Fluctuation relations in a nonequilibrium system: Surface tension and effective temperature in an Ising-doped voter model

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(Received 21 March 2022; revised 14 May 2022; accepted 25 May 2022; published 17 June 2022)

Fluctuation relations of Jarzynski and Crooks enable efficient calculations of a free-energy difference between equilibrium states. In the present paper, we provide some numerical evidence that these relations can also be used for a two-dimensional Ising-doped voter model, which is a nonequilibrium system with a violated detailed balance. Adopting the method of Híjar and Sutmann, we implement a protocol that switches between periodic and antiperiodic boundary conditions and induces formation of an interface in the model. Assuming that a suitably interpreted Ising Hamiltonian can be considered as a pseudoenergy of the model, we examine fluctuations of work performed during these processes and estimate the surface tension. Our results confirm that the surface tension remains positive in this model except a limiting case of the voter model, where it seems to vanish. Comparing the free-energy estimates at different speeds of the switching process, we also estimate an effective temperature in the model. Perhaps coincidentally, the effective temperature of the voter model appears to be close to the critical temperature of the Ising model.

DOI: 10.1103/PhysRevE.105.064120

I. INTRODUCTION

Equilibrium statistical mechanics provides a solid foundation to investigate many-body systems [1]. Indeed, the existence of the Gibbs measure enables us to determine thermodynamic potentials or correlation functions for a variety of systems. However, for most natural processes, conditions for a thermal equilibrium are not met and as a result the system remains in nonequilibrium. An analysis of such systems is much more difficult and requires a fundamentally different approach [2] but, in some cases, progress has been achieved [3].

Recent studies show that fluctuation theorems provide valuable insight into nonequilibrium processes. Of particular interest is the theorem obtained by Jarzynski [4] that relates free-energy change ΔF to the probability distribution of work A extracted during the experiment that moves the system between two equilibrium states,

$$\langle \exp(-\beta A)\rangle = \exp(-\beta\Delta F), \tag{1}$$

where β is the inverse of the temperature. Subsequently, Crooks has shown that Eq. (1) can be considered as a special case of the more general relation [5],

$$P_F(A) = P_R(-A)\exp[\beta(A - \Delta F)], \tag{2}$$

where $P_F(A)$ and $P_R(-A)$ are probability distributions for the so-called forward and backward protocols.

Relations Eqs. (1) and (2) offer an interesting and efficient method to estimate free-energy differences, as demonstrated with the use of Monte Carlo simulations, molecular dynamics [6], and in some single-molecule experiments [7]. Let us emphasize that the transitions in relations Eqs. (1) and (2) are between equilibrium states. It would be very desirable to develop analogous relations for transitions between nonequilibrium steady states. Research along these lines for systems described by the Langevin dynamics was initiated by Hatano and Sasa [8] but the absence of a statistical description in the form of the Gibbs measure makes such an approach very challenging.

Statistical mechanics concepts are often formulated or verified with the use of lattice models, the Ising model being perhaps a prime example. In addition to numerous magnetic or lattice-gas studies, the Ising model was also examined in the context of opinion formation [9]. In such an interpretation, opinion of a given spin is set according to the cumulative effect of all neighboring spins, possibly perturbed with some (social) temperature noise. In an alternative approach, the so-called voter model [10], opinion of a spin is set as the opinion of a randomly chosen neighbor.

Taking into account the heterogeneity of human population and multiplicity of factors affecting opinion formation processes prompted us to examine the Ising-doped voter model that is a mixture of the Ising and voter-model dynamics [11]. Let us notice that such a model combines the equilibrium dynamics, which generates the surface tension (Ising), and the dynamics, which is tensionless (voter) [12]. In the Ising-doped voter model, the detailed balance is broken and is thus a nonequilibrium system. Simulations [11] indicate that the dynamics of the model shares some similarity to the Ising model, suggesting that a certain effective surface tension is generated. Let us notice that such tension appears also in some other nonequilibrium models of opinion [13] or language [14] formation as might be inferred from some dynamical behavior, e.g., power-law coarsening. In equilibrium systems, the surface tension is defined as a certain free-energy difference [15], but such an approach is usually not available for nonequilibrium systems.

