N^+)$ and $N_d^+ = \sum n(E+\Delta E,N^+)$. Then we have $\Omega(E+\Delta E) = \Omega(E)N_d^+/N_d$ and $\omega(E,N^+) = \Omega(E)n(E,N^+)/N_d$. This completes the new MCT.

3. Monte Carlo results

In order to test the efficiency of the new method we took an $N = 30 \times 30$ square lattice with toroidal boundary condition and obtained data using a PC. We compared the results from the data with the exact calculation of Kaufman (1949) for finite-sized lattices using the formula given by Ferdinand and Fisher (1969). We also calculated the magnetisation and susceptibility and compared them with Onsagar's exact magnetisation (Yang 1952) for an infinite system and the asymptotic susceptibility expression for infinite systems of Barouch *et al* (1973).

For the sake of simplicity in the discussion below, we will denote $E/\Delta E$ by N_e and a function $A(E)$ by $A(N_e)$ indiscriminately so that $\Omega(N_e)$ is the same as $\Omega(E)$ where $E = N_e\Delta E = 4JN_e$. For $N = 900$, N_e runs from 0 to 450 for the ferromagnetic or positive temperature side. In the first run the random walk was stopped at $N_d = 20\,000$ for all N_e. However N_d samples taken at the energy band with $N_e - 1$ are added to the N_d^+ samples for the calculation of microcanonical averages making the total number of samples for each N_e,

$$N_d(1 + R(N_e - 1)) \tag{10}$$

where $R(N_e) = \Omega(N_e+1)/\Omega(N_e) \simeq N_d^+/N_d$.

Since $R(N_e)$ decreases as N_e increases as can be seen from table 1 of appendix 2, the number of samples for each N_e is not uniform although N_d is uniform in this work. It is always possible to control N_d according to the demanded degree of accuracy at a given thermodynamic domain. As an example, we have performed a run with an extra $50\,000\,N_d$ in the energy range $N_e \in (80,249)$, which contributes to the critical region significantly, to obtain a more accurate estimate of the thermodynamic functions in the critical region. In our data taking, samples taken with $N^+ > N/2$ are put to $n(N_e,N^+ - N/2)$ since $\omega(N_e,N^+)$ is symmetric about $N^+ = N/2$, so that all raw data about distribution of the order parameter N^+ is restricted to $N^+ \in [0,N/2]$.

In figure 1 the free energy, internal energy, entropy and specific heat are plotted superimposed on exact curves. On this scale deviations from the exact curves are not visible except for the specific heat where the exact curve (thin line) is barely discernible

in a few places. In order to show the numerical values of these deviations we plot in figure 2(*a*) the relative deviation, defined by $(A_{MC} - A_{exact})/A_{exact}$, which measures the precision of the result, in the critical region. In figure 2(*b*), similar curves to figure 2(*a*) are plotted using reinforced data. By visual inspection alone we can say that the precision is remarkably improved. Average absolute deviations are calculated using values from 100 uniformly spaced points by the formula:

$$\sum_{i=1}^{100} \{|A_{MC}(i) - A_{exact}(i)|/A_{exact}(i)\}.$$

They are 1.31×10^{-4}, 4.57×10^{-4}, 10.95×10^{-4} and 6.69×10^{-3} for the free energy, internal energy, entropy and specific heat in figure 2(*a*) and 0.98×10^{-4}, 2.38×10^{-4}, 5.50×10^{-4} and 2.53×10^{-3} for the same quantities in figure 2(*b*) respectively. As figure 2(*b*) shows, these precisions are equal to or even better than that of the conventional MCT that uses a special purpose processor (Hoogland 1983) for $N = 16 \times 16$ and $N = 32 \times 32$ lattices (of comparable size with our system). We will show in the next section that the time it takes to complete our result is only a fraction of the time it takes to get data for a single temperature point using a conventional MCT. Except for figure 2(*b*) all the plots (figures 1–6 and 8) are with first run data to give the reader the general idea of the efficiency and accuracy.

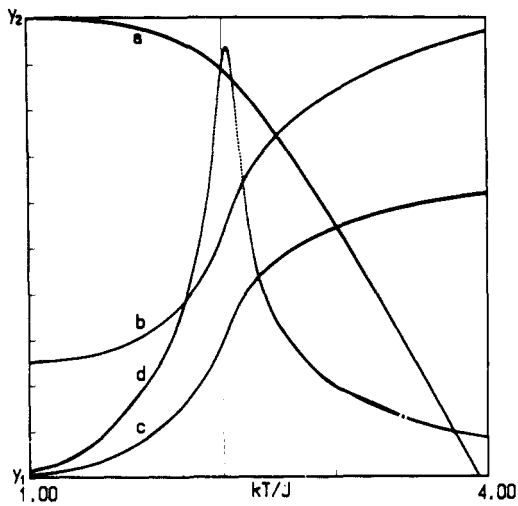

Figure 1. Free energy (a), internal energy (b), entropy (c) and specific heat (d) per spin plotted against temperature. $(y1, y2) = (-3, -2)$, $(-2.5, 0.5)$, $(0, 1)$ and $(0, 2)$ for a, b, c and d respectively. The vertical bar marks T_c, the critical temperature of the infinite system.

The internal energy is calculated using the canonical average, $\langle E \rangle/(J/N) - q/2$, and specific heat is calculated using the fluctuation formula, $\beta(\langle E^2 \rangle - \langle E \rangle^2)/N$, in these figures. However numerical derivatives from the free energy yield almost the same result. In figure 3 we plot magnetisation M and reduced susceptibility χ on a semi-log scale together with the exact magnetisation (Yang 1952) and asymptotic susceptibility of an infinite system (Barouch 1973). The deviation from the exact susceptibility curve on the low-temperature side is due to the fact that the exact susceptibility is known

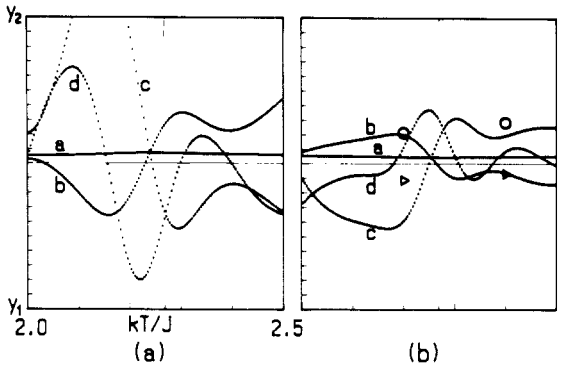

Figure 2. The relative deviation from the exact values, $(A_{MC} - A_{exact})/A_{exact}$ plotted against temperature. Symbols are the same as figure 1. $(y1, y2) = (-2 \times 10^{-3}, 2 \times 10^{-3})$ for a, b, c and $(-2 \times 10^{-2}, 2 \times 10^{-2})$ for d. (*a*) The result with the first run data. (*b*) The same quantities with reinforced data for $E/4J \in [80, 249]$. Circles (energy) and triangles (specific heat) represent the typical accuracy of conventional MC result at temperatures 2.2 and 2.4 for 16 × 16 square lattice (from Hoogland 1983).

