Critical behavior of a displacive structural phase transition in two dimensions

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The critical behavior of the displacive structural phase transition in a two-dimensional model solid due to Benassi et al. [Phys. Rev. Lett. 106, 256102 (2011)] is analyzed using Monte Carlo simulations and finite-size scaling. The transition temperature in the thermodynamic limit is determined, as well as the critical exponents. The exponents differ distinctly from those of Ising/Potts universality. The exponent of the specific heat is negative, implying that the specific heat at the transition does not diverge.

I. INTRODUCTION

Complex oxide solids are known to exhibit structural phase transitions. A famous example is the perovskite material BaTiO$_3$ which undergoes such a transition at $T_c = 393$ K. The transition is characterized by a shift of Ti and O atoms in the unit cell, while the positions of Ba atoms remain essentially unchanged. These transitions are relevant for applications, as material properties below and above $T_c$ typically differ, but are also interesting in their own right regarding the fundamentals of solid phase behavior. Consequently, these transitions have received considerable theoretical attention, including increasingly, by means of computer simulation.

An example of the latter is a molecular dynamics investigation by Benassi et al. which considered how sliding friction changes when the underlying substrate undergoes a (displacive) structural phase transition. These simulations used particle interactions for the substrate tailored to support a transition, but otherwise kept the complexity at a minimum. As such, the model is ideal for high-resolution numerical studies concerning the generic effects of structural phase changes in materials, though it does not address a specific real material in particular. In addition to sliding friction, which at the transition reaches a maximum, the authors also briefly address the complexity at a minimum. As such, the model is ideal for high-resolution numerical studies concerning the generic effects of structural phase changes in materials, though it does not address a specific real material in particular. In addition to sliding friction, which at the transition reaches a maximum, the authors also briefly address the complexity at a minimum.

The outline of this paper is as follows: We first describe the Benassi model. Next, a brief summary of critical behavior is provided, including the definitions of the critical exponents. The details of our simulation method are described thereafter. The application of finite-size scaling to our simulation data is presented in the results section. We conclude in Section IV with a brief summary and outlook to future work.

II. MODEL AND METHODS

A. Benassi particle model

The Benassi model provides a simple description of a material exhibiting a structural phase transition. It qualitatively resembles a system whereby, during the transition, one of the particle species remains fixed (as do, e.g. Ba atoms in the case of BaTiO$_3$). The fixed species is assumed to provide an underlying lattice structure, as well as to give rise to a (static) external field acting on the mobile species. It is assumed there is only one type of mobile particle species, and the total number of these particles is denoted $N$. In addition, there is a pair interaction between the mobile species, described in the form of permanent anharmonic bonds. The total energy of the system is thus given by $E = \sum_{ij} u_{ij} + \sum_{i=1}^{N} h_i$, where $[ij]$ is a sum over bonded pairs of particles $i$ and $j$, $u_{ij}$ the corresponding bond energy, and $h_i$ the external field acting on particle $i$.

The underlying crystal structure is assumed to be a hexagonal lattice, i.e. the model is purely two-dimensional. The nearest neighbor distance between lattice points is denoted $a$. To each lattice position $\vec{R}_i$, a single particle is assigned ($i = 1, \ldots, N$). The displacement of particle $i$ from its lattice position $\vec{R}_i$ is denoted $\vec{r}_i = (x_i, y_i)$. During the simulations, the particle displacements $\vec{r}_i$ are allowed to fluctuate, but the lattice positions $\vec{R}_i$ remain fixed.

Each particle is bonded to its six nearest neighbors by means of an anharmonic spring. The spring energy is given by $u_{ij} = b_2(d_{ij} - a)^2 + b_4(d_{ij} - a)^4$ with $d_{ij} = |\vec{R}_i + \vec{r}_j - \vec{R}_j - \vec{r}_i|$ the distance between the two particles. The bonds (3N in total) are assigned once at the start of the simulation. During the simulations, there is no
breaking of bonds, nor the formation of new bonds.