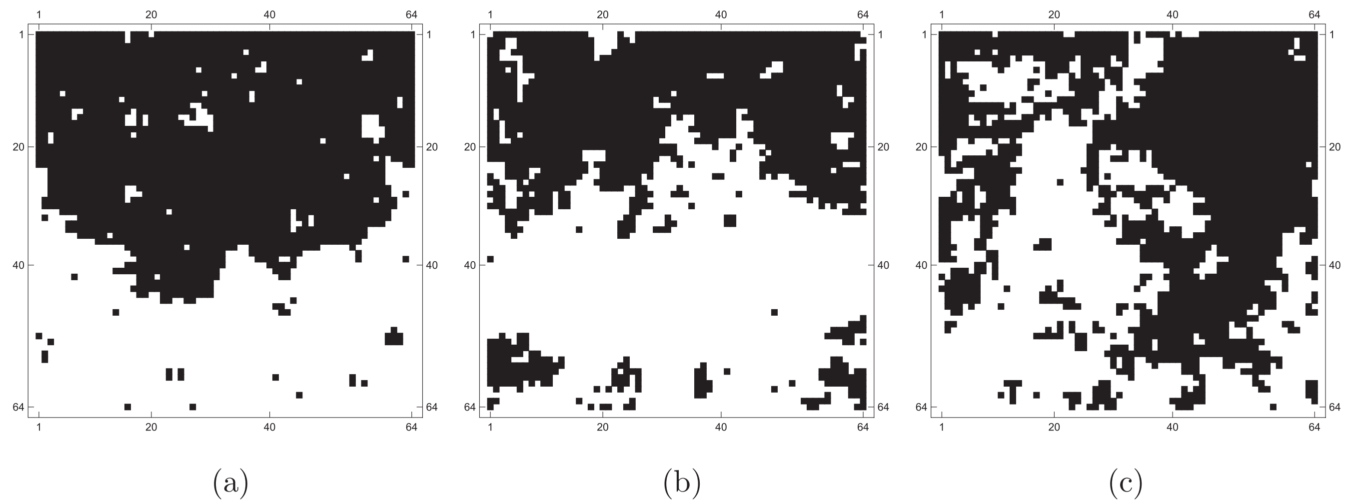

FIG. 1. Exemplary steady-state configurations with antiperiodic boundary conditions at the horizontal boundary (see Fig. 2) and periodic ones at the vertical boundary for 64×64 lattices and different concentrations of the Ising spins p. The temperature is equal to $T = 1.8$, which for $p = 0.7$ and 0.1 is below the critical point. As the concentration of Ising spins is reduced (and the temperature is kept constant), the system moves toward the transition point [11] and for $p = 0.01$ it is already in the disordered regime. (a) $p = 0.7$. (b) $p = 0.1$. (c) $p = 0.01$.

In the present paper, we use relations Eqs. (1) and (2) to estimate the surface tension in a two-dimensional Ising-doped voter model [11]. For the Ising model, the calculation of the surface tension using fluctuation theorems has already been made [16] and our work constitutes an extension of these calculations for a nonequilibrium model with a broken detailed balance. Assuming that the work extracted during nonequilibrium protocols can be related to a certain pseudoenergy of the model, we calculate the surface tension and show that the fluctuation relations enable us to extract information about the properties of such systems.

II. MODEL

We examine a two-dimensional Ising-doped voter model [11]. On each site i of a square lattice of size $L \times L$, we have a binary variable (spin) $s_i = \pm 1$, which initially is assigned to evolve according to an Ising-type heat bath dynamics or using the voter model dynamics [12]. Our model is thus a quenched mixture of the Ising and voter variables selected randomly with probability p and $1 - p$, respectively. An elementary step of the dynamics in our model is defined as follows.

(1) Select an agent, say i.

(2) If the variable s_i is of the Ising type, update it according to the heat-bath dynamics, namely, set as $+1$ with probability

$$r(s_i\!=\!1) = \frac{1}{1+\exp(-2h_i/T)}, \quad h_i = \sum_j J_{i,j} s_j, \tag{3}$$

and as -1 with probability $1 - r(s_i\!=\!1)$. The temperaturelike parameter T controls the noise of the system and the summation in Eqs. (3) is over the four neighbors of the site i.