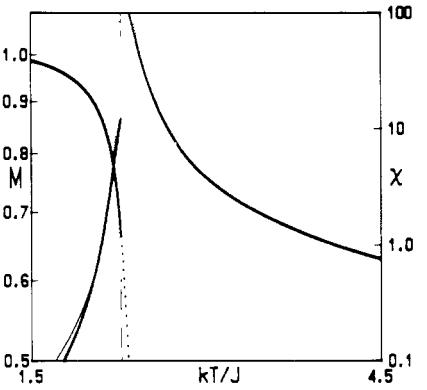

Figure 3. Magnetisation and susceptibility per spin plotted against temperature. Thin lines are exact magnetisation (Yang 1952) and exact asymptotic susceptibility curve of infinite system (Barouch *et al* 1973).

only in the asymptotic form as $\chi = C_0^{\pm}\epsilon^{7/4} + C_1^{\pm}\epsilon^{3/4}$, where $\epsilon = |1 - T_c/T|$. The MC curve must be close to the true susceptibility values of an infinite system in this region.

In figure 4 we plot M and χ against ϵ on a log–log scale. Along the magnetisation curve the exact $M(\epsilon)$ and its asymptotic curve given by $M = \{-2^{5/2}\ln(\sqrt{2} - 1)\epsilon\}^{1/8}$ of an infinite system are plotted. Alongside the two $\chi^{\pm}$ curves the exact asymptotic curve $\chi = C_0^{\pm}\epsilon^{7/4}$ is plotted. From figure 4 one can easily estimate the susceptibility exponent γ on the high-temperature side without even resorting to the finite-size scaling analysis. For the low-temperature side, however, the temperature range between the beginning of the asymptotic region and the beginning the finite-size rounding is too narrow to estimate the critical exponent of the infinite system. In fact, at this lattice size the finite-size rounding occurs before the asymptotic region is reached denying a direct estimate of the magnetisation exponent. In figures 3 and 4, M is defined by $M = \langle|(N - 2N^+)|\rangle/N$ and

$$\chi = 4(\langle(N^+)^2\rangle - \langle N^+\rangle^2)/N \qquad \text{for } T < T_c \tag{11}$$

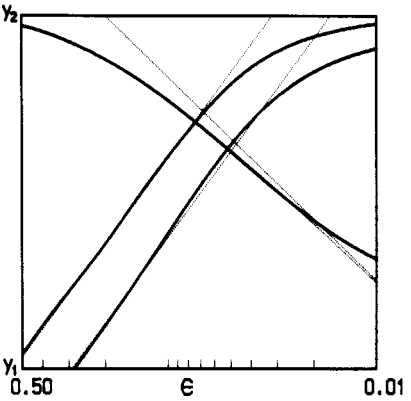

Figure 4. Log–log plot of M and χ against ϵ. $(y1, y2) = (-0.5, 1)$ for $\ln M$ and $(1.0, 6.0)$ for $\ln\chi$ of $T > T_c$ (left) and $(-1.5, 3.5)T < T_c$ (right). For the magnetisation the exact magnetisation curve and its asymptotic curve for an infinite system are plotted as dotted lines. For the two MC $\chi^{\pm}$ curves the exact asymptotic curve $\chi^{\pm} = C_0^{\pm}\epsilon^{-7/4}$ of Barouch *et al* (1973) for an infinite system is plotted as dotted lines.

but

$$\chi = 4\langle(N^+)^2\rangle/N \qquad \text{for } T > T_c. \tag{12}$$

Figure 5 shows microcanonical energy $E = N_e\Delta E$ and entropy $S(N_e) = k\ln\Omega(N_e)$ plotted against microcanonical temperature $kT/J = 4/[\ln\{\Omega(N_e + 1)/\Omega(N_e)\}]$. There are only $qN/8$ points for microcanonical quantities. It is interesting to note that in spite of the irregular behaviour of the microcanonical entropies and temperatures at low energies (see also table 1 of appendix 2) they give rise to smooth well behaving thermodynamic functions when they are averaged canonically. In figure 6 we plot the normalised canonical weight factor $\Omega(N_e)\exp(-\beta N_e\Delta E)/Q$ against N_e for six typical temperatures, $kT/J = 1.5$, 2.2, 2.2692 $(= T_c)$, 2.4, 4 and 15. Notice that at the critical temperature configurations within 1/3 of the available energies (60 210) contribute to the canonical averages! Furthermore configurations with N_e values ranging from 100 to 175 contribute to the thermodynamic averages significantly at two fairly separated temperatures 2.2 and 2.4 of figure 2(*b*). This proves the point mentioned in the introduction that many of the configurations contributing to the thermodynamic averages at nearby temperatures must overlap.

4. Efficiency analysis

In this section we will discuss the efficiency of the new MCT and its advantages over the conventional MCT. Let us first consider the number of spin-flip attempts necessary to obtain a set of data for single N_e with given N_d. The configuration space spanned by a random walker given by (8) consists of $(q+2)$ energy layers. The total number of spin-flip trials per data is on average the ratio of the total number of configurations to $\Omega(N_e)$, i.e.

$$N_t = \sum_{k=-2}^{3} \Omega(N_e + k)/\Omega(N_e). \tag{13}$$

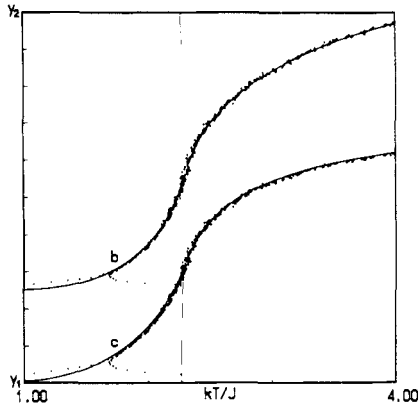

Figure 5. The microcanonical internal energy and entropy plotted against temperature. The symbols and scale are the same as figure 1. Thin full curves are exact canonical values.

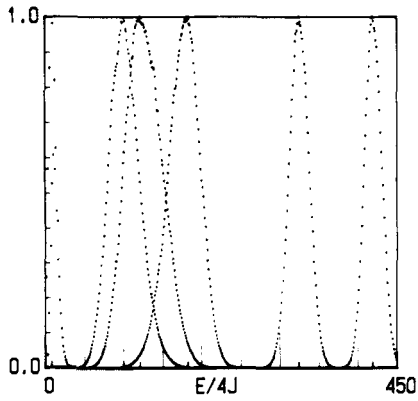

Figure 6. The scaled canonical weight factor $\Omega(E)\exp(-\beta E)$ plotted against $N_e = E/4J$ for temperatures $kT/J = 1.5$, 2.0, 2.2692 (T_c), 2.4, 4.0 and 15.

