Simulation of an ensemble with varying magnetic field: A numerical determination of the order-order interface tension in the $D=2$ Ising model

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In analogy with a recently proposed multicanonical ensemble we introduce an ensemble where the partition function is simulated with a term in the action containing a varying magnetic field. Using this ensemble we demonstrate on lattices with periodic boundary conditions that it is possible to enhance the appearance of order-order interfaces by many orders of magnitude. To perform a stringent test of the method we consider the $D=2$ Ising model at $\beta=0.5$ and simulate square lattices up to size 100×100. By a finite-size scaling analysis, the order-order interface tension per unit area is obtained. Our best infinite-volume extrapolation is in excellent agreement with Onsager's exact result.

Interfaces between ordered and disordered and, correspondingly, between ordered and ordered physical states play an important role in statistical mechanics, as well as in field theoretic models of fundamental gauge interactions.[1-3] Past numerical studies of the properties of interfaces were, however, hampered by a problem of principle. The surface tension per unit area F^s between ordered and disordered states or between ordered and ordered states has a finite value. Thus in the canonical ensemble, where configurations are samples with the Boltzmann weight $\mathcal{P}^{\mathcal{B}} \propto e^{-\beta H}$, configurations containing interfaces with an area A of typical size $O(L^{D-1})$ on the D-dimensional lattice with linear extension L are suppressed by exponentially small factors e^{-AF^s}. The aim of numerical studies of interfaces consists in obtaining many statistical independent interfaces on large lattices. This is prevented by the exponentially small suppression of configurations containing interfaces, resulting in a corresponding exponentially fast increase of the tunneling time with the area A between pure phases of the system, when the system is simulated with local Monte Carlo (MC) algorithms. To overcome these difficulties two of the present authors recently proposed MC simulations of a *multicanonical* ensemble.[4] Originally the ensemble was formulated for a temperature driven, order-disorder first order phase transition and the two-dimensional (2D) 10-state Potts model has been the first applicational target.[5] In the present paper we generalize the method to the case of a magnetic field driven order-order phase transition. We introduce a multimagnetic ensemble and illustrate how things work by simulating the 2D Ising model. The aim of the present paper is to check the numerical approach versus the exactly known[6] interface tension of 2D Ising model. The discrepancy between Refs. 1 and 2 illuminates that such stringent tests are desirable.

Let us introduce the notation. Spins $s_i=\pm1$ are defined on sites of a square lattice of volume $V=L\times L$ with periodic boundary conditions and the symbol $\langle i,j\rangle$ is used to denote nearest neighbors. The Ising Hamiltonian

$$H=H_I-hM, \quad \text{with } H_I=-\sum_{\langle i,j\rangle} s_i s_j \quad \text{and } M=\sum_i s_i \ , \tag{1}$$

contains the nearest-neighbor interaction term H_I and a term which couples the magnetic field h to the magnetization $M=\sum_i s_i$. For the 2D model the exact planar interface surface tension is, since long, known to be given by[6]

$$F^s=2\beta-\ln[(1+e^{-2\beta})/(1-e^{-2\beta})] \quad \text{for } \beta\geq\beta_c=\tfrac{1}{2}\ln(1+\sqrt{2})=0.4406\ldots . \tag{2}$$

Following Binders,[7,8] we are going to extract the interface tension from the probability distribution of the magnetization M. Probability distributions $P_L(M)$, as for $h=0$ obtained with our new algorithm, are depicted in Fig. 1, where we have adopted the normalization $\sum_M P_L(M)=1$. The distributions are sharply double peaked and we denote the positions of the maxima by $\pm M_L^{\max}$. Our measured distributions show deviations from the symmetry $P_L(M)=P_L(-M)$, due to statistical fluctuations, and the average of the absolute values of the positions of the measured maxima is taken to define $M_L^{\max}$. Correspondingly we define $P_L^{\max}$ as $P_L^{\max}=[P_L(-M_L^{\max})+P_L(+M_L^{\max})]/2$. The distribution takes its maximum at $P_L^{\min}=P_L(0)$. The logarithmic scale of Fig. 1 displays that more than twenty orders of magnitude are involved. The standard MC algorithm would only sample configurations corresponding to $P_{100}^{\min}$ if one could generate of the order $O(10^{20})$ or more statistically independent configurations. Here we overcome this difficulty by sampling configurations with a multimagnetical weight factor

$$\mathcal{P}_L^{mm}(M)\sim\exp(\alpha_L^k+h_L^k\beta M-\beta H_I) \quad \text{for } M_L^k<M\leq M_L^{k+1} \tag{3}$$

