Sheared Ising models in three dimensions

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Abstract - The nonequilibrium phase transition in sheared three-dimensional Ising models is investigated using Monte Carlo simulations in two different geometries corresponding to different shear normals. We demonstrate that in the high shear limit both systems undergo a strongly anisotropic phase transition at exactly known critical temperatures $T_c$ which depend on the direction of the shear normal. Using dimensional analysis, we determine the anisotropy exponent $\theta = 2$ as well as the correlation length exponents $\nu_\parallel = 1$ and $\nu_\perp = 1/2$. These results are verified by simulations, though considerable corrections to scaling are found. The correlation functions perpendicular to the shear direction can be calculated exactly and show Ornstein-Zernike behavior.

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Introduction. – While the occurrence of nonequilibrium phase transitions is ubiquitous in nature, its investigation in the framework of nonequilibrium statistical mechanics is intricate and restricted to a few simple models, like the driven lattice gas (DLG) [1–3] or, recently, to the driven two-dimensional Ising model [4]. In this model the system is cut into two halves parallel to one axis and moved along this cut with velocity $v$. The model exhibits energy dissipation and subsequently friction due to spin correlations, which also occurs in a suitable Heisenberg model [5–8] and, of interest for the current context, undergoes a nonequilibrium phase transition from an ordered low-temperature phase to a disordered high-temperature phase. This transition has been investigated analytically as well as with Monte Carlo (MC) simulations for various geometries [9]. Since then, this model has been generalized to the driven Potts models [10], and finite-size effects were calculated analytically in the driven Ising chain [11].

A lot of similarities and comparable critical behavior between the Ising model with friction and the very famous and well-investigated DLG have been found [12]. Both models are characterized by a critical temperature $T_c$, which increases with the external drive, which is the field or the shift/shear velocity $v$, respectively, and saturates in the high driving limit. The critical temperature has been calculated analytically in the limit $v \to \infty$ for various geometries of the Ising model with friction [9].

Moreover, it was discovered that the DLG and two-dimensional sheared Ising systems with non-conserved order parameter [12–14] show strongly anisotropic critical behavior, with direction-dependent correlation length exponents $\nu_\parallel$ and $\nu_\perp$. For the 2d and 1 + 1d geometry of the Ising model with shear the same exponents $\nu_\parallel = 3/2$ and $\nu_\perp = 1/2$ [12] as in the two-dimensional DLG have been determined. Additionally, finite velocities $v$ have been studied and it was found that for all finite $v$ the 2d model and 1 + 1d model cross over from isotropic Ising-like behavior to strongly anisotropic mean-field behavior in the thermodynamic limit, demonstrating that the external drive is a relevant perturbation.

In the following we shall extend the investigations to a three-dimensional model with two different shear geometries and focus on the high shear velocity limit $v \to \infty$. This three-dimensional model is experimentally accessible in the framework of sheared binary liquids [15–18], albeit the order parameter is not conserved here. Using dimensional analysis, we predict the correlation length exponents for arbitrary dimension $d$. These predictions are verified by simulations; however we find strong corrections to scaling at small system sizes.

Model. – The systems considered in this work are denoted $2 + 1d$ and $1 + 2d$ and are shown in fig. 1, for a classification see ref. [9]. In the $2 + 1d$ geometry shear is applied such that two-dimensional Ising models are moved relative to their upper (lower) neighboring layer with velocity $v$ ($-v$) along one axis. In the following we denote the direction parallel to the shear with $\parallel$, the direction perpendicular to the planes with $\perp_1$ and the
inplane direction perpendicular to the shear direction with $\perp 2$. The model contains $L_{\perp 1} \times L_{\perp 2} \times L_{\parallel}$ spins (lattice sites), where we choose $L_{\perp 1} = L_{\perp 2} = L_{\perp}$ throughout this work, and periodic boundary conditions are applied in all directions. The shear velocity $v$ corresponds to a shear rate, which is often denoted as $\dot{\gamma}$ [13,14]. Using the notation $(\perp 1 \perp 2 ||)$ for directions, the shear is in $(001)$-direction and the shear normal is in $(100)$-direction.