Therefore the average number of spin-flip trials to obtain N_d data for an N_e is given by:

$$N_d \sum_{k=-2}^{3} \Omega(N_e + k)/\Omega(N_e).$$

We estimated these numbers using our knowledge of $\Omega(N_e)$ and compared them with the actual time it took to perform in the random walk run. We did this for three typical values of N_e: 7, 120 and 280. The estimated numbers are 8737, 241 and 60, while the actual numbers of spin-flip trials it took for each N_d are 8471, 244 and 61 which is in agreement within a few per cent. Incidentally this fact suggests that one can count the time the random walker spends at each energy layer in the band (9) without any restriction for data taking to estimate $R(N_e)$ or even perform sampling to estimate $\omega(N_e, N^+)$. However, if we do so, repeated counting of the same configuration

in case the spin-flip attempt fails would mean the data was of poor statistical quality unless the sampling is done at large time intervals.

The estimated total number of spin-flip trials to obtain this set of data ($N_e \in [5, 450]$) is calculated using $N_d = 20\,000$, except $N_d = 70\,000$ for N_e values ranging 80 to 249. It is 0.39×10^{10}.

On the other hand Hoogland *et al* (1983) made 20 series of observations, each of which comprises 25 000 samples taken with an interval of 32 MC steps per spin in order to obtain data at a single temperature, such as a single pair of circle and triangle as in figure 2(*b*). Had we carried out a similar simulation, we would have attempted 20 (series of observation) $\times$ 25 000 (samples) $\times$ 32 (MC steps per spin) $\times$ 900 (spin-flip trials) $= 1.44 \times 10^{10}$ trials in order to obtain data at a single temperature since the number of lattice sites in our system is 900. In other words, we can determine whole thermodynamic functions with only a quarter of the effort that is needed to obtain a single data point in the conventional MC method! Furthermore the new technique requires less than half the effort since in this new technique one needs only to calculate δE to decide whether to allow or reject the move. On the other hand in the conventional MCT, one has to calculate not only the δE of the attempted spin-flip move, but also perform an extra comparison with a random number for the decision which is necessary to attain the equilibrium canonical distribution.

The advantages of this new method besides the points we have mentioned already are (i) the algorithm consists of only integer operations which are best suited to digital computers; (ii) it is extremely lenient in its demands on the random number generator since the complexity of the system itself serves as a random number generator; and (iii) there is no critical slowing down because the configuration space is restricted to a narrow energy band at each separate energy.

In order to demonstrate the second point, we have carried out the sampling run by selecting lattice sites sequentially for the spin-flip trial, eliminating the random number generator entirely except for the generation of a random initial spin configuration of given E. We compared these raw data with those of the random selection method. The sequential selection technique works very well except at extremely small N_e values where the configurations are not complex enough since only few spins are upturned. Comparisons are made at two values of N_e, 121 and 281. We detect no difference at all in the quality of the data. Indeed the raw data, which give the normalised distribution function of the order parameter, $n(N_e, N^+)/N_d$ approach a common smooth distribution as the number of data N_d increases as figures 7 and 9 clearly show.

In order to expatiate the last point, the absence of critical slowing down, let us examine the origin of the difficulty in the conventional MCT at criticality. It is due to large fluctuations which cause adverse effects in two ways. Because of large fluctuations in energy and magnetisation in the critical region, the realisation of a canonical ensemble by some simulated 'thermal motion' takes a long time. Secondly since the energy and magnetisation variables are spread over a wide range at criticality as is clear from figures 6 and 8(*a*), a large number of samplings would be required to calculate the thermodynamic averages of the quantities of interest with reasonable accuracy.

The new technique avoids the first problem altogether since we do not realise a canonical ensemble by some simulated 'thermal motion' but generate a uniform distribution in a narrow energy band, namely a microcanonical ensemble for data taking. The second problem is also naturally solved in the new technique. Although we take the same amount of data for all N_e, a large number of data points naturally

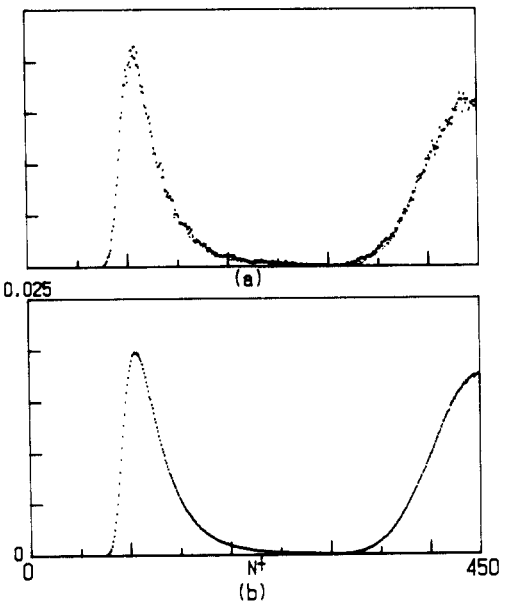

Figure 7. Two plots of MC data for the normalised distribution function of the order parameter, $n(N_e, N^+)/N_d$, which were obtained with the sequential selection method (bold dots) and the random selection method (small dots). (*a*) $N_d = 1.2 \times 10^5$ for $N_e = 121$ and $N_d = 7 \times 10^4$ for $N_e = 281$. (*b*) There are 50 times more N_d than in (*a*), i.e. $N_d = 6 \times 10^6$ and 3.5×10^6. The scales are the same for both figures. (See also figure 9 for another example of data obtained using the sequential selection method.)

contribute to the canonical average of the thermodynamic functions in the critical region because of large fluctuations in energy as figure 6 clearly indicates. Therefore as figures 1 and 2 shows no change in precision near the critical region although the number of data N_d are uniform for all N_e. Actually the precision in the critical region is even enhanced compared with the high and low temperature regions because of this effect. In figure 8(*a*) we show that raw data $n(N_e, N^+)/N_d$ for several N_e values, namely 51, 121, 165, 281 and 419 for the same number of data N_d. In general the quality of the data gets poorer as N_e increases because the total number of data (13) decreases. Actually, for the 'critical' N_e value ($\simeq$ 160) for which the fluctuation, $\overline{N^{+2}} - \overline{N^+}^2$, is largest, the quality of the raw data is poorest if we fix the number of data N_d to be uniform for all N_e. This is because $\omega(E, N^+)$ spreads over a wide range of N^+ at criticality and the number of samples for each N^+ becomes small compared with that for low or high N_e values, where $\omega(E, N^+)$ is rather sharply peaked thereby increasing the statistical error. However, even this effect is overcome by the effect discussed in the last paragraph. In a sense the difficulty caused by the large fluctuations in the magnetisation is resolved by the large fluctuations of energy in the new MCT.

To be more specific let us consider this behaviour at $T = T_c$ in detail. We can show that N_e for which the canonical weight factor exceeds 50% of the peak value which occurs at $N_e = 121$ ranges from 98 to 154, and above 25%, 88 to 167. Now we can estimate the total number of samples contributing to thermodynamic averages at T_c. The number of samples at $N_e = 121$ with $R(N_e) = 5.8$ is, by formula (10), 476 000, and if we assume data of 50 N_e contributing to the average, the total number becomes 23 800 000. And all these samples are from freshly generated configurations!