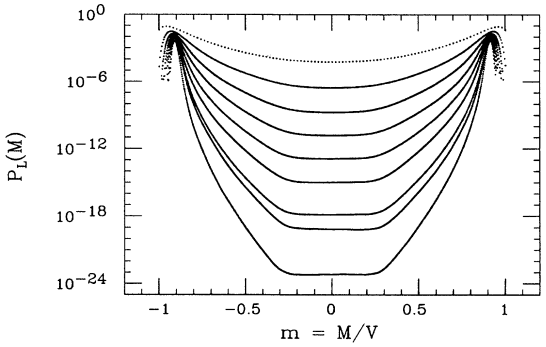

FIG. 1. Boltzmann probability distributions $P_L(M)$ for the magnetization.

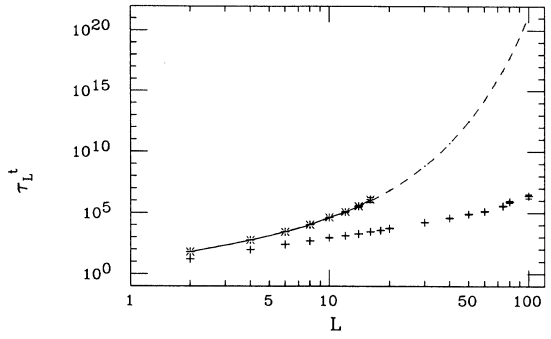

FIG. 2. Tunneling times vs lattice size. The upper data are for the standard heat bath algorithm and the broken line extrapolates by means of fit (6) into the region where no data exist. The lower data points are obtained with our multimagnetical algorithm.

instead of sampling with the usual Boltzmann factor $\mathcal{P}^B$. In Eq. (3) we partition the magnetization $-V \le M \le V$ into $k=0,\ldots,N$ (N odd) intervals $I_k=(M_L^k, M_L^{k+1}]$ with $M^{k+1}>M^k$ and the idea is to choose the intervals I_k and parameters h_L^k, α_L^k such that the resulting multimagnetical probability density $\mathcal{P}_L(M)$, as opposed to $P_L(M)$, has an approximately flat behavior. Let $M_L^1=-V$ and for $k=2,\ldots,N/2$ we define $M_L^k<0$ such that $P_L(M_L^k)=r^{1-k}P_L^{\max}$, where $r>1$. Similarly, we define $M_L^{N+1}=V$ and $P_L(M_L^k)=r^{k-N-1}P_L^{\max}$ with $M_L^k>0$ for $k=N/2+1,\ldots,N$. It follows from Ref. 4 that, in the limit $r\to 1$, the multimagnetical probability distribution $\mathcal{P}_L(M)$ can be made arbitrarily flat by adapting the following choice of parameters:

$$h_L^k=\begin{cases} 0 \text{ for } k=0,N/2,N\ , \\ +\beta^{-1}\ln(r)/(M_L^{k+1}-M_L^k) \\ \qquad \text{for } k=1,\ldots,N/2-1\ , \\ -\beta^{-1}\ln(r)/(M_L^{k+1}-M_L^k) \\ \qquad \text{for } k=N/2+1,\ldots,N-1\ , \end{cases} \tag{4}$$

where we require validity of the recursion relation

$$\alpha_L^{k+1}=\alpha_L^k+(h_L^k-h_L^{k+1})\beta^{-1}M_L^{k+1},\quad \alpha_L^0=0\ . \tag{5}$$

The standard Markov process is well suited to generate configurations which are in equilibrium with respect to this multimagnetical distribution and the probability distribution $P_L(M)$ corresponding to the Boltzmann weight is then obtained from $\mathcal{P}_L(M)$ by weighting with $\exp(-\alpha_L^k-h_L^k\beta M)$.