(3) If the variable s_i is of the voter type, select one of its neighbors, say j, and set $s_i = s_j$.

We define a unit of time (Monte Carlo step) as L^2 elementary steps and $J_{i,j}$ is the coupling constant between spins i and j. Let us note that the presence of the voter agents ($p < 1$) implies a violation of the detailed balance. Indeed, when a voter-type agent and all its neighbors are in the same state, then a flip of this agent is strictly forbidden. Since the reversed transition is allowed, it means that the detailed balance in our model (for $p < 1$) does not hold. Numerical simulations indicate [11] that certain steady-state and dynamical characteristics of the Ising-doped voter model on two- and three-dimensional lattices, even for a very small concentration of the Ising spins p, show some similarity to the pure Ising model. Figure 1 demonstrates some typical interfacial and disordered configurations in the system.

III. METHOD

The surface tension in the Ising model has already been determined with the use of fluctuation theorems by Híjar and Sutmann [16] and we will adapt their method. First, we sketch the method for the Ising model ($p = 1$). The idea is based on the observation that antiperiodic boundary conditions induce an interface in the Ising model, which raises the free energy of the model. Then one examines protocols that quasicontinuously change the boundary conditions from periodic to antiperiodic or vice versa. It means that the coupling $J_{i,j}$ in the Ising model along a certain, e.g., horizontal line (see Fig. 2) changes from $+1$ to -1 (or inversely for reverse processes) in n equal steps $\Delta = \pm\frac{2}{n}$. Outside this line, the coupling constant equals unity. After each of these steps, the system is allowed to thermalize for $t = 1$ Monte Carlo steps.

The work A extracted after these changes equals the change of the energy, which is defined by the Ising model Hamiltonian

$$H = -\sum_{(i,j)} J_{i,j} s_i s_j, \tag{4}$$

where the summation is over square lattice bonds and the indices in $J_{i,j}$ indicate that due to the changing boundary conditions, the coupling constant is spatially dependent. With such a definition of the energy, the extracted work A can be

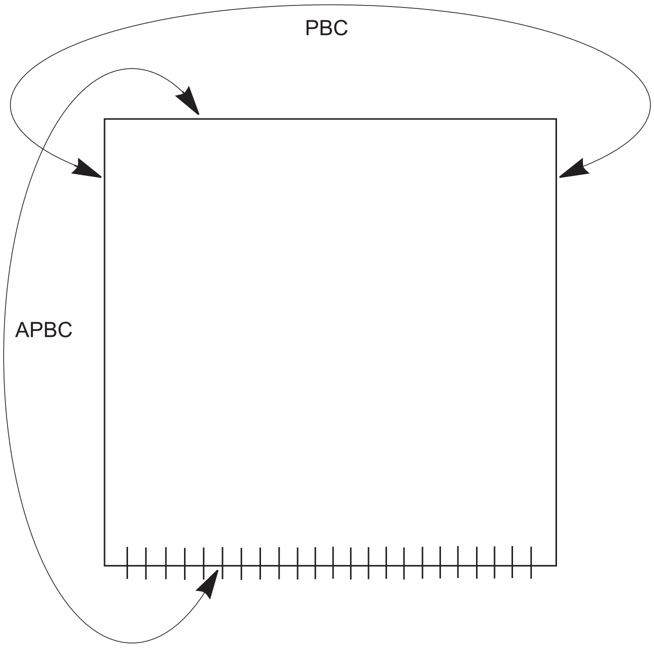

FIG. 2. For the antiperiodic boundary conditions that we imposed, the coupling constants at the bottom line (short vertical dashes) are switched to -1. During nonequilibrium protocols, these interactions quasicontinuously change from 1 to -1 or vice versa.