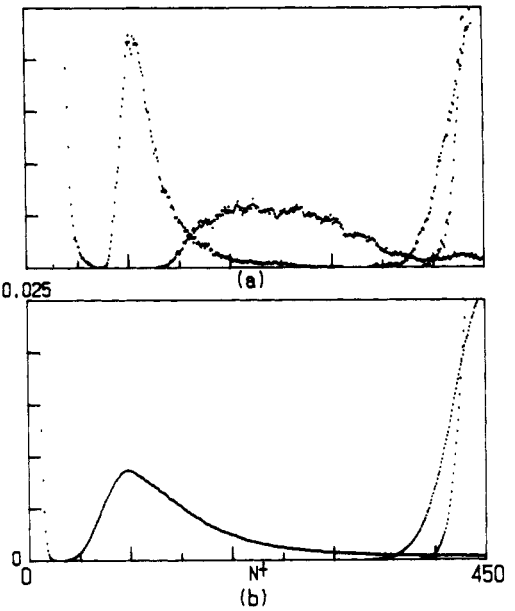

Figure 8. (*a*) MC data for the normalised distribution functions of the order parameter at N_e = 51, 121, 165, 281 and 419. (*b*) Canonical average of the distribution function at temperatures 1.5, 2.2692 (T_c), 4.0 and 15.0 from the left. The scales are the same for both figures. These data are taken with the sequential sampling method without the use of a random number generator. All the random nature in this data taking process is contained in the single random initial configuration.

In figure 8(*b*) we plot the canonically averaged distribution function of the order parameter, the significance of which was discussed recently in conjunction with the finite-size test of hyperscaling (Binder *et al* 1985, Barber *et al* 1985), at four typical temperatures, 1.5, 2.2692, 4.0 and 15. They all look smooth, well behaving functions although they are all from the fuzzy looking raw data of figure 8(*a*). Indeed if the number of data approaches this size even the raw data for a single N_e itself shows smoothness of comparable quality as can be seen in figure 9.

In short, data taking with a uniform number of N_d for each N_e has no special adverse effect when E passes critical 'E_c' to get thermodynamic functions of more or less uniform precision, which is our assertion about the absence of critical slowing down.

We will make a brief analysis of the effective MC steps per spin used in this new scheme. Since we only have control over the sampling of freshly generated configurations because of the allowance of the energy width given by (8) and (9), we can obtain a large number of samplings without any risk of repeated sampling of the same configuration within a much shorter time interval (the number of spin-flip trials). Indeed we can estimate the effective 'MC step per spin' of this technique. Let us take as a typical example N_e = 160 which may be considered as the 'critical N_e' and estimate the number of spin-flip trials to obtain a single data point near this N_e value. From table 1 of appendix 2, we know N_t = 205 which is the average number of spin-flip trials between two consecutive visits on the energy layer of N_e = 160, and $R(N_e)$ = 5.51 which is the the average number of visits on the energy layer of $N_e + 1$ = 161 in this same time interval. Therefore the average number of samples taken within the time interval N_t is 6.51 (see (10)) and the average time interval between two samples used

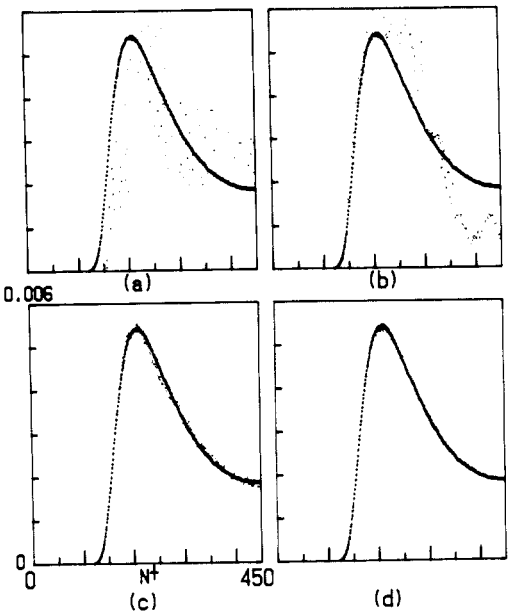

Figure 9. Normalised distribution function for various levels of the total number of data N_d. Plots (in small dots) are for $n^+(N_e,N^+)/N_d^+$ at (*a*) $N_d = 2000$, (*b*) 20 000, (*c*) 200 000 and (*d*) 2 000 000, superimposed with a plot at $N_d = 4\,000\,000$ (in bold dots). The scales are the same for all four figures.

for data is $N_t/(1 + R(N_e)) = 205/6.51 = 31.5$ which is equivalent to $31.5/900 = 0.035$ 'MC steps per spin'.

At first one might get a little suspicious of getting data of such quality on samples taken with such a short time interval. To see the dynamics of this sampling scheme, we watched the dynamical aspect of the random walk on the computer. Although N^+ does not change very much between two successive samples, they are nonetheless independent and furnish information on the local distribution of the order parameter. Subsequently if N_d is sufficiently large, the random walker sweeps configurations of the accessible range of N^+ (at most $N = 900$ and usually it is less than N at any N_e) so many times that the fuzziness of raw data decreases and the distribution function approaches a rather smooth and sharply defined function. Although the dynamics may depend on the structure of configuration space (such as the existence of metastable states), our contention is that if $n(N_e,N^+)$ ($\simeq N_d(1 + R(N_e))/N$) is sufficiently large we would get the distribution function of the order parameter within the statistical error. In figure 9 we plot the raw data with varying N_d near the 'critical' N_e value, i.e. 164, to show how the sampled distribution function approaches a smooth, well defined curve as the N_d increases. Data in these figures are obtained using a sequential selection method for the spin sites.

Lastly we should remark that expanding the energy band (8) would lower the efficiency drastically. The reason is that the ratio of the two numbers of data at the highest energy and the lowest energy in the same band, $R(N_e)^n, n+1$ being the number of the data-taking energy layer ($n \geq 2$), is too big, and in order to obtain data on the lowest energy layer would make the number of data of the highest energy layer unnecessarily large, wasting much MC time.

5. Conclusion and discussion

In this paper we have shown that the new MCT is simple, accurate and efficient. With only a fraction of the effort that is needed to obtain a single data point in the conventional MCT, one can calculate whole thermodynamic functions including free energy and entropy functions. The origin of the accuracy and efficiency is due to two facts. In the new MC method the canonical ensemble is not generated by some 'simulated thermal motion' but input from the information obtained using a much simpler sampling scheme in the microcanonical ensemble. Secondly sampling from the microcanonical ensemble allows us to control the sampling method best suited for high quality of data such as allowing a small width in the energy band so that all the configurations sampled are independent, while keeping the sampling interval very short, only a fraction of 'MC steps per spin'.

In fact the most offending part of data taking is not at criticality but at low energies. The worst case appears to be at $N_e = 7$ where it took time $N_t = 8737$ to obtain $41 + 1$ samples. Even in this case the average effective MC steps per spin is less than 0.25. In any case inefficiency at low energies (equivalently at low temperatures) is not a unique problem of the new MCT but is also present in the conventional MCT for which various remedies are discussed by Binder (1973). These techniques can also be applied to the new MCT. There is also another remedy to this problem. Since at low energies configurations are simple as only a few spins are upturned, we can calculate $\omega(E, N^+)$ applying the counting method commonly used in calculations of the coefficients of the low temperature series expansion (Domb and Green 1974). We have used an elementary method to calculate $\omega(N_e, N^+)$ for N_e up to 8 and listed it in appendix 1. However if one is not interested in free energy or entropy one can always start data taking at some high E.