Our simulations were performed at $\beta=0.5$ on square lattices with linear size $L=2$ up to $L=100$. On the smallest systems we get the parameters in Eq. (3) from standard heat bath simulations. This is no longer possible for $L\ge 18$ and in this case we chose them by making everytime a finite size scaling (FSS) prediction of the quantity $P_L(M)$ from the smaller systems. To optimize the parameters we performed a second run and in some cases further runs to control our results. Our statistics for this investigation was $4\cdot 10^6$ sweeps per run and lattice size for $L=2$ up to $L=50$; for the larger lattices we increased our statistics to $8\cdot 10^6$ sweeps. In each case 200 000 additional, initial sweeps were performed for reaching equilibrium with respect to the multimagnetical distribution. One sweep updates each spin on the lattice once.

To compare the efficiency of our method with standard MC we measured the tunneling time τ_L^t. Similarly as in Ref. 5 we define the tunneling time τ_L^t as the average number of sweeps needed to get from a configuration with magnetization $M=-M_L^{\max}$ to a configuration with $M=M_L^{\max}$ *and* back. (The tunneling time is a direct measure for the number of statistically independent generated interfaces in the simulation, because for every completed tunneling the system has to pass twice through a region in phase space with $M\simeq 0$.) Our data are collected in Table I and in Fig. 2 we display on a log to log scale both the tunneling times for the multimagnetic MC algorithm and the heat bath algorithm. A reliable direct calculation of τ_L^t (heat bath) was only possible for lattices with $L\le 16$, for the larger systems standard MC runs would not tunnel often enough to allow for a reliable estimate. To compare with the multimagnetical algorithm, we use the fit

$$\tau_L^t(\text{heat bath})=6.80L^{2.14}e^{2\times 0.185\times L}\ , \tag{6}$$

as depicted in Fig. 2. The ratio $R=\tau_L^t(\text{heat bath})/\tau_L^t(\text{multicanonical})$ is a direct measure for the improvement due to our method. R increases from a factor 4 for the smallest lattice ($L=2$) up to $R\approx 450$ for $L=16$, the biggest lattice size where it was with our statistics possible to get data from standard MC. The extrapolation to $L=100$ yields $R\approx 6.1\times 10^{15}$, i.e., an improvement by more than fifteen orders of magnitude. The real improvement is presumably even bigger as we cannot reliably determine the parameters in the fit (6). Our multimagnetic data allow a highly precise determination of the interface tension per unit area. Following Binder,[8] the interface tension F^s can be defined from the infinite volume limit of the quantity of $P_L^{\min}/P_L^{\max}$, which for sufficiently large L takes the form

$$P_L^{\min}/P_L^{\max}=\text{const}L^p\exp(-2LF^s) \tag{7}$$

on lattices with periodic boundary conditions. Physically

TABLE I. The tunneling times and effective interface tensions as functions of the lattice size.

L	τ_L^t multimagnetic	τ_L^t heat bath	F_L^s
2	16.57(5)	62.87(23)	0.6516(79)
4	94.81(36)	588(5)	0.5852(54)
6	256(12)	2808(49)	0.4780(06)
8	498(3)	10 750(383)	0.4028(04)
10	856(43)	42 872(2136)	0.3641(04)
12	1365(14)	121 786(16 004)	0.3369(14)
14	1909(24)	361 055(69 141)	0.3201(07)
16	2851(45)	1 265 491(540 106)	0.3075(06)
18	3669(68)		0.2991(04)
20	5369(118)		0.2914(07)
30	16 688(550)		0.2689(07)
40	37 875(1861)		0.2580(05)
50	80 526(7562)		0.2509(09)
60	135 908(10 444)		0.2478(07)
74	376 843(32 804)		0.2443(09)
80	857 073(162 730)		0.2442(07)
100	2 469 200(924 055)		0.2403(12)

this definition assumes that at values of the mean magnetization $M \simeq 0$ a rectangular domain enclosed by two interfaces spanning the lattice via the periodic boundary condition is formed. On finite lattices we define the effective tension by means of

$$F_L^s = (1/2L)\ln(P_L^{\max}/P_L^{\min}) . \tag{8}$$

Our thus obtained F_L^s estimates are also contained in Table I.