written as [16]

$$A = -\Delta \sum_{i=0}^{n-1} \sum_{j,j'} s_j^{(i)} s_{j'}^{(i)}, \tag{5}$$

where the first summation is over steps where the coupling constant changes and the second summation is over all (L) pairs of spins along the boundary, where the coupling is modified. The upper index in $s_j^{(i)} s_{j'}^{(i)}$ indicates the spin variables at the ith step. Simulations start by equilibrating the system for 10^5 Monte Carlo steps and then the nonequilibrium protocol that changes the boundary conditions is implemented. To estimate the free-energy difference, the nonequilibrium protocol should be reversible, which means that the number of steps n when the coupling J changes should be large. Such simulations are repeated many times and the values of the extracted work are collected. We distinguish forward processes as such where the boundary conditions change from periodic to antiperiodic and reverse processes where they change from antiperiodic to periodic. Having the probability distributions of A, one can estimate the free-energy difference ΔF either from the Jarzynski relation for the forward processes $\Delta F = -\frac{1}{\beta} \ln \langle \exp(-\beta A) \rangle_F$ or for the reverse processes $\Delta F = \frac{1}{\beta} \ln \langle \exp(-\beta A) \rangle_R$. Alternatively, from the Crooks relation, we obtain that $\Delta F = A$ at the intersection point of these distributions, namely, for $P_F(A) = P_R(-A)$. Having estimated the free-energy difference, we can calculate the surface tension σ of the Ising model that is defined as $\sigma = \Delta F / L$.

We adopt the above scheme for the Ising-doped voter model. It is relatively simple to implement antiperiodic boundary conditions in the presence of voter agents. The antiferromagnetic link for a voter agent means that the agent gets the opposite orientation of the chosen neighbor. To have a possibility of gradual transition from periodic to antiperiodic boundary conditions, we introduce a probability r with which a given voter-type agent gets the same orientation (and with probability $1 - r$, it gets the opposite orientation). The change from periodic to antiperiodic boundary conditions along a chosen line implies a gradual change of the coupling J from 1 to -1, which depending on the type of a chosen agent, is either interpreted as the Ising coupling for an Ising-type agent or a parameter that sets $r = (1 + J)/2$ for a voter.

Although for $p < 1$, the model lacks the Hamiltonian description, we would like to suggest that the ordinary Ising Hamiltonian Eq. (4) may be interpreted as the pseudoenergy of our Ising-doped voter model, with the interpretation of the coupling $J_{i,j}$ depending on the agents it connects. Let us note that for the pure voter model, the value of the expression Eq. (4) is (approximately) related to the distance from the absorbing state (where all spins are aligned), perhaps similarly as the energy Eq. (4) in the Ising model specifies the distance from the ground state. We expect that such a similarity can be also reflected in the dynamical behavior, which could be captured by the fluctuation-theorem methodology. Additional hints supporting such an assumption come from a recent work on the Ising-doped voter model on the complete graph [17]. In this case, one can show that for an arbitrary concentration of the Ising spins, the steady-state magnetization obeys the same equation as for the pure Ising model. It can suggest that even though the Ising-doped voter model is nonequilibrium, the Ising Hamiltonian is (to some extent) still related to its behavior. On finite-dimensional lattices, the behavior of the model is different since, for example, the critical temperature depends on the concentration of the Ising spins [11]. Nevertheless, one might hope that even in this case the pseudoenergy, which has a form of the Ising Hamiltonian, to some extent governs the dynamics of our model. We admit that our assumption that Eq. (4) defines the pseudoenergy in our model is somewhat speculative. However, taking the assumption, we find that the work extracted during the protocols that change boundary conditions is given by the same Eq. (5).

IV. RESULTS

We made simulations for lattices of size $L = 8$, 16, and 32 and $p = 1$ (pure Ising model), 0.7, 0.3, and 0 (pure voter model). First, we distribute randomly Ising and voter agents, with probability p and $1 - p$, respectively. Simulations start from setting random initial values of variables s_i and subsequently the model is equilibrated for 10^5 Monte Carlo steps. Then we implement nonequilibrium protocols that switch boundary conditions from periodic to antiperiodic or vice versa. The switch is quasicontinuous with n steps ($n = 5$, 10, 20, 50, 100, and 200). For the pure Ising ($p = 1$) and pure voter ($p = 0$) models, the experiment is repeated 10^7 times. For the mixed cases $p = 0.7$ and 0.3, the distribution of the Ising and voter variables introduces a certain quenched disorder and we average over 10^3 of such distributions with 10^5 experiments for each distribution. Simulations were made for temperature $T = 1$, which for $p = 1$, 0.7, and 0.3 is below the critical temperature in this model [11]. For the voter model ($p = 0$), the parameter T is meaningless. During