A finite shear velocity $v$ is implemented by shifting neighboring layers $v$ times by one lattice constant during one MC step (for details see [4,9]). A simplification of the implementation is yielded by reordering the couplings between moved layers instead, and by introducing a time-dependent displacement $\Delta(t) = vt$. Hence we get the Hamiltonian

$$\beta H(t) = -\sum_{k=1}^{L_{\perp 1}} \sum_{l=1}^{L_{\perp 2}} \sum_{m=1}^{L_{\parallel}} \sigma_{klm} \left( K_{\perp} \sigma_{k,l,m+1} + K_{\parallel} \sigma_{k,l+1,m} + K_{\parallel} \sigma_{k+1,l,m} + \Delta(t) \right),$$

(1)

where $K_{\mu} = \beta J_{\mu}$ is the reduced nearest-neighbor coupling with $\mu = \{\perp 1, \perp 2, ||\}$, and $\beta = 1/k_BT$. In the following we shall concentrate on the infinite shear velocity limit $v \to \infty$, which can easily be implemented by choosing $1 \leq \Delta(t) \leq L_{||}$ randomly. In this limit an analytical calculation [9] yield the equation

$$\chi^{(0)}_{\text{eq}}(K_{\perp}) \tanh K_{\perp} = 1,$$

(2)

from which we can determine the critical temperature, where $\chi^{(0)}_{\text{eq}}$ is the zero-field equilibrium susceptibility of the subsystems moved relative to each other and $f$ the number of fluctuating adjacent fields. Here $\chi^{(0)}_{\text{eq}}$ of the two-dimensional Ising model is required, which has been calculated to higher than 2000th order by a polynomial algorithm [19]. Using $f = 2$ and $J_{\parallel} = J_{\perp 1} = J_{\perp 2}$ we get

$$T_{c}^{2+1d}(\infty) = 5.2647504145147435505980 \ldots$$

(3)

The second considered geometry $1+2d$ is similar to the previous case, but now the shear normal is in the $(110)$-direction. As a consequence, all four perpendicular coupling partners of a spin $\sigma$ are in neighboring shear planes. The corresponding Hamiltonian reads

$$\beta H(t) = -\sum_{k=1}^{L_{\perp 1}} \sum_{l=1}^{L_{\perp 2}} \sum_{m=1}^{L_{\parallel}} \sigma_{klm} \left( K_{\parallel} \sigma_{k,l,m+1} + K_{\perp} \sigma_{k,l+1,m} + K_{\ll} \sigma_{k+1,l,m} + \Delta(t) \right),$$

(4)

where $K_{\perp 1} = K_{\perp 2} = K_{\perp}$. For $v \to \infty$ we set $f = 4$ and use $\chi^{(0)}_{\text{eq}}(K_{\perp}) = e^{2K_{\perp}t}$ from the one-dimensional Ising model in eq. (2) to get, for $J_{\parallel} = J_{\perp 1} = 1$, the critical temperature

$$T_{c}^{1+2d}(\infty) = \frac{2}{\ln[\frac{1}{2}(5 + \sqrt{14})]} = 5.642611138 \ldots,$$

(5)

which notably is different from eq. (2). Hence the critical temperature depends on the direction of the shear normal.

Finally we comment on the simulation method: in MC simulations of nonequilibrium models the critical temperature often depends on the used acceptance rates [20]. It has been shown that the multiplicative rate [9]

$$p_{\text{lip}}(\Delta E) = e^{-\frac{1}{2}(\Delta E - E_{\text{min}})}$$

(6)

with the energy change $\Delta E$ and the minimal energy change $E_{\text{min}} = \min\{\Delta E\}$ must be used in order to reproduce the critical temperatures, eqs. (3) and (5).

Anisotropic scaling. – Our aim is to prove that both models exhibit a strongly anisotropic phase transition and calculate the corresponding exponents. Such a phase transition is characterized by bulk correlation lengths $\xi_{\mu}$ diverging with direction-dependent critical exponents $\nu_{\mu}$ at criticality$^1$,

$$\xi_{\mu}(t) \sim t^{-\nu_{\mu}},$$

(7)

with direction $\mu = \{\perp 1, \perp 2, ||\}$, amplitude $\xi_{\mu}$, and reduced critical temperature $t = T/T_{c} - 1$. Usually one defines the anisotropy exponent $\theta = \nu_{\perp}/\nu_{||}$, which is $\theta = 1$ for isotropic scaling and $\theta \neq 1$ for strongly anisotropic scaling [2,21–24].