The external field acting on particle $i$ is defined in terms of its displacement $\mathbf{r}_i$ as follows:

$$h_i = \varepsilon \left( \frac{\mathbf{r}_i}{a_0} \right)^4 - 2\varepsilon \left[ (3 \cos \theta_i - 4 \cos^3 \theta_i) \frac{\mathbf{r}_i}{a_0} \right]^2,$$

with $r_i = \sqrt{x_i^2 + y_i^2}$ and $\cos \theta_i = x_i/r_i$. Due to the external field $h_i$, each lattice position $\mathbf{R}_i$ is “surrounded” by six local energy minima, at coordinates $\mathbf{R}_i + a_0(\cos \pi \lambda/3, \sin \pi \lambda/3)$, with $\lambda = 1, 2, 3, 4, 5, 6$. A single particle can thus minimize its field energy by selecting one of the surrounding minima. In order to simultaneously minimize the bond energy requires that all particles choose the same value of $\lambda$. The model thus features a high-temperature phase (all values of $\lambda$ equally likely), and a low-temperature phase (one dominating value of $\lambda$), with the transition occurring at $T_c$. As the temperature is lowered through the transition, the particles collectively shift into the same minimum, reminiscent of a displaceable structural phase transition.

In what follows, $b_2 = 28.32U/a^2$, $b_4 = 784.35U/a^4$, $\varepsilon = 0.2U$, and $a_0/a = 0.05$, which are the values of the original reference [2]. The lattice constant $a$ will be our unit of length, and temperature will be expressed in units of $U/k_B$, with $k_B$ the Boltzmann constant. We use rectangular $L_x \times L_y$ simulation cells with periodic boundary conditions in both dimensions. To prepare the initial hexagonal lattice, we take as unit cell a $t_x \times t_y$ rectangle, with $t_x = a$ and $t_y = \sqrt{3}a$. The unit cell contains two lattice sites, at coordinates (0, 0) and ($t_x/2, t_y/2$). This unit cell is then replicated 2n times in the $x$-direction, and $n$ times in the $y$-direction, with integer $n$. Consequently, $N = 4n^2$, $L_x = 2an$, $L_y = \sqrt{3}an$, and it is ensured that, irrespective of $n$, all our simulation cells have the same aspect ratio $L_x/L_y$.

### B. Order parameter distribution and criticality

A key quantity in the numerical analysis of phase transitions is the order parameter distribution $P(m)$ (OPD), defined as the probability to observe a micro-state with order parameter $m$. For the Benassi model, a suitable definition is $m = \langle \sum_{i=1}^{N} \mathbf{r}_i \rangle/(a_0 N)$. We emphasize that the OPD depends on the temperature $T$, as well as on the system sizes $L_x, L_y$.

Assuming the OPD is known, thermal averages can readily be computed. The thermally averaged order parameter, for instance, follows as $\Delta = \langle m \rangle = \int m P(m) dm$, where it is assumed that $P(m)$ is properly normalized. In the ordered phase (low temperature), where the majority of particles have selected the same minimum, $\Delta \sim 1$. In the disordered phase (high temperature), where the distribution of the particles over the minima is random, $\Delta \sim 0$. In the vicinity of the (continuous) transition, at temperature $T = T_c$, one expects a power law dependence, $\Delta \propto (t/T_c)^{\beta}$, $t = T/T_c - 1$, with critical exponent $\beta$. This power law describes the variation of $\Delta$ with $T$ in the thermodynamic limit (infinite system size) for $T \leq T_c$ (for $T > T_c$, $\Delta = 0$). Similarly, we can define the order parameter fluctuation (susceptibility) as $\chi = N \langle (\langle m^2 \rangle - \langle m \rangle^2) / N \rangle$, with the required thermal averages $\langle \cdots \rangle$ again be obtained from the OPD. The susceptibility diverges at the transition, $\chi \propto |t|^{-\gamma}$, with critical exponent $\gamma$. Also of interest is the specific heat, $c_V = \langle (E^2) - \langle E \rangle^2 \rangle / N$, with $E$ the energy of the system. It is common for the specific heat to diverge at the transition, $c_V \propto |t|^{-\alpha}$, provided the critical exponent $\alpha > 0$. As it turns out, for the Benassi model, $\alpha < 0$, in which case the specific heat remains finite. We note that, in order to compute $c_V$, the OPD $P(m)$ alone is not sufficient, and that information about the energy fluctuations is then also required, to be explained later. Finally, at the transition, the correlation length diverges as well, $\xi \propto |t|^{-\nu}$, defining the critical exponent $\nu$.