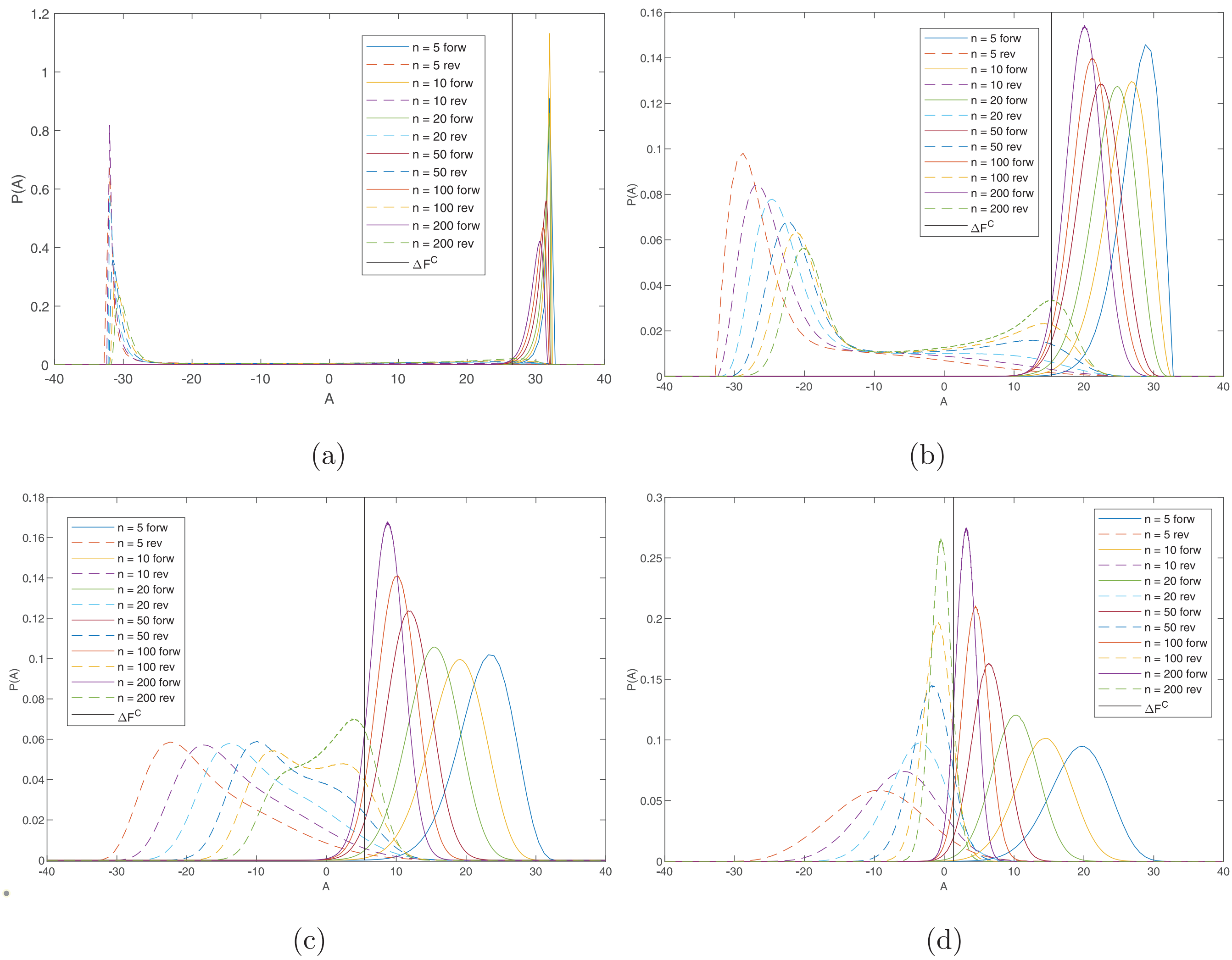

FIG. 3. Probability distributions of work $P_F(A)$ and $P_R(-A)$ for a 16×16 lattice, $\beta = 1$, and four different concentrations of the Ising spins p. Distributions for forward processes are plotted with solid lines and for reverse ones with dashed lines. Black vertical lines indicate intersections of respective distributions and correspond to the free-energy differences obtained using the Crooks method. (a) $p = 1$, Ising model. (b) $p = 0.7$, mixed model. (c) $p = 0.3$, mixed model. (d) $p = 0$, voter model.