As mentioned above, the phase transitions of the Ising model with shear in the 2d geometry and the 1+1d model with shear in the 2d geometry and the 1+1d geometry become strongly anisotropic for $v > 0$ in the thermodynamic limit, with $\theta = 3$ [12].

In ref. [12] it was shown that the application of a stripe geometry $L_{||} \to \infty$ with finite $L_{||}$ is an appropriate way to determine the anisotropy exponent and subsequently the correlation length exponents. Here we measure the perpendicular correlation function

$$G_{\perp}(L_{||}; r_{\perp}) = \langle \sigma_{000} \sigma_{r_{\perp},r_{\perp},0} \rangle$$

(8)

at the critical point $T_{c}$, from which we can determine the correlation lengths $\xi_{\mu}$ with $\mu = \{\perp 1, \perp 2\}$ as shown below (in the following the index $\mu$ only represents

$^1$Throughout this work the symbol $\simeq$ means “asymptotically equal” in the respective limit, e.g., $f(L) \simeq g(L) \iff \lim_{L \to \infty} f(L)/g(L) = 1$. 

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the perpendicular directions $\perp_1$ and $\perp_2$). Note that by symmetry $G_\perp(L||,r_{\perp_1}) = G_{\perp}(L||,r_{\perp_2})$ for the 1+2d system. From $\xi_\mu$ we can then determine $\theta$ using the relation \[23,25\]
$$
\xi_\mu(L||) \simeq A_\mu L_{\parallel}^{1/\theta}.
$$
(9)

The above-mentioned stripe geometry is a film geometry in three dimensions, and we choose $L_{\parallel}/\xi_\perp(L||) \gtrsim 10$ sufficient for our purpose \[12\].

**Dimensional analysis.** – For $v \to \infty$ it was shown in ref. \[9\] that the 1+1d model can be mapped onto an equilibrium system consisting of one-dimensional chains that only couple via fluctuating magnetic fields. Now we generalize these ideas to a $d$-dimensional driven system. Due to the film geometry with confining length $L_{\parallel}$ and the periodic boundary conditions in parallel direction the magnetization $\mathbf{m}(\mathbf{x})$ with $\mathbf{x} = (\mathbf{x}_\perp, x_{\parallel})$ is homogeneous in this direction, and parallel correlations are irrelevant. Hence we can use the zero-mode approximation in this direction, leading to an order parameter $m = m(\mathbf{x}_\perp)$ only.

The resulting Ginzburg-Landau-Wilson (GLW) Hamiltonian
$$
\beta H = L_{\parallel} \int dx^{d-1}_\perp \left( \frac{t}{2} \mathbf{m}^2 + \frac{1}{2} (\nabla m)^2 + \frac{u}{4!} m^4 \right),
$$
(10)
cannot, however, be mapped onto a Schrödinger equation for systems with $d > 2$ as done in ref. \[12\], as the $(d - 1)$-dimensional integral cannot be interpreted as a time integral. Instead we use dimensional analysis in order to predict the critical exponents: starting from the GLW Hamiltonian (10) in $d$ dimensions we eliminate $L_{\parallel}$ with the substitution
$$
m \to \tilde{m} L_{\parallel}^{-1/(5-d)},
$$
(11a)
$$\mathbf{x}_\perp \to \tilde{\mathbf{x}} L_{\parallel}^{1/(5-d)},
$$
(11b)
$$t \to \tilde{t} L_{\parallel}^{-2/(5-d)}
$$
(11c)
to get the $(d - 1)$-dimensional Hamiltonian
$$
\beta H = \int dx^{d-1} \left( \frac{\tilde{t}}{2} \tilde{m}^2 + \frac{1}{2} (\nabla \tilde{m})^2 + \frac{u}{4!} \tilde{m}^4 \right),
$$
(12)
with $\tilde{m} = \tilde{m}(\tilde{\mathbf{x}})$, where quantities in the $(d - 1)$-dimensional system are denoted by a tilde. From eqs. (11b) and (11c) we directly read off\(^2\) the exponents
$$
\theta = 5 - d,
$$
$$\nu_{\parallel} = \frac{5 - d}{2} \quad \Rightarrow \quad \nu_{\perp} = \frac{1}{2},
$$
(13)
reproducing the results for $d = 1$ \[9\] and $d = 2$ \[12\] and fulfilling the generalized hyperscaling relation \[26\]
$$
\nu_{\parallel} + (d - 1) \nu_{\perp} = 2 - \alpha
$$
(14)
with $\alpha = 0$ \[9,12\]. For our case $d = 3$ we find
$$
\theta = 2, \quad \nu_{\parallel} = 1, \quad \nu_{\perp} = \frac{1}{2},
$$
(15)
while for $d \geq 4$ we predict isotropic or weakly anisotropic behavior with $\theta = 1$ and $\nu_{\parallel} = \nu_{\perp} = 1/2$, as then the upper critical dimension $d_c = 4$ is reached and the shear becomes an irrelevant perturbation.