There are more critical exponents that can be defined, but the above suffices for our purposes. Various mathematical relations between critical exponents have been derived [3, 4], in particular the Rushbrooke and hyperscaling relations, $2 - \alpha = 2\beta + \gamma = d\nu$, where $d$ is the spatial dimension ($d = 2$ presently). We stress again that power law behavior is only observed in the thermodynamic limit, which simulations cannot probe directly. The standard procedure is to perform simulations of different system sizes, and to systematically extrapolate to the thermodynamic limit using finite-size scaling, to be explained later.

### C. Monte Carlo methods

As stated in the Introduction, the Monte Carlo (MC) method is used to analyze the phase behavior. The central aim of these simulations is to accurately obtain the OPD $P(m)$, from which the critical temperature $T_c$ and critical exponents $\beta, \gamma, \nu$ can be determined. The MC move that we use consists of the random selection of one of the particles, which is then displaced by a (two-dimensional) vector drawn randomly from inside a circle of radius $0.1a$. A common choice is to then accept the move with the Metropolis probability, $P_{\text{acc}} = \min[1, \exp(-\Delta E/k_BT)]$, with $\Delta E$ the energy difference between initial and proposed state, and $T$ the temperature (for rejected moves, the particle is shifted back to its position at the start of the move). In principle, by using standard Metropolis, the OPD $P(m)$ can be straightforwardly obtained, by maintaining a histogram of observed $m$ values. However, this approach is far from optimal.

To boost efficiency, we instead use Wang-Landau sampling [5, 6], in conjunction with the collection of transition matrix elements [7, 8], as well as a scheme to systematically extrapolate simulation data to different (nearby) temperatures [10]. In order to apply these methods, the (micro-state) order parameter $m$ needs to be discretized,
which in this work is done in steps of $\Delta m = 0.25/N$ (larger systems require a finer discretization). A continuous value of $m$ may then be converted to an integer index $\tilde{m} = \text{int}(m/\Delta m)$, where “int” means rounding down to the nearest integer. In what follows, whenever the symbol $m$ appears with an overbar, it is to be interpreted as the integer index of the corresponding micro-state order parameter. To convert the index back, we use the relation $m \simeq (\tilde{m} + 0.5)\Delta m$. This relation has a binning error associated with it, but for the resolution $\Delta m$ used by us, no ill side effects were noticed.

The purpose of Wang-Landau sampling is to force the simulation to visit a larger portion of phase-space. It does so by adding a bias function $W$ to the potential energy of the system, such that MC moves must now be accepted with $P_{\text{WL}} = \min[1, \exp(-\Delta E/k_B T - \Delta W)]$, with $\Delta W$ the bias function difference between initial and proposed state. In the present work, we choose a bias function that depends on the (discretized) micro-state order parameter: $W \equiv W(m)$. MC moves proposing states for which $W(\tilde{m})$ increases (decreases), are now less (more) likely to be accepted, see the equation for $P_{\text{WL}}$. Hence, by tuning the bias, one can systematically “force” the simulation to also “visit” micro-states with values of $m$ that would otherwise rarely be sampled. Ideally, one seeks a bias function such that all values of $\tilde{m}$, over some specified range of interest, are sampled equally often on average. The Wang-Landau algorithm [5, 6] provides a way to achieve this, and we refer the reader to the original references for the details.

The second optimization is the collection of transition matrix elements $M_{kl}$ [7, 9]. Each time a MC move is proposed, from a state with $\tilde{m} = k$ to one with $\tilde{m} = l$, one adds the corresponding Metropolis probability $P_{M}^{kl}$ (not the Wang-Landau version $P_{\text{WL}}^{kl}$) to the matrix element $M_{kl}$. The matrix element is updated irrespective of whether the MC move is accepted. Hence, also rejected moves contribute to the data collection process, which is a huge bonus. From the transition matrix elements, free energy differences between states can be computed. To this end, one defines $P_{kl} = M_{kl}/\sum_{l} M_{kl}$, which can be interpreted as the probability that, being in a state with $\tilde{m} = k$, a state with $\tilde{m} = l$ is proposed. The latter is related to the free energy difference between the states: $\Delta F_{kl} = F(l) - F(k) = k_B T \ln(p_{kl}/p_{kl})$. Hence, from the transition matrix, a large set of free energy differences is obtained. To construct, from this set, the best estimate of the free energy $\tilde{F}(\tilde{m})$ as a function of $\tilde{m}$, one minimizes the error $\Sigma^2 = \sum_{l} (\tilde{F}(l) - \tilde{F} - \Delta F_{kl})^2$, where the sum is over all free energy differences in the set [9]. This yields a system of linear equations for the values $\tilde{F}(\tilde{m})$, which can be solved with standard numerical routines. From the free energy, the OPD trivially follows using $\tilde{F}(\tilde{m}) = -k_B T \ln P(\tilde{m})$.