In summary the new MCT can be applied to any system with a discrete energy, where the conventional MCT can be used, for calculating static properties with very high efficiency.

Acknowledgments

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Appendix 1. Exact $\omega(N_e, N^+)$ of the square lattice for small N_e

Only non-vanishing $\omega(N_e, N^+)$ for general N are given.

$\omega(0,0) = 1.$

$\omega(1,j) = 0$ for all j.

$\omega(2,1) = N.$

$\omega(3,2) = 2N.$

$\omega(4,2) = N^2/2 - 5N/2$ $\omega(4,3) = 6N$ $\omega(4,4) = N.$

$$\omega(5,3) = 2N^2 - 16N \qquad \omega(5,4) = 18N \qquad \omega(5,5) = 8N \qquad \omega(5,6) = 2N.$$

$$\omega(6,3) = N^3/6 - 5N^2/2 + 31N/3 \qquad \omega(6,4) = 8N^2 - 85N \qquad \omega(6,5) = N^2 + 43N$$

$$\omega(6,6) = 40N \qquad \omega(6,7) = 22N \qquad \omega(6,8) = 6N \qquad \omega(6,9) = N.$$

$$\omega(7,4) = N^3 - 21N^2 + 118N \qquad \omega(7,5) = 30N^2 - 400N \qquad \omega(7,6) = 10N^2 + 30N$$

$$\omega(7,7) = 2N^2 + 136N \qquad \omega(7,8) = 134N \qquad \omega(7,9) = 72N$$

$$\omega(7,10) = 30N \qquad \omega(7,11) = 8N \qquad \omega(7,12) = 2N.$$

$$\omega(8,4) = N^4/24 - 5N^3/4 + 13\tfrac{11}{24}N^2 - 52\tfrac{1}{4}N \qquad \omega(8,5) = 5N^3 - 132N^2 + 926N.$$

$$\omega(8,6) = N^3/2 + 94\tfrac{1}{2}N^2 - 1651N \qquad \omega(8,7) = 62N^2 - 486N$$

$$\omega(8,8) = 26\tfrac{1}{2}N^2 + 194\tfrac{1}{2}N.$$

$$\omega(8,9) = 6N^2 + 540N \qquad \omega(8,10) = N^2 + 461N \qquad \omega(8,11) = 310N$$

$$\omega(8,12) = 151N.$$

$$\omega(8,13) = 68N \qquad \omega(8,14) = 22N \qquad \omega(8,15) = 6N \qquad \omega(8,16) = N.$$

Appendix 2. Table of microcanonical Monte Carlo data

In this appendix we tabulate microcanonical MC data for $N_e = 7 \sim 450$. The second column is $\ln\Omega(N_e)$, the third, $R(N_e) \equiv \Omega(N_e+1)/\Omega(N_e)$, the fourth, $M \equiv \overline{|1 - N^+/N|}$, the fifth, $\Delta M^2 \equiv \overline{(1 - N^+/N)^2} - M^2$, the sixth, MC time which is defined by (13). Although ΔM^2 is not used directly to calculate the canonical susceptibility (see (12) and (13)) it is included in the table because this quantity gives a measure of the spread of $\omega(N_e, N^+)$ over N^+.

Table 1. Table of microcanonical Monte Carlo data.

N_e	S/k	$R(N_e)$	M	ΔM^2	N_t	N_e	S/k	$R(N_e)$	M	ΔM^2	N_t
7	21.122	41.20	0.9910	0.0000	8737	8	24.840	7.60	0.9908	0.0000	2025
9	26.868	26.78	0.9886	0.0000	4902	10	30.155	8.91	0.9883	0.0000	1908
11	32.343	19.42	0.9862	0.0000	3294	12	35.309	9.97	0.9856	0.0000	1799
13	37.609	15.91	0.9837	0.0000	2381	14	40.376	10.28	0.9830	0.0000	1614
15	42.706	13.46	0.9812	0.0000	1878	16	45.305	10.59	0.9802	0.0000	1510
17	47.665	12.07	0.9785	0.0000	1631	18	50.156	10.72	0.9774	0.0000	1425
19	52.528	11.50	0.9758	0.0000	1444	20	54.971	10.47	0.9746	0.0000	1300
21	57.319	10.89	0.9731	0.0000	1294	22	59.707	10.30	0.9718	0.0000	1185
23	62.039	10.42	0.9703	0.0000	1130	24	64.383	9.93	0.9690	0.0000	1068
25	66.678	9.81	0.9675	0.0000	1034	26	68.962	9.85	0.9660	0.0000	997
27	71.250	9.58	0.9645	0.0000	951	28	73.510	9.44	0.9629	0.0000	918
29	75.755	9.40	0.9615	0.0000	901	30	77.995	9.23	0.9598	0.0000	868
31	80.217	9.27	0.9583	0.0000	845	32	82.444	9.03	0.9568	0.0000	792
33	84.645	8.96	0.9553	0.0000	763	34	86.838	8.65	0.9537	0.0000	728
35	88.996	8.71	0.9521	0.0000	722	36	91.161	8.53	0.9505	0.0000	699

Table 1. (continued)