**Correlation functions.** – The perpendicular correlation function can be calculated from eq. (12) using a Gaussian approximation, which is valid, since we investigate the system at the critical temperature of the bulk, which is higher than the critical temperature of the studied film geometry. Setting $u = 0$ in eq. (12) and using $\xi \propto \tilde{t}^{-1/2}$ we get the Ornstein-Zernike structure factor
$$
\tilde{S}(\mathbf{k}) \propto \frac{1}{k^2 + \xi^{-2}}.
$$
(16)
In our case the dimension is $d - 1 = 2$, and a Fourier transformation yields the correlation function
$$
\tilde{G}(\mathbf{r}) \propto K_0(\tilde{r}/\xi),
$$
(17)
with modified Bessel function of the second kind $K_0$. Using $\tilde{G} \propto \tilde{m}^2$ and back-substituting with eqs. (11) gives the result
$$
G(L_{\parallel}, r_{\perp}) \propto L_{\parallel}^{1-\nu_{\parallel}} K_0[r_{\perp}/\xi_\perp(L_{\parallel})]
$$
(18)
for the perpendicular correlation function of the GLW Hamiltonian (10).

The $2 + 1$d geometry is weakly anisotropic in perpendicular direction at least for different couplings $J_{\perp_1} \neq J_{\perp_2}$, i.e., the correlation lengths $\xi_{\perp_1}$ and $\xi_{\perp_2}$ have the same exponent $\nu_{\perp}$ but different amplitudes $\xi_\mu$ \[23\]. This anisotropy can be removed by the rescaling
$$
l_\mu \to \tilde{l}_\mu = \frac{l_\mu}{A_\mu},
$$
(19)
with amplitude $A_\mu$ from eq. (9). Now the perpendicular directions are isotropic and we can use eq. (18) to get the final result
$$
G_{\perp}(L_{\parallel}; r_\mu) \simeq \tilde{G} L_{\parallel}^{1-\nu_{\parallel}} K_0[r_\mu/\xi_\mu(L_{\parallel})].
$$
(20)
Here we already have back-substituted with eq. (19). Note that especially in the $2+1$d case the amplitude $\tilde{G}$ should not depend on the direction $\mu$.

**Results.** – We measured $G_{\perp}(L_{\parallel}; r_\mu)$ at criticality for both models using extensive Monte Carlo simulations and fitted the results against eq. (20) to get $\xi_\mu(L_{\parallel})$ shown in fig. 2. Similar to the 1+1d case we find corrections to scaling for $L_{\parallel} \lesssim 300$ which are problematic in these three-dimensional cases, as we cannot\(^3\) simulate systems

\(^3\)Remember that $L_{\parallel}$ is the confining length and that $L_{\parallel} \gtrsim 10\xi_{\perp}(L_{\parallel})$ (see above), leading to system sizes up to $128 \times 128 \times 1024$ which took $\approx 1$ CPU year on an Opteron cluster for the required $3 \times 10^6$ MC sweeps.