To estimate F^s requires a FSS extrapolation towards $L=\infty$. Equation (7) converts into a fit of the form $F_L^s = F^s + a/L + b\ln(L)/L$. We arrive at the result $F^s = 0.2325(7)$ from lattices of size $L = 8$–100, an estimate by several standard deviations inconsistent with Onsager's exact value $F^s = 0.228\,06\ldots$ at $\beta = 0.5(2)$. When we omit the $\ln(L)/L$ correction, i.e., assume $p=0$, and include instead the $1/L^2$ next order correction to the interface tension into the fit, we arrive at the three parameter fit $F_L^s = F^s + a/L + b/L^2$, as depicted in Fig. 3. For the range $L = 8$–100 this fit turns out to be about equally well acceptable as the previous one, but yields $F^s = 0.2281(5)$. This value is now in excellent agreement with the exact result. From this we are very tempted to

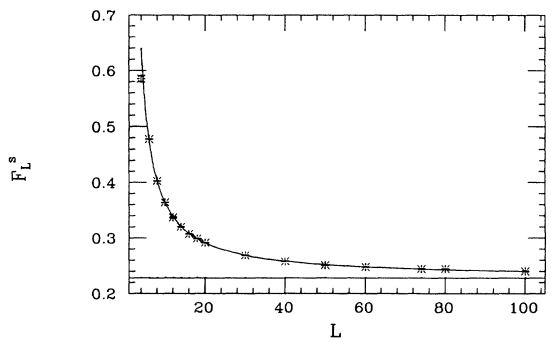

FIG. 3. Infinite-volume estimate of the interfacial tension by means of Eq. (8).

suggest that, indeed, $p=0$. Combining both fits into a four parameter fit reduces greatly our precision. Again, the first self-consistent result is found for the range $L = 8$–100 with $F^s = 0.2312(18)$ and the prefactor of the $\ln(L)/L$ term comes out to be $-0.146(86)$, compatible with zero on a two σ level. More important, we have seen that excluding the $\ln(L)/L$ term altogether does not spoil the goodness of the fit in a statistically significant way. Performing the two parameter fit $F_L^s = F^s + a/L$, we have to omit some more smaller lattices to get a self-consistent fit. This is now obtained for the range $L = 30$–100 with the estimate $F^s = 0.2281(8)$, a result clearly favorable for the assumption that $1/L$ is the leading order correction. In summary, we would like to quote

$$F^s = 0.2281 \pm 0.0005 , \tag{9}$$

as our best and final numerical result.

It is worthwhile to inspect the distributions $P_L(M)$ of Fig. 1 more closely. As the lattice size increases we observe a pronounced flattening of the logarithm of the probability distribution close to values of the magnetization $m=0$ and it appears that in the thermodynamic limit the probability distribution becomes constant in a finite range of mean magnetization $m \le m^c$. Such a behavior for the $D=2$ Ising model with periodic boundary conditions was in fact rigorously predicted. It was demonstrated in Ref. 9 that in this situation there exists a value of m^c such that for values of $m \le m^c$ the probability distribution is a constant. The value of m^c is calculable from the Wulf construction[10] for the asymptotic shapes of droplets of one phase floating in the opposite phase. Physically this result means that in the region $m \le m^c$ the minimum free energy excess is dominated by a single rectangular domain, extending throughout the lattice by making use of its periodic boundary conditions. In order to gain a visual impression, we decided to write configurations on the computer disk which describe a tunneling transition on our 100×100 lattice. We depict some examples in Figs. 4(a)–4(d). On a qualitative level we find support for the droplet model. Figure 4(a) depicts a fairly ordered configuration with magnetization $m \approx -0.9$. With increasing m a single droplet cluster begins to dominate the configuration Fig. 4(b) for $m \approx -0.6$. This cluster grows, Fig. 4(c), for $m \approx -0.4$, until it extends throughout the lattice by means of the periodic boundary conditions, Fig. 4(d), for $m \approx 0$. With further increasing m ($m \ge 0$), similar pictures, with black and white interchanged, are seen to emerge.