N_e	S/k	$R(N_e)$	M	ΔM^2	N_t	N_e	S/k	$R(N_e)$	M	ΔM^2	N_t
37	93.304	8.59	0.9488	0.0000	686	38	95.454	8.42	0.9473	0.0000	655
39	97.585	8.35	0.9455	0.0000	638	40	99.707	8.18	0.9439	0.0000	624
41	101.809	8.20	0.9422	0.0000	622	42	103.914	8.16	0.9407	0.0001	611
43	106.013	8.15	0.9394	0.0000	591	44	108.111	8.04	0.9371	0.0001	571
45	110.196	7.88	0.9357	0.0001	560	46	112.260	7.87	0.9339	0.0001	556
47	114.322	7.90	0.9323	0.0001	537	48	116.389	7.81	0.9305	0.0001	516
49	118.444	7.57	0.9288	0.0001	496	50	120.468	7.59	0.9263	0.0001	485
51	122.494	7.49	0.9247	0.0001	480	52	124.508	7.39	0.9227	0.0001	475
53	126.508	7.52	0.9215	0.0001	472	54	128.525	7.39	0.9191	0.0001	460
55	130.526	7.34	0.9174	0.0001	459	56	132.519	7.32	0.9154	0.0001	457
57	134.510	7.39	0.9135	0.0001	455	58	136.510	7.29	0.9117	0.0001	444
59	138.497	7.28	0.9095	0.0001	439	60	140.482	7.20	0.9076	0.0002	425
61	142.456	7.22	0.9058	0.0002	417	62	144.433	7.01	0.9032	0.0002	403
63	146.380	7.08	0.9018	0.0002	403	64	148.337	6.96	0.9002	0.0002	393
65	150.278	7.01	0.8979	0.0002	389	66	152.225	6.88	0.8953	0.0002	382
67	154.154	6.89	0.8936	0.0002	383	68	156.085	6.89	0.8903	0.0003	379
69	158.015	6.89	0.8884	0.0003	375	70	159.945	6.81	0.8867	0.0003	366
71	161.864	6.81	0.8855	0.0002	360	72	163.783	6.71	0.8823	0.0003	353
73	165.686	6.70	0.8802	0.0003	352	74	167.589	6.68	0.8760	0.0004	347
75	169.488	6.68	0.8756	0.0003	344	76	171.387	6.61	0.8738	0.0003	339
77	173.276	6.62	0.8691	0.0005	335	78	175.167	6.56	0.8672	0.0006	333
79	177.048	6.52	0.8659	0.0004	331	80	178.923	6.61	0.8630	0.0005	330
81	180.811	6.52	0.8608	0.0005	321	82	182.685	6.48	0.8580	0.0006	319
83	184.554	6.42	0.8554	0.0005	316	84	186.413	6.50	0.8533	0.0006	317
85	188.285	6.39	0.8477	0.0009	311	86	190.140	6.43	0.8478	0.0007	309
87	192.001	6.38	0.8456	0.0006	305	88	193.855	6.34	0.8426	0.0007	300
89	195.702	6.34	0.8371	0.0013	297	90	197.549	6.28	0.8335	0.0013	294
91	199.386	6.28	0.8329	0.0010	292	92	201.223	6.28	0.8310	0.0011	292
93	203.060	6.22	0.8271	0.0010	290	94	204.888	6.29	0.8261	0.0009	291
95	206.726	6.24	0.8211	0.0011	288	96	208.557	6.23	0.8178	0.0014	283
97	210.387	6.20	0.8117	0.0019	281	98	212.212	6.14	0.8103	0.0015	278
99	214.026	6.20	0.8093	0.0013	277	100	215.850	6.11	0.8025	0.0017	271
101	217.660	6.12	0.8012	0.0016	270	102	219.472	6.06	0.7983	0.0017	265
103	221.273	6.08	0.7918	0.0022	264	104	223.079	6.00	0.7930	0.0017	262
105	224.871	6.04	0.7910	0.0015	263	106	226.670	6.01	0.7846	0.0021	261
107	228.464	6.03	0.7797	0.0030	260	108	230.260	6.01	0.7707	0.0061	259
109	232.053	5.99	0.7723	0.0030	256	110	233.844	5.99	0.7694	0.0026	255
111	235.633	5.95	0.7705	0.0021	255	112	237.416	5.97	0.7670	0.0023	255
113	239.203	5.99	0.7518	0.0052	253	114	240.993	5.93	0.7359	0.0130	248
115	242.774	5.91	0.7463	0.0035	246	116	244.550	5.88	0.7457	0.0032	245
117	246.322	5.86	0.7459	0.0030	243	118	248.091	5.89	0.7288	0.0063	245
119	249.864	5.83	0.7251	0.0058	242	120	251.628	5.91	0.7340	0.0032	241
121	253.404	5.82	0.7218	0.0039	236	122	255.166	5.80	0.7220	0.0048	237
123	256.925	5.78	0.7082	0.0089	237	124	258.679	5.85	0.6997	0.0092	237
125	260.445	5.82	0.6829	0.0138	234	126	262.206	5.76	0.6971	0.0065	233
127	263.957	5.77	0.6888	0.0073	234	128	265.710	5.82	0.6743	0.0106	234
129	267.470	5.76	0.6737	0.0096	234	130	269.221	5.78	0.6683	0.0118	235
131	270.974	5.81	0.6548	0.0133	234	132	272.734	5.80	0.6475	0.0138	229
133	274.491	5.74	0.6429	0.0150	228	134	276.239	5.69	0.6397	0.0182	227
135	277.977	5.77	0.6480	0.0112	231	136	279.729	5.72	0.6217	0.0173	229
137	281.474	5.78	0.6188	0.0196	229	138	283.228	5.73	0.5906	0.0264	226
139	284.973	5.71	0.5841	0.0240	223	140	286.716	5.68	0.5829	0.0219	222
141	288.454	5.65	0.5911	0.0161	223	142	290.185	5.71	0.5820	0.0183	221

Table 1. (continued)

N_e	S/k	$R(N_e)$	M	ΔM^2	N_t	N_e	S/k	$R(N_e)$	M	ΔM^2	N_t
143	291.927	5.68	0.5603	0.0256	216	144	293.665	5.59	0.5559	0.0240	216
145	295.385	5.59	0.5737	0.0212	218	146	297.106	5.69	0.5523	0.0255	218
147	298.844	5.63	0.5484	0.0241	215	148	300.573	5.59	0.5526	0.0196	215
149	302.293	5.63	0.5379	0.0228	215	150	304.021	5.61	0.5183	0.0260	212
151	305.746	5.58	0.5238	0.0239	211	152	307.465	5.57	0.5122	0.0233	212
153	309.182	5.58	0.5194	0.0203	212	154	310.902	5.60	0.4743	0.0279	212
155	312.624	5.57	0.4546	0.0321	211	156	314.341	5.59	0.4505	0.0317	208
157	316.062	5.56	0.4701	0.0256	205	158	317.778	5.48	0.4375	0.0292	203
159	319.480	5.51	0.4598	0.0281	204	160	321.187	5.51	0.4516	0.0260	205
161	322.893	5.49	0.4460	0.0277	205	162	324.595	5.54	0.4253	0.0307	205
163	326.308	5.52	0.3987	0.0308	201	164	328.016	5.49	0.3907	0.0323	199
165	329.719	5.42	0.3966	0.0286	196	166	331.408	5.47	0.4003	0.0281	196
167	333.108	5.38	0.3621	0.0324	195	168	334.790	5.43	0.3954	0.0288	196
169	336.483	5.43	0.3643	0.0307	194	170	338.175	5.40	0.3534	0.0274	194
171	339.861	5.38	0.3471	0.0292	193	172	341.544	5.43	0.3363	0.0315	193
173	343.237	5.38	0.3132	0.0282	190	174	344.920	5.36	0.3272	0.0285	189
175	346.599	5.37	0.3347	0.0269	188	176	348.280	5.35	0.3152	0.0277	186
177	349.956	5.32	0.3128	0.0264	186	178	351.627	5.33	0.2939	0.0253	185
179	353.300	5.33	0.2788	0.0264	183	180	354.973	5.29	0.2860	0.0263	181
181	356.638	5.28	0.2846	0.0264	180	182	358.302	5.27	0.2786	0.0267	179
183	359.963	5.24	0.2714	0.0246	178	184	361.620	5.25	0.2647	0.0242	177
185	363.278	5.24	0.2689	0.0239	175	186	364.934	5.21	0.2503	0.0229	173
187	366.584	5.19	0.2511	0.0234	171	188	368.231	5.17	0.2517	0.0215	169
189	369.874	5.13	0.2551	0.0220	166	190	371.510	5.12	0.2401	0.0204	165
191	373.144	5.06	0.2282	0.0201	164	192	374.765	5.10	0.2525	0.0208	164
193	376.395	5.10	0.2376	0.0223	162	194	378.024	5.04	0.2320	0.0193	159
195	379.642	5.05	0.2307	0.0199	159	196	381.262	5.01	0.2209	0.0206	157
197	382.872	5.04	0.2130	0.0175	158	198	384.490	4.99	0.2053	0.0183	157
199	386.097	5.03	0.2137	0.0183	158	200	387.712	5.01	0.1888	0.0159	157
201	389.323	5.02	0.1946	0.0166	155	202	390.936	4.99	0.2012	0.0157	152
203	392.544	4.93	0.1793	0.0152	149	204	394.140	4.93	0.1922	0.0157	148
205	395.735	4.87	0.1880	0.0145	145	206	397.319	4.89	0.1903	0.0139	145
207	398.906	4.84	0.1753	0.0134	144	208	400.484	4.84	0.1800	0.0140	143
209	402.061	4.86	0.1828	0.0144	142	210	403.643	4.81	0.1655	0.0130	140
211	405.213	4.81	0.1670	0.0130	138	212	406.783	4.79	0.1795	0.0133	137
213	408.350	4.74	0.1731	0.0131	135	214	409.906	4.76	0.1624	0.0126	133
215	411.466	4.71	0.1519	0.0117	131	216	413.015	4.68	0.1575	0.0118	130
217	414.558	4.69	0.1542	0.0107	130	218	416.103	4.66	0.1430	0.0103	129
219	417.641	4.69	0.1590	0.0113	128	220	419.187	4.62	0.1541	0.0114	127
221	420.718	4.65	0.1502	0.0110	126	222	422.254	4.63	0.1524	0.0106	123
223	423.786	4.58	0.1470	0.0098	121	224	425.308	4.54	0.1484	0.0105	119
225	426.821	4.52	0.1414	0.0093	119	226	428.329	4.54	0.1344	0.0090	119
227	429.842	4.51	0.1324	0.0093	118	228	431.349	4.52	0.1429	0.0096	116
229	432.858	4.48	0.1345	0.0088	113	230	434.358	4.44	0.1275	0.0083	112
231	435.848	4.41	0.1308	0.0084	111	232	437.332	4.43	0.1293	0.0087	111
233	438.821	4.41	0.1273	0.0080	110	234	440.305	4.40	0.1278	0.0083	109
235	441.787	4.36	0.1241	0.0076	108	236	443.261	4.39	0.1235	0.0079	108
237	444.739	4.36	0.1240	0.0077	106	238	446.212	4.33	0.1174	0.0072	104
239	447.677	4.29	0.1193	0.0074	103	240	449.133	4.29	0.1181	0.0076	102
241	450.591	4.30	0.1158	0.0071	100	242	452.049	4.21	0.1110	0.0063	98
243	453.487	4.21	0.1141	0.0067	98	244	454.924	4.22	0.1157	0.0068	97
245	456.365	4.20	0.1093	0.0060	96	246	457.800	4.18	0.1070	0.0061	94
247	459.230	4.13	0.1031	0.0055	93	248	460.649	4.13	0.1044	0.0056	92