As a last optimization, we use the scheme of Ref. [10] to facilitate the extrapolation of the OPD obtained at temperature $T = T_0$ to a different (nearby) temperature $T = T_1$ without having to do additional simulations. To this end, we introduce the energy moments $\langle E^k \rangle_m$, with $E$ the energy, and $\langle \cdot \rangle_m$ an average over all micro-states whose order parameter index equals $\tilde{m}$. The moments are readily collected in our Monte Carlo simulations: At the end of each move, one simply identifies the current order parameter bin $\tilde{m}$, and “updates” the corresponding energy moment bins. If $P_0(\tilde{m})$, $\rho_{0,m} = \langle E \rangle_{0,m}$, and $\sigma^2_{0,m} = \langle E^2 \rangle_{0,m} - \langle E \rangle_{0,m}^2$ denote the OPD and energy moments measured at $T = T_0$, then the OPD at $T = T_1$, may be approximated as

$$\ln P_1(\tilde{m}) \approx \ln P_0(\tilde{m}) - \rho_{0,m} \Delta \beta + \frac{\sigma^2_{0,m}(\Delta \beta)^2}{2},$$

with $\Delta \beta = 1/k_B T_1 - 1/k_B T_0$ (note that one must not forget to normalize $P_1(\tilde{m})$ after extrapolation).

By using the above extrapolation formula, the variation of the order parameter $\Delta$ and susceptibility $\chi$ with $T$, is readily obtained. If also the temperature dependence of the specific heat $C_V$ is desired, one additional step is needed because, by changing $T$, also the energy moments $\langle E \rangle_m$ will change. Hence, given $\langle E \rangle_m$ obtained at $T = T_0$, we still need to explain how to extrapolate these moments to obtain $\langle E \rangle_m$ at $T = T_1$. To this end, we assume that the distribution of energy values $H_m(E)$ between micro-states with the same value of $\tilde{m}$ is Gaussian. In particular, at $T = T_0$, $H_m(E) \propto e^{-(E - \mu_m)^2/2 \sigma^2_{m}}$. The latter can be extrapolated to $T = T_1$ using standard histogram reweighting [11], $H_{1,m}(E) \propto H_m(E)e^{-\Delta \beta E}$, which, after some straightforward algebra, yields:

$$\langle E \rangle_{1,m} \approx \mu_{0,m} - \sigma^2_{0,m}(\Delta \beta),$$

$$\langle E^2 \rangle_{1,m} \approx \sigma^2_{0,m} + (\mu_{0,m} - \sigma^2_{0,m}(\Delta \beta))^2.$$

The thermally averaged energy moments at $T = T_1$ thus become $\langle E \rangle_{1,m} = \sum_{m} \langle E \rangle_{1,m} P_1(\tilde{m})$, from which the specific heat can be computed. We emphasize that, since the extrapolation of the energy moments relies on the assumption of Gaussian energy distributions, the temperature range over which the specific heat can be accurately obtained is smaller than that of the order parameter and susceptibility.

In our simulations, for a given system size and temperature, the order parameter range $0 \leq m \leq 0.9$ is sampled using the Wang-Landau method. We typically split the range into $5 - 15$ subintervals, and assign a single processor to each subinterval. The collected data is then combined afterward to obtain the OPD. In the vicinity of $T_c$, we found that $\sim 2$ simulations performed at different temperatures suffice to sample the entire transition, using the above extrapolation scheme to obtain data at “in between” temperatures.