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larger than $L_\parallel = 1024$. Hence we have to introduce a lattice correction term in the perpendicular correlation length and improve relation (9) using the ansatz

$$\xi_\mu(L_\parallel) = A_\mu(L_\parallel + c_0 L_\parallel^{1/2} + \ldots)^{1/\theta}$$

(21)

with $\theta = 2$, which gives the best fit to the data. From the numerical data we find the amplitudes $A_\mu$ and $\hat{G}$ as well as the correction parameter $c_0$ listed in table 1, and the resulting fit is shown as a solid line in fig. 2. For large systems the curve approaches the theoretical limit, eq. (9), with slope $\theta^{-1} = 1/2$. Note that for $L_\parallel \lesssim 64$ we could also find a reasonable data collapse with exponent $\theta_{\text{eff}} = 3$ (dotted line).

The resulting rescaled correlation functions for both models are presented in fig. 3. In all cases the data can be rescaled with $L_\parallel$ as predicted, without notable corrections, to obtain a convincing data collapse onto the mean-field correlation function $K_0(r/\xi)$ from eq. (20). For small distances $r_{\perp \perp} = O(1)$ the correlation function $G_\perp(L_\perp; r_{\perp \perp})$ differs from eq. (20) due to the inplane nearest-neighbor interactions.

Now we comment on the four-dimensional geometry 1+3d, with decouples to a three-dimensional array of interacting chains, with $f = 6$ in eq. (2). We performed test simulations for system sizes up to $32^3 \times 32$ and found very strong, possibly logarithmic corrections to scaling. From the scaling behavior of the available data we estimate that system sizes $L_\parallel, L_\perp \gtrsim 1000$ would be required to find the correct scaling behavior.

Finally, we extend the dimensional analysis to the general case of a $d$-dimensional hyper-cubic sheared lattice with $d_\parallel$ driven dimensions and $d_\perp$ perpendicular dimensions. We again must distinguish between the $d_\perp$ dimensions normal to the shear and $d_{\perp \perp}$ “inplane” dimensions without shear motion, with $d_\perp = d_{\perp \perp} + d_{\perp \perp}$. The critical temperature $T_\xi$ at infinite shear velocity $v$ is given by eq. (2), with the equilibrium zero-field susceptibility $\chi^{(0)}_\mu$ of the $d_{\perp \perp}$-dimensional system having $f$ fluctuating fields at each lattice point, where $d_{\perp \perp} = d_{\parallel} + d_{\perp \perp}$, and $f = 2d_{\perp \perp}$.

From a simple generalization of eq. (13) we find the exponents

$$\theta = 4 - d_{\perp \perp}, \quad \nu_{\parallel} = \frac{4 - d_{\parallel}}{2d_{\perp}}, \quad \nu_{\perp} = \frac{1}{2},$$

(22)

fulfilling the hyperscaling relation $d_{\parallel} \nu_{\parallel} + d_{\perp} \nu_{\perp} = 2$.

We conclude with a tabular summary of the found exponents and critical temperatures $T_\xi$ at infinite driving velocity $v$ given in table 2, including two cases denoted “mix” where we assumed a suitable two-dimensional motion of the interacting planes. These systems have $d_{\parallel} = 2$, but notwithstanding the same $T_\xi$ as the corresponding systems with unidirectional motion at infinite $v$. For the layered case $2 + 4d_{\perp \perp}$ we predict the exponents $\theta = 3/2$ and $\nu_{\parallel} = 3/4$. A test of these predictions is left for future work.

Table 1: Amplitudes and corrections to scaling parameter $c_0$ for both models.

| Model | $\mu$ | $A_\mu$ | $\hat{G}$ | $c_0$ |
|-------|-------|---------|-----------|-------|
| 1+2d  | $\perp$ | 0.254(5) | 0.93(1)   | 14(1) |
| 2+1d  | $\perp_1$ | 0.320(5) | 0.85(1)   | 12(1) |
|       | $\perp_2$ | 0.331(5) | 0.85(1)   | 12(1) |

Fig. 2: (Colour on-line) Perpendicular correlation lengths $\xi_\mu(L_\parallel)$ for the 1+2d geometry (red circles), the 2+1d geometry in the $\perp_1$-direction (green diamonds) and in the $\perp_2$-direction (blue squares) at criticality. The statistical error is smaller than the symbol size. Due to corrections to scaling, small systems have effective anisotropy exponent $\theta_{\text{eff}} \approx 3$ (dotted line), which is obtained from the logarithmic derivative and shown exemplary for system 1+2d in the inset.