In summary, we have introduced a multimagnetic ensemble which on lattices with periodic boundary conditions is suitable for the numerical simulation of order to order interfaces in statistical mechanics as well as field theoretic models. The multimagnetic simulation eliminates super critical slowing down—or an exponentially fast increase of the tunneling time between the pure phases of the system with increasing area A of the interfaces. The remaining critical slowing down is of the type of a power law divergence. Due to our method it is possible to explore configurations in phase space, which in the canonical ensemble are suppressed by many orders of

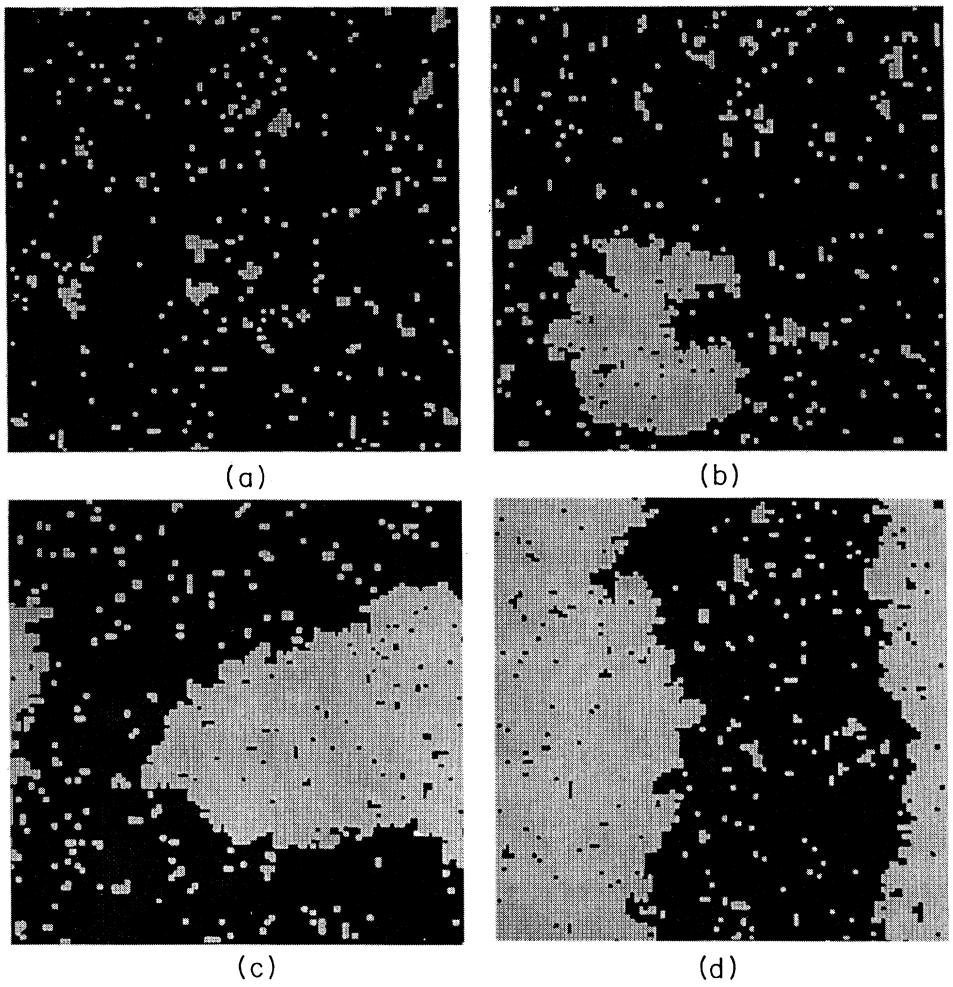

FIG. 4. (a) Configuration at $m \approx -0.9$ on the 100×100 lattice. (b) Configuration at $m \approx -0.6$ on the 100×100 lattice. (c) Configuration at $m \approx -0.4$ on the 100×100 lattice. (d) Configuration at $m \approx 0$ on the 100×100 lattice.