each experiment, we calculate the extracted work A Eq. (5) and collect the data to produce two probability distributions. Forward processes that change periodic boundary conditions into antiperiodic (creation of the interface) produce $P_F(A)$ and reverse processes give $P_R(A)$. From the Jarzynski Eq. (1) and Crooks Eq. (2) relations, we can then infer the (effective) free-energy change and the (effective) surface tension.

A. Surface tension

Probability distributions $P_F(A)$ and $P_R(-A)$ for $L = 16$ are presented in Fig. 3 and similar distributions were obtained for $L = 8$ and 32. We did some simulations also for $L = 64$ but for such a large system at a relatively low temperature, fluctuations are small and estimations of the free energy are subject to considerable errors. For $p = 1$, our results are very similar to those obtained by Híjar and Sutmann [16]. Using these distributions, we estimate the surface tension σ and the results are presented in Fig. 4. In analogy to transitions between equilibrium states, we plot numerical data as a function of $1/n$ and analyze the data in the limit $n \rightarrow \infty$.

For $p = 1$ [Fig. 4(a)], the estimation of σ is close to 1.7. In this case, our estimate can be compared with an exact result for the pure Ising model, due to Onsager [18],

$$\sigma = 2 - \frac{1}{\beta} \ln[\coth(\beta)], \tag{6}$$

which gives $\sigma \approx 1.7277\ldots$ for $\beta = 1$.

For $p = 0.7$ [Fig. 4(b)] and 0.3 [Fig. 4(c)], only a fraction of spins operate according to the Ising heat-bath dynamics. Consequently, the parameter β, which enters the fluctuation relations Eqs. (1) and (2), most likely is different than $1/T$. In such a case, we estimate the surface tension using only the Crooks relation Eq. (2) since this method does not depend on the explicit value of temperature. The obtained results indicate that the surface tension for $p = 0.7$ and 0.3 remains positive. Such a result confirms the earlier findings [11] that the model coarsening dynamics indicates the existence of a certain effective surface tension. Values of the surface tension