III. RESULTS

In what follows, we define $L \equiv L_x$ to denote the size of the system.
Fig. 1: Susceptibility $\chi$ as a function of temperature $T$ for system size $L = 40$. The temperature at the maximum defines $T_{c,L}$, the value of $\chi$ at the maximum $\chi_{\text{max},L}$. To assess the magnitude of the statistical error in the data, three curves are shown, each corresponding to a different set of Poissonian random noise. On the scale of the graph, the curves overlap perfectly, showing that the statistical error is negligible.

A. Susceptibility

We begin our finite-size scaling study by analyzing the susceptibility $\chi$. Fig. 1 shows the variation of $\chi$ with the temperature $T$ using system size $L = 40$. To quantify the magnitude of the statistical error in our data, we have added, to each transition matrix element $M_{kl}$, a Poissonian deviation $\Delta M_{kl} = r \sqrt{M_{kl}}$, with uniform random numbers $0 \leq r \leq 1$. Fig. 1 actually contains three curves, corresponding to three different sets of the random numbers $r$, but the overlap is essentially perfect. Hence, on the scale of the graph of Fig. 1 and those to follow, we believe that the statistical error is negligible.

Consistent with a continuous phase transition in a finite system, the graph of $\chi$ versus $T$ reveals a maximum, but there is no divergence. We now define $T_{c,L}$ as the temperature where $\chi$ obtains its maximum, as measured in a system of size $L$. We also define $\chi_{\text{max},L}$, as the corresponding value of $\chi$ at the maximum. Following finite-size scaling theory [12], at a continuous phase transition, one expects $T_{c,L} - T_c \propto L^{-1/\nu}$ and $\chi_{\text{max},L} \propto L^{\gamma/\nu}$, with $T_c$ the transition temperature in the thermodynamic limit ($L \to \infty$), and critical exponents $\gamma, \nu$ defined earlier. Hence, by performing simulations for several system sizes $L$, and then fitting the data to the finite-size scaling relations, $T_{c,L}, \gamma, \nu$ can be obtained. Following this procedure, we plot in Fig. 2(a) the temperatures $T_{c,L}$ versus $L^{-1/\nu}$, where system sizes $L = 20 - 60$ were used. By plotting versus $L^{-1/\nu}$, the data should collapse on a straight line, provided the correct value of $\nu$ is used, which we obtained by fitting. From the fit, $\nu \approx 1.32$, and the linear dependence is strikingly confirmed. The intercept of the line yields as critical temperature $T_c \approx 0.0623$. Fig. 2(b) shows $\chi_{\text{max},L}$ versus $L$. The data are well described by a power law, and by fitting we obtain $\gamma/\nu \approx 1.70$. We emphasize that, for the analysis of the susceptibility, short simulations were performed beforehand to roughly locate $T_{c,L}$. Production runs were then performed at these values. The range in temperature over which extrapolations were performed to generate the data of Fig. 2 was therefore minimal.

B. Binder cumulant

To test the consistency of our estimate of $T_c$, we plot in Fig. 3 the Binder cumulant, $U_4 = 1 - \langle m^4 \rangle / (3 \langle m^2 \rangle^2)$, versus $T$, for several system sizes $L$. The vertical line indicates our estimate of $T_c$. For the data of Fig. 3, simulations were performed close to the temperature $T_c$ derived from Fig. 2(a). Hence, also in Fig. 3, the extrapolation range was kept at a minimum. In line with a critical phase transition [13-14], the curves for different $L$ intersect at $T_c$. The intersection is not perfect, especially the data for $L = 20$ appear off, which we attribute to corrections to scaling (in order for finite-size scaling theory to be applicable, the system size $L$ must be large enough [14]).
D. Specific heat

Finally, we consider the critical behavior of the specific heat $c_V$. Analogously to the susceptibility, the graph of $c_V$ versus $T$ reveals a maximum. Let $c_V^{\text{max},L}$ denote the value of the specific heat at the maximum, as obtained in a system of size $L$. In Fig. 5, we plot $c_V^{\text{max},L}$ versus $L$. Comparing this to Fig. 2(b) of the susceptibility, one sees that the behavior of $c_V^{\text{max},L}$ is fundamentally different: Instead of diverging with $L$, $c_V^{\text{max},L}$ appears to saturate at a finite value. Our results thus indicate that the specific heat does not diverge at the transition, implying that the critical exponent $\alpha$ is negative. Indeed, our measured value of the correlation length critical exponent implies, due to hyperscaling, $\alpha = 2 - d\nu \approx -0.63$, which is distinctly negative.