Table 1. (continued)

N_e	S/k	$R(N_e)$	M	ΔM^2	N_t	N_e	S/k	$R(N_e)$	M	ΔM^2	N_t
249	462.067	4.12	0.1023	0.0058	92	250	463.483	4.09	0.1021	0.0056	92
251	464.893	4.14	0.0969	0.0050	91	252	466.314	4.11	0.1052	0.0054	89
253	467.729	4.03	0.1039	0.0056	87	254	469.123	4.05	0.0947	0.0049	86
255	470.521	4.00	0.0874	0.0044	84	256	471.908	4.01	0.0986	0.0051	83
257	473.296	3.93	0.0988	0.0049	82	258	474.664	3.92	0.0992	0.0051	81
259	476.031	3.96	0.0928	0.0044	81	260	477.408	3.87	0.0980	0.0052	78
261	478.761	3.92	0.0993	0.0047	78	262	480.127	3.82	0.0932	0.0049	78
263	481.468	3.86	0.0926	0.0044	77	264	482.818	3.92	0.0891	0.0039	75
265	484.185	3.74	0.0886	0.0040	72	266	485.505	3.73	0.0864	0.0038	72
267	486.821	3.78	0.0931	0.0044	73	268	488.150	3.74	0.0863	0.0036	71
269	489.468	3.78	0.0835	0.0036	69	270	490.797	3.65	0.0813	0.0039	67
271	492.093	3.65	0.0825	0.0039	67	272	493.388	3.65	0.0900	0.0041	67
273	494.684	3.64	0.0824	0.0035	65	274	495.974	3.63	0.0832	0.0037	64
275	497.265	3.55	0.0878	0.0040	63	276	498.530	3.57	0.0822	0.0034	63
277	499.802	3.57	0.0751	0.0032	64	278	501.073	3.60	0.0803	0.0034	63
279	502.353	3.57	0.0784	0.0032	61	280	503.626	3.53	0.0727	0.0028	60
281	504.886	3.47	0.0768	0.0029	59	282	506.131	3.49	0.0815	0.0035	59
283	507.381	3.46	0.0811	0.0034	58	284	508.621	3.47	0.0779	0.0031	58
285	509.866	3.44	0.0728	0.0029	57	286	511.102	3.43	0.0733	0.0031	56
287	512.334	3.42	0.0698	0.0026	55	288	513.563	3.39	0.0722	0.0029	55
289	514.783	3.38	0.0693	0.0027	53	290	516.000	3.35	0.0686	0.0028	53
291	517.210	3.30	0.0699	0.0028	52	292	518.404	3.34	0.0723	0.0030	52
293	519.609	3.30	0.0761	0.0032	51	294	520.802	3.30	0.0732	0.0029	50
295	521.996	3.23	0.0734	0.0029	49	296	523.168	3.23	0.0604	0.0021	48
297	524.340	3.22	0.0703	0.0025	47	298	525.510	3.18	0.0712	0.0025	46
299	526.667	3.16	0.0687	0.0024	47	300	527.818	3.17	0.0685	0.0025	47
301	528.970	3.21	0.0695	0.0024	46	302	530.137	3.16	0.0658	0.0022	45
303	531.287	3.12	0.0640	0.0024	45	304	532.423	3.14	0.0606	0.0022	44
305	533.566	3.11	0.0680	0.0026	42	306	534.699	3.03	0.0667	0.0024	41
307	535.808	2.99	0.0673	0.0024	41	308	536.903	3.03	0.0638	0.0022	41
309	538.012	2.98	0.0632	0.0021	39	310	539.105	3.01	0.0668	0.0024	39
311	540.207	2.90	0.0592	0.0020	38	312	541.273	2.91	0.0577	0.0019	38
313	542.341	2.93	0.0590	0.0019	37	314	543.415	2.89	0.0580	0.0019	37
315	544.478	2.90	0.0572	0.0019	36	316	545.543	2.87	0.0575	0.0017	36
317	546.596	2.86	0.0576	0.0018	36	318	547.647	2.85	0.0591	0.0020	35
319	548.694	2.85	0.0563	0.0017	34	320	549.739	2.78	0.0574	0.0018	33
321	550.762	2.74	0.0556	0.0016	33	322	551.771	2.78	0.0569	0.0017	32
323	552.792	2.77	0.0544	0.0016	32	324	553.811	2.67	0.0540	0.0016	31
325	554.793	2.73	0.0546	0.0017	31	326	555.796	2.69	0.0539	0.0016	30
327	556.785	2.66	0.0607	0.0019	30	328	557.765	2.67	0.0543	0.0017	29
329	558.747	2.62	0.0536	0.0017	29	330	559.708	2.61	0.0536	0.0017	29
331	560.667	2.65	0.0500	0.0014	29	332	561.640	2.62	0.0512	0.0016	28
333	562.602	2.59	0.0533	0.0016	27	334	563.553	2.51	0.0525	0.0015	26
335	564.474	2.55	0.0518	0.0015	26	336	565.411	2.49	0.0483	0.0015	26
337	566.322	2.48	0.0500	0.0015	26	338	567.230	2.49	0.0478	0.0014	26
339	568.144	2.48	0.0459	0.0012	25	340	569.051	2.51	0.0505	0.0014	25
341	569.970	2.45	0.0485	0.0013	24	342	570.868	2.43	0.0461	0.0012	24
343	571.756	2.38	0.0482	0.0014	23	344	572.621	2.43	0.0503	0.0015	23
345	573.509	2.37	0.0467	0.0012	23	346	574.373	2.32	0.0467	0.0012	22
347	575.213	2.38	0.0460	0.0012	22	348	576.081	2.30	0.0450	0.0011	21
349	576.912	2.30	0.0478	0.0012	21	350	577.743	2.27	0.0489	0.0012	21
351	578.564	2.25	0.0454	0.0012	20	352	579.373	2.25	0.0447	0.0012	20
353	580.185	2.23	0.0452	0.0011	20	354	580.988	2.24	0.0447	0.0012	20