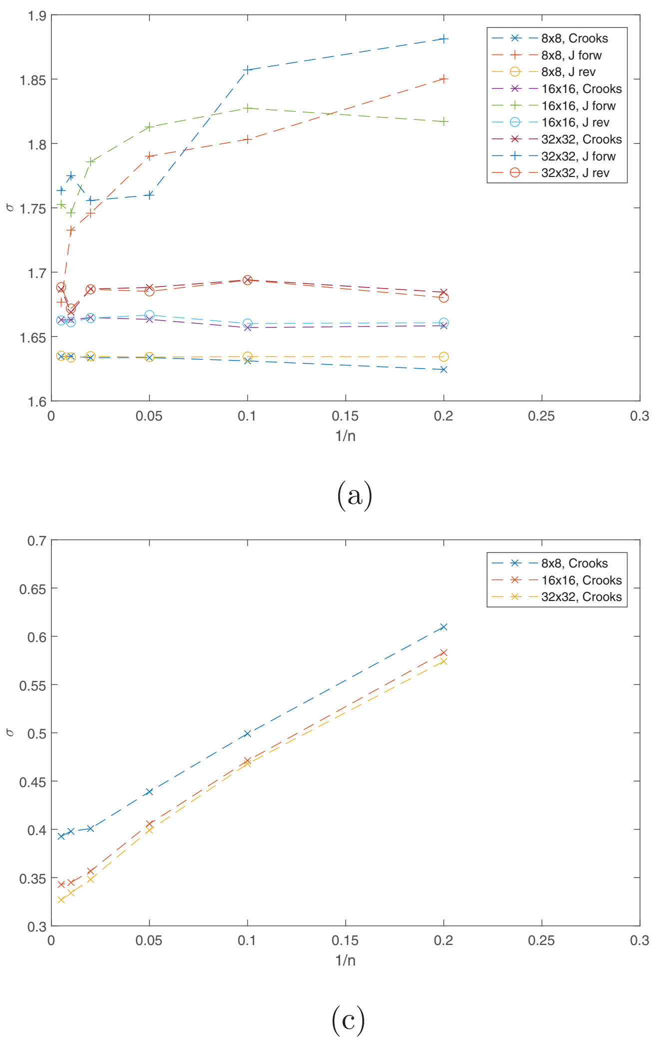

FIG. 4. Surface tension estimates σ for $\beta = 1$ and four different concentrations of the Ising spins p. For the pure Ising model (a), three methods were used because the temperature is known. For other cases, only the effective temperature exists but the Crooks method is still applicable. (a) $p = 1$, Ising model. (b) $p = 0.7$, mixed model. (c) $p = 0.3$, mixed model. (d) $p = 0$, voter model.

that are lower than for $p = 1$ are also plausible since the critical temperature decreases for decreasing p and thus the model shifts toward to the transition point.

We also ran simulations for the pure voter model ($p = 0$) [Fig. 4(d)]. In this case, the surface tension seems to have much smaller values and the bending of our data indicates that it can even converge to 0. Such a result is consistent with some other indications that the voter model can be tensionless [12].

An important property of the surface tension in the Ising model is its vanishing at the critical point. To verify this behavior, we did calculations of the surface tension for $p = 0.7$ and for several values of temperature. The obtained results (Fig. 5) suggest that the surface tension vanishes around $T = 2.2$ and such behavior is consistent with the estimation of the critical temperature based on the behavior of magnetization [11].

B. Effective temperature

As we have already mentioned, for $p < 1$ due to a fraction of the voter agents, there are some strictly forbidden transitions between configurations in our model and the detailed balance is broken. In such a case, the model is

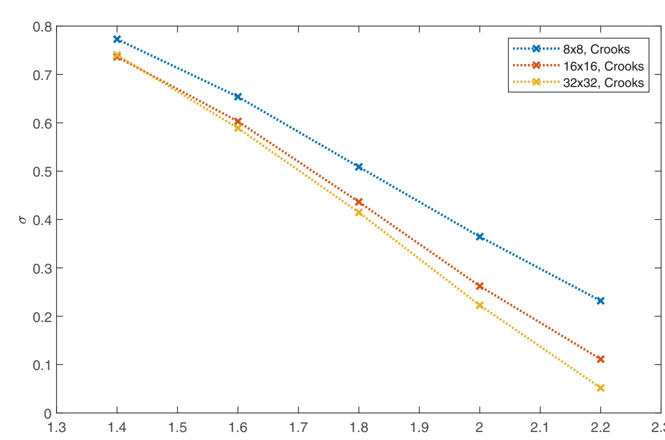

FIG. 5. Surface tension σ as a function of temperature T for $p = 0.7$ and $n = 200$.