Fig. 3: (Colour on-line) Rescaled correlation function $G_\perp(L_\perp; r_{\perp \perp})$ with $\mu = \{\perp, \perp_1, \perp_2\}$ for both models at criticality. We show varying system extensions $L_\parallel = \{8, 16, 32, 64, 128, 256, 512, 1024\}$ for both cases. A rescaling of the abscissa with $\xi_\mu(L_\parallel)$ and of the ordinate with $L_\parallel$ results in an excellent data collapse, verifying $\theta = 2$ and $\nu_{\parallel} = 1$. The solid lines represent the calculated Ornstein-Zernike correlation function, eq. (20). Note that we multiplied the collapsed data by different factors as indicated in order to show them in one plot.
Table 2: Relevant dimensions, exponents and parameters of the considered models as defined in the text, together with geometries from the literature [9]. 1d, 2d and 3d denote two d-dimensional Ising models (with $d = 1, 2, 3$) moved against each other such that every spin in one system has a coupling partner in the other system, while 2d$_b$ and 3d$_b$ denote two d-dimensional Ising models (with $d = 2, 3$) moved along a $(d − 1)$-dimensional boundary. For details and a classification see ref. [9].

| Model    | $d$ | $d_{∥}$ | $d_{⊥}$ | $d_{∥⊥}$ | $d_{⊥∥}$ | $θ_{∥}$ | $ν_{∥}$ | $f$ | $d_{eq}$ | $T_c(∞)/J$ |
|----------|-----|---------|---------|----------|----------|--------|--------|----|--------|-------------|
| moved    | 1d  | 1       | 1       | 1         | 1         | 2      | 1      | 1  | 2.2691853 | 3.4659074... |
|          | 2d  | 2       | 1       | 0         | 1         | 3      | $3/2$  | 1  | 4.0587824 | 5.983835(1)  |
|          | 3d  | 3       | 1       | 2         | 0         | 2      | 1      | 1  | 5.2647504 | 7.728921...  |
|          | 2d$_b$ | 1   | 1       | 0         | 0         | 2      | 1      | 2  | 2.2691853 | 4.0587824... |
|          | 3d$_b$ | 2   | 1       | 1         | 0         | 3      | $3/2$  | 1  | 4.8(1)   | 5.2647504... |

**Conclusion.** – We investigated the nonequilibrium phase transition in three-dimensional Ising models with shear and two different shear normals by means of Monte Carlo simulations. In the limit of infinitely high shear velocity $v$ we found a critical temperature $T_c(∞)$ that depends on the direction of the shear normal. At criticality, strongly anisotropic diverging correlation lengths with exponents $ν_{∥} = 1$ and $ν_{⊥} = 1/2$ occur, leading to an anisotropy exponent $θ = 2$, which confirms the results of a dimensional analysis of the corresponding Ginzburg-Landau-Wilson Hamiltonian. Furthermore, the dimensional analysis reproduces the anisotropy exponents as well as the correlation length exponents of the previously studied two-dimensional cases [12] and the parallel correlation length exponent of the one-dimensional cases [9]. The dimensional analysis also gives predictions for two-dimensional shear directions, leading to, e.g., the exponents $θ = 3/2$ and $ν_{∥} = 3/4$ in a three-dimensional model. This strongly anisotropic behavior provides a natural explanation for the string domains found in real three-dimensional sheared binary liquids [15–18].

Fluctuations perpendicular to the shear were shown to be Gaussian, resulting in a correlation function with Ornstein-Zernike behavior. Additionally, in the case of the 2 + 1d geometry we found weakly anisotropic perpendicular correlations. As for $v = 0$ both the 2 + 1d geometry and the 1 + 2d geometry reduce to the three-dimensional equilibrium Ising model, we expect a crossover from this case to strongly anisotropic mean-field behavior, similar to the 1 + 1d geometry. In ref. [12] an expensive analysis for finite velocities has been done leading to a crossover scaling, pointing out that all $v ≠ 0$ provoke strongly anisotropic mean-field behavior, which is expected to occur in the current systems as well. However, we did not prove this in detail, due to the additional complexity in three-dimensional systems.

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