IV. CONCLUSION

In conclusion, we have accurately determined the critical temperature $T_c$ and critical exponents of a displacive phase transition in a two-dimensional model originally proposed by Benassi et al. [2]. The thermodynamic limit estimate $T_c \approx 0.0623$ of the present work is somewhat below $T_c \approx 0.075$ of Ref. [2] obtained in a finite system, a finding that makes sense since the apparent transition temperature decreases with system size, see Fig. 2(a).

More surprisingly, our analysis reveals a rather large value of the critical exponent of the correlation length. Consequently, the specific heat critical exponent is negative, meaning that the specific heat at the transition remains finite, as opposed to diverging. Comparing to the critical behavior of the two-dimensional Potts model (which includes the Ising model), the exponents obtained by us differ markedly. In particular, our estimates for $\beta/\nu$ and $\gamma/\nu$ cannot be matched to those of the Potts model, for any value of the number of states $0 \leq q \leq 4$ where the transition in the Potts model is continuous [10]. Hence, the universality class of the Benassi model is a different,

C. Critical OPD

Next, we consider the shape of the OPD, $P(m)$, at the critical temperature. Following finite-size scaling, at $T = T_c$, the OPD becomes scale invariant [15]. That is, by plotting the scaled distribution, $P(x)$, with scaling variable $x = mL^{\beta/\nu}$, the distributions for different system sizes $L$ should become identical, provided the correct value of $\beta/\nu$ is used. From our previous estimate of $\gamma/\nu$, and using the hyperscaling relation, we obtain $\beta/\nu = (d - \gamma/\nu)/2 \approx 0.15$. Using the latter value, as well as our estimate of $T_c$, the scaled distribution can be explicitly obtained. The result is shown in Fig. 4 and the collapse of the data for the various system sizes onto a single master curve is strikingly confirmed. In Fig. 3, the data for $L = 20$ was omitted since, judging from the cumulant plot, corrections to scaling are then quite strong.

FIG. 3: Binder cumulant $U_4$ versus $T$ for different system sizes $L$. The intersection of the curves yields an estimate of $T_c$, which, indeed, is close to the estimate of Fig. 2(a), indicated here by the vertical line.

FIG. 4: Scaled order parameter distribution $P(x)$, with scaling variable $x = mL^{\beta/\nu}$, obtained at the critical temperature $T = T_c$, for various system sizes $L$ as indicated. The collapse onto a single master curve is strikingly confirmed. The value of $\beta/\nu$ used in this plot is the one implied by hyperscaling and our previous estimate of $\gamma/\nu$.

FIG. 5: Variation of the specific heat maximum $c_V^{\text{max},L}$ with system size $L$. The specific heat appears to saturate at a finite value, implying a negative critical exponent $\alpha$. 
possibly novel, one.

As demonstrated in Fig. 1, the statistical error in the simulation data of the present work is small. Hence, running the simulations for longer times, we do not expect our $T_c$ and exponent estimates to significantly change. In addition, since the simulation temperatures were carefully chosen to be close to the temperature of interest, the systematic error introduced by our extrapolation scheme is also small. The one remaining systematic error is therefore the before-mentioned “correction to scaling” [4]. In principle, it cannot be ruled out that, for larger values of $L$ beyond our present scope, a cross-over to a different universality class occurs [17]. For the Benassi model, due to its six-fold symmetry, a cross-over to the $q = 6$ Potts model might seem plausible. If this were the case, the transition should ultimately become first-order [16]. However, for the values of $L$ currently accessible, no sign of such a cross-over is visible, and all the evidence strongly indicates a continuous transition.

Having studied the equilibrium properties of the transition in the Benassi model, we are currently studying non-equilibrium dissipative processes (friction) using the same model. One question we seek to answer is to what extent friction measurements depend on system size. While the study of finite-size effects in simulations at (equilibrium) phase transitions is well established, much less is known regarding non-equilibrium situations.

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