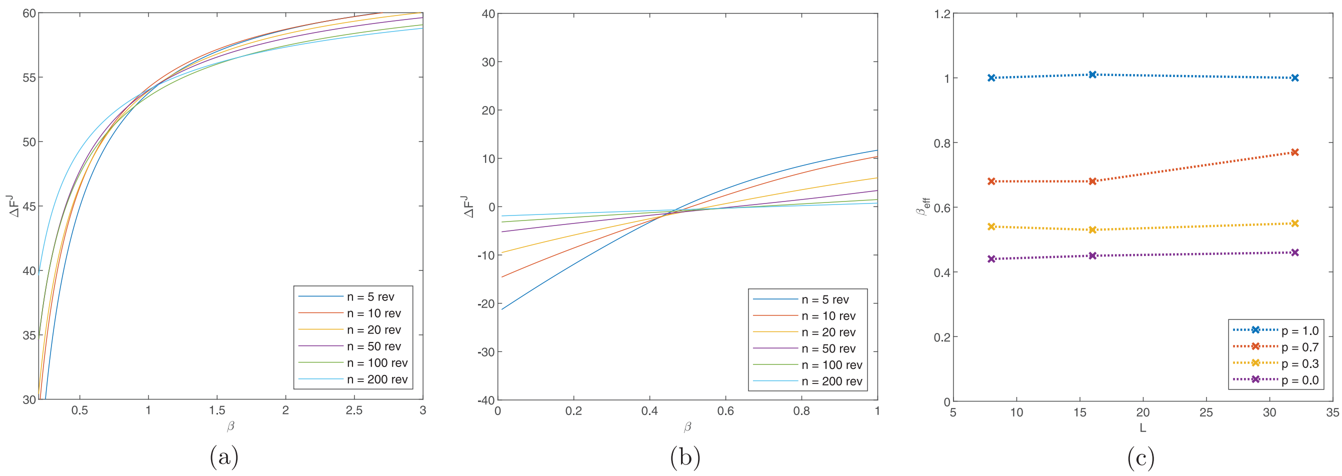

FIG. 6. Crossings of the free-energy differences for the 32×32 Ising model (a) and the voter model (b). Based on the crossings, we estimated the effective temperature, which is plotted as a function of the system size L (c). (a) $p = 1$, Ising model. (b) $p = 0$, voter model. (c) $\beta_{\text{eff.}}$

nonequilibrium and the temperature T has only a dynamical meaning, namely, it is a parameter governing the evolution of the Ising spins. Nevertheless, one can assume that the steady state of our model is characterized by a certain effective temperature, which for $p < 1$ is most likely different than T. In this section, we would like to suggest that probability distributions $P(A)$ and fluctuation theorems can allow us to determine such an effective temperature.

In particular, we examined the free-energy difference as calculated from the Jarzynski relation for reverse processes $\Delta F = \frac{1}{\beta} \ln \langle \exp(-\beta A) \rangle_R$ and the results are plotted as a function of β in Figs. 6(a) and 6(b). One can note that when plotted for several values of n, these results seem to cross at a certain value of β and such behavior is particularly transparent for the voter model [Fig. 6(b)]. One might expect that for the plotted free-energy differences, the dependence on the number of steps n is similar to the size dependence for some equilibrium quantities. For example, for the Binder cumulant, such crossing is a frequently used method to locate the phase transition [19]. Based on the intersection of the highest n data ($n = 50, 100, 200$), we estimate the effective β and the results are plotted in Fig. 6(c) For the Ising model ($p = 1$), our method fairly well reproduces the expected value $\beta = 1$. For decreasing p, the estimated β decreases and for the voter model ($p = 0$), we obtain $\beta \sim 0.44$. This value corresponds to $T = 2.27$, which is very close to the critical temperature of the Ising model [18]. Let us notice that at the critical point, the Ising model becomes tensionless, similarly to the voter model. However, the Ising model remains tensionless at any temperature higher than the critical temperature and further studies would be needed to verify whether this is just a numerical coincidence or a manifestation of an interesting relation between Ising and voter models dynamics. Let us also note that for some nonequilibrium systems, the effective temperature can be determined using generalized fluctuation-dissipation relations [20]. Such an approach used for the voter model predicts the effective temperature $T = 3.641$ [21].

V. CONCLUSIONS

In our paper, we presented numerical evidence that the fluctuation relations of Jarzynski and Crooks can be used to study transitions between the stationary states of a nonequilibrium model. In particular, we calculated the surface tension and the effective temperature for an Ising-doped voter model. We adapted the method developed for the Ising model [16], which utilizes switching between periodic and antiperiodic boundary conditions.

The obtained results confirm the earlier observation [11] that the model dynamics generates an effective surface tension. In the limiting case of the voter model, our simulations support the expectation [12] that in this case the dynamics is tensionless. From the crossing of the free-energy differences calculated at various speeds of the numerical protocol, we estimated the effective temperature of the model. It is perhaps worth further studying why the effective temperature of the voter model happened to be very close to the temperature where the Ising model loses the surface tension.

To extract the work performed during nonequilibrium processes that switch boundary conditions, we assumed that the expression analogous to the Ising Hamiltonian defines a pseudoenergy of our model. We suggested that for the Ising-doped voter model, there can be some reasons justifying such an assumption, although, in general, a possible existence and the form of such a pseudoenergy certainly remains an open problem.

ACKNOWLEDGMENTS

This work was supported by funds from the project Inicjatywa Doskonałości—Uczelnia Badawcza, Adam Mickiewicz University in Poznań-Study@research, Grant No. 034/34/UAM/0003.

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