Table 1. (continued)

N_e	S/k	$R(N_e)$	M	ΔM^2	N_t	N_e	S/k	$R(N_e)$	M	ΔM^2	N_t
355	581.796	2.21	0.0429	0.0011	19	356	582.587	2.24	0.0443	0.0011	19
357	583.396	2.14	0.0441	0.0011	18	358	584.156	2.14	0.0423	0.0010	18
359	584.917	2.16	0.0451	0.0012	18	360	585.688	2.10	0.0439	0.0011	18
361	586.429	2.15	0.0450	0.0012	18	362	587.196	2.08	0.0449	0.0011	17
363	587.928	2.12	0.0434	0.0010	17	364	588.678	2.04	0.0432	0.0010	16
365	589.390	2.00	0.0438	0.0010	16	366	590.081	2.02	0.0403	0.0009	16
367	590.786	1.96	0.0386	0.0009	15	368	591.460	2.00	0.0404	0.0009	15
369	592.152	1.97	0.0414	0.0010	15	370	592.831	1.97	0.0397	0.0009	15
371	593.508	1.97	0.0409	0.0010	15	372	594.189	1.94	0.0405	0.0008	14
373	594.851	1.91	0.0396	0.0009	14	374	595.498	1.91	0.0402	0.0009	14
375	596.146	1.89	0.0395	0.0009	14	376	596.780	1.86	0.0383	0.0008	14
377	597.402	1.87	0.0369	0.0007	14	378	598.029	1.89	0.0356	0.0007	13
379	598.664	1.85	0.0384	0.0008	13	380	599.278	1.78	0.0386	0.0008	13
381	599.852	1.84	0.0385	0.0008	13	382	600.460	1.79	0.0371	0.0008	12
383	601.041	1.76	0.0364	0.0007	12	384	601.606	1.71	0.0369	0.0008	12
385	602.145	1.74	0.0382	0.0008	12	386	602.697	1.75	0.0386	0.0008	12
387	603.257	1.75	0.0380	0.0008	12	388	603.815	1.71	0.0365	0.0008	11
389	604.353	1.69	0.0359	0.0007	11	390	604.879	1.67	0.0356	0.0007	11
391	605.393	1.68	0.0363	0.0008	11	392	605.910	1.67	0.0359	0.0008	11
393	606.423	1.63	0.0349	0.0007	10	394	606.914	1.62	0.0352	0.0007	10
395	607.394	1.60	0.0335	0.0006	10	396	607.866	1.60	0.0342	0.0007	10
397	608.339	1.61	0.0353	0.0007	10	398	608.815	1.55	0.0348	0.0007	10
399	609.252	1.53	0.0335	0.0007	10	400	609.677	1.56	0.0315	0.0006	10
401	610.120	1.52	0.0318	0.0006	9	402	610.541	1.53	0.0324	0.0006	9
403	610.965	1.52	0.0322	0.0006	9	404	611.387	1.49	0.0313	0.0006	9
405	611.783	1.48	0.0328	0.0006	9	406	612.174	1.47	0.0330	0.0006	9
407	612.562	1.46	0.0337	0.0006	8	408	612.938	1.41	0.0343	0.0007	8
409	613.283	1.38	0.0332	0.0006	8	410	613.607	1.42	0.0311	0.0005	8
411	613.957	1.39	0.0314	0.0006	8	412	614.286	1.40	0.0324	0.0006	8
413	614.619	1.37	0.0327	0.0006	8	414	614.934	1.37	0.0312	0.0005	8
415	615.249	1.38	0.0309	0.0005	8	416	615.574	1.33	0.0309	0.0005	8
417	615.863	1.33	0.0310	0.0006	8	418	616.149	1.31	0.0299	0.0005	7
419	616.418	1.29	0.0292	0.0005	7	420	616.673	1.28	0.0298	0.0005	7
421	616.919	1.29	0.0309	0.0005	7	422	617.176	1.27	0.0303	0.0005	7
423	617.416	1.28	0.0293	0.0004	7	424	617.663	1.25	0.0295	0.0004	7
425	617.882	1.24	0.0299	0.0004	7	426	618.101	1.23	0.0304	0.0005	7
427	618.312	1.22	0.0299	0.0005	7	428	618.509	1.19	0.0302	0.0005	7
429	618.683	1.20	0.0298	0.0005	7	430	618.866	1.21	0.0301	0.0005	7
431	619.055	1.20	0.0293	0.0005	7	432	619.235	1.20	0.0287	0.0005	7
433	619.421	1.16	0.0290	0.0005	7	434	619.571	1.15	0.0289	0.0005	6
435	619.709	1.14	0.0281	0.0005	6	436	619.841	1.12	0.0282	0.0004	6
437	619.952	1.12	0.0284	0.0005	6	438	620.070	1.12	0.0288	0.0005	6
439	620.184	1.10	0.0277	0.0005	6	440	620.278	1.11	0.0275	0.0004	6
441	620.384	1.08	0.0277	0.0004	6	442	620.457	1.07	0.0269	0.0004	6
443	620.527	1.06	0.0272	0.0004	6	444	620.583	1.05	0.0260	0.0004	6
445	620.633	1.02	0.0267	0.0004	6	446	620.653	1.02	0.0271	0.0004	6
447	620.677	1.04	0.0260	0.0004	6	448	620.713	1.02	0.0258	0.0004	6
449	620.734	1.02	0.0260	0.0004	6	450	620.753	1.02	0.0000	0.0000	6

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