magnitude. In a region of configurations with mean magnetization close to zero we have found clear numerical evidence for the formation of a rectangular domain, which is enclosed by two interfaces. We have performed a finite-size scaling analysis of the finite volume estimates of the interface tension and our infinite volume value for the interface tension of a planar rigid surface. Another interesting approach to the numerical calculation of surface tensions exploits correlation functions,[11] and it may be worthwhile to try to combine this with a multimagnetical simulation.

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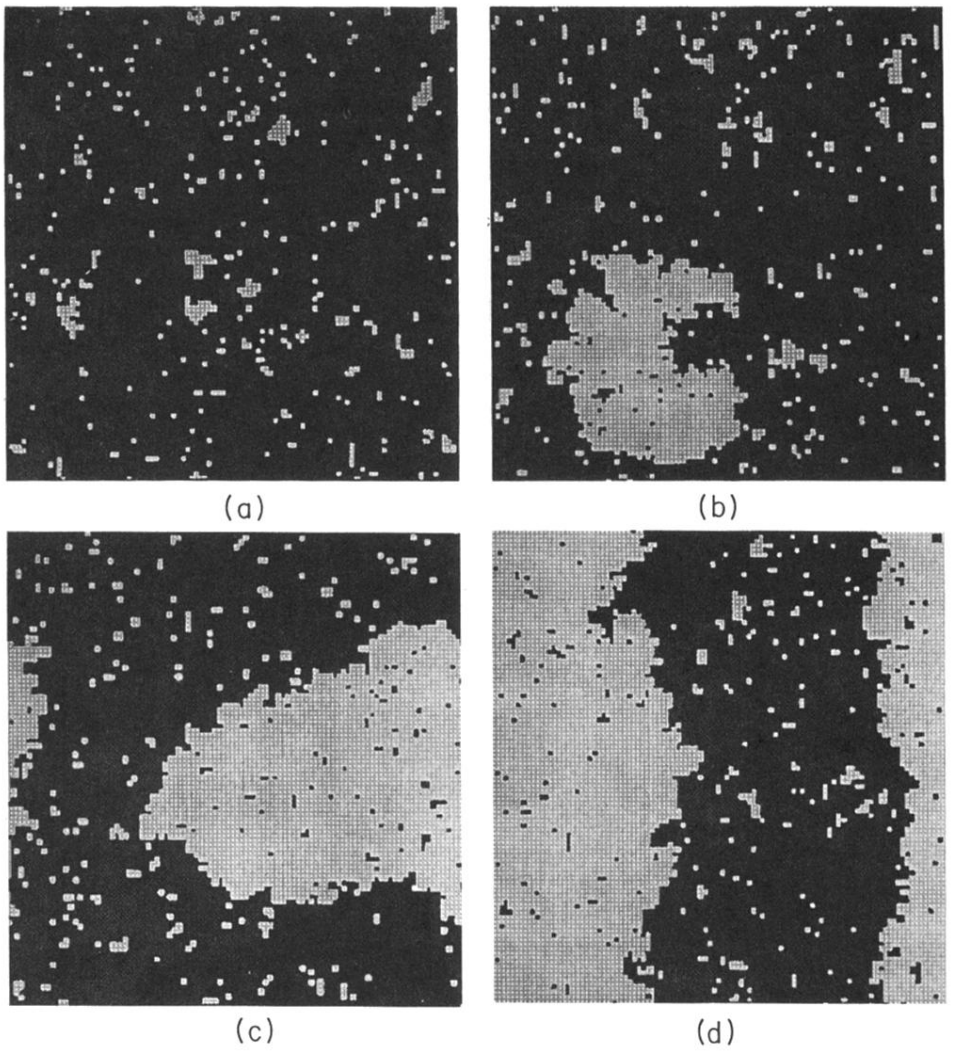

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