Letter

Arresting dynamics in hardcore spin models

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We study the dynamics of hardcore spin models on the square and triangular lattice, constructed by analogy to hard spheres, where the translational degrees of freedom of the spheres are replaced by orientational degrees of freedom of spins on a lattice and the packing fraction as a control parameter is replaced by an exclusion angle. In equilibrium, models on both lattices exhibit a Kosterlitz-Thouless transition at an exclusion angle Δ_{KT}. We devise compression protocols for hardcore spins and find that *any* protocol that changes the exclusion angle nonadiabatically, if endowed with only local dynamics, fails to compress random initial states beyond an angle $\Delta_{\mathrm{J}} > \Delta_{\mathrm{KT}}$. This coincides with a doubly algebraic divergence of the relaxation time of compressed states toward equilibrium. We identify a remarkably simple mechanism underpinning this divergent timescale: topological defects involved in the phase ordering kinetics of the system become incompatible with the hardcore spin constraint, leading to a vanishing defect mobility as $\Delta \to \Delta_{\mathrm{J}}$.

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Introduction. Within the realm of condensed-matter physics, examples abound of continuum systems whose critical phenomena can be well captured by simplified lattice models. For instance, the liquid-gas transition can, remarkably, be described using the lattice gas model, which then maps onto the Ising model [1]. Similarly, the Edwards-Anderson model and related spin-glass Hamiltonians provide a fruitful avenue toward understanding random impurities in magnetic alloys [2].

In this Letter, we take a lattice approach toward what might be called vitrifaction, i.e., the emergence of slow dynamics which has played an important role under the headings of glassiness, freezing, jamming, and the like. To do so, we devise a particularly simple yet versatile and tractable family of models of what we have termed hardcore spins. These insulating (nonitinerant) spin models are constructed by analogy to hard spheres/disks, which are the common idealized model systems for the phenomenon of jamming. Much progress has been made to understand the random jamming transition of hard spheres both numerically [3,4] as well as in infinite dimensions [5]. In particular, it is possible to define random jamming without the need to invoke any particular dynamics, the hallmark being a jump of the contact number z as a function of packing fraction at "point J" Φ_J.

In contrast, our work takes a different tack: addressing the broad issue of dynamical arrest of an athermal system—one in which thermal fluctuations make a negligible contribution to its dynamics—far from equilibrium, we study whether, and by what mechanism, this phenomenon can arise in a lattice model. Concretely, we address its relation to the physics of phase ordering kinetics, i.e., the extent to which an underlying, but under a given dynamics inaccessible, ordered state and its concomitant topological defects play a fundamental role, an idea that dates back several decades in the glass literature [6–10].

The hardcore spin models are defined by a local constraint, whereby no two neighboring hardcore spins are allowed to enclose an angle smaller than their exclusion angle [see Fig. 1(a)]. This can be viewed as an orientational lattice analog to the nonlocal constraint on the translational degrees of freedom of hard spheres, for which two sphere centers must not be closer than the sum of their radii. The exclusion angle Δ serves as a tuning parameter for the equilibrium behavior of the system, which we have investigated in Ref. [11]. The simplest possible phase diagram of hardcore spins is shown in Fig. 1(c). At low exclusion angle, the system is weakly constrained and hence, in a paramagnetic phase. As the exclusion angle is increased in equilibrium, the system undergoes an entropically driven Kosterlitz-Thouless (KT) transition at Δ_{KT}.

Crucially, in a constrained system topological defects can not only become confined but their existence can even become strictly incompatible with the hardcore constraint. This happens at a point $\Delta_{\mathrm{J}} > \Delta_{\mathrm{KT}}$, and the defect density vanishes with a power law as $\Delta \to \Delta_{\mathrm{J}}$ [12].

In this Letter, we generalize compression protocols originally developed for hard spheres [13] and study dynamics of hardcore spins far from equilibrium. Importantly, we uncover a remarkably simple mechanism precipitating of what might be called "arresting" or perhaps "jamming dynamics" in our model. In particular, any adiabatic compression protocol,

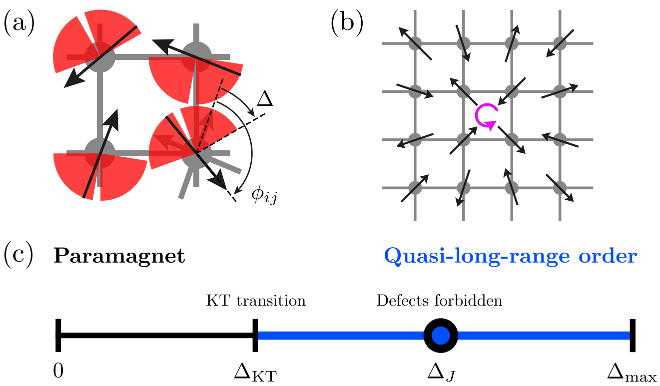

FIG. 1. (a) Illustration of the hardcore constraint. For a given spin, red shading indicates the orientations forbidden by its nearest neighbors. (b) An antiferromagnetic vortex on the square lattice. The vortex core is marked in purple. (c) Minimal phase diagram of the model.

namely one in which the system stays in equilibrium as Δ is driven through Δ_{J}, reaches the ordered state with maximal exclusion angle Δ_{max}, analogous to the close packing. In contrast, a nonadiabatic protocol starting from a random initial state at $\Delta = 0$ will fall out of equilibrium and reach $\Delta = \Delta_{\mathrm{J}}$ with nonzero defect density. As the existence of defects is incompatible with the hardcore constraint for $\Delta > \Delta_{\mathrm{J}}$, the protocol will fail beyond this point. The failure of compression at Δ_{J} coincides with a doubly algebraic divergence of the relaxation time of compressed states toward equilibrium—as a function of both system size as well as the distance to Δ_{J}. This can be fully understood in terms of a diffusion-annihilation process of topological defects, with a vanishing defect mobility.

In the remainder of this Letter we first present hardcore XY spins on the square lattice as a minimal model exhibiting all the abovementioned features. We then show that on the triangular lattice, the relevant physics is realized in a more complex way: the additional chiral symmetry in the model leads to the presence of two kinds of topological defects, that is, domain walls in addition to vortices. This leads to a more structured slow dynamics, but crucially, the behavior of the model can be accounted for by the same fundamental mechanism as before.

Model and phase diagram on the square lattice. We consider a system of XY spins, that is two-component unit vectors $\{\mathbf{S}_j\}$, on a lattice $\mathcal{L}$ subject to the constraint

$$\phi_{ij} := \arccos(\mathbf{S}_i \cdot \mathbf{S}_j) > \Delta \;\; \forall \langle ij \rangle \in \mathcal{L}, \tag{1}$$

where $\langle ij \rangle$ denotes an edge between site i and j.

For XY spins on the square lattice, the hardcore constraint is illustrated in Eq. (1), where for each spin we denote in red the orientations forbidden while keeping all neighbors fixed. This model realizes the minimal equilibrium phase diagram sketched in Fig. 1(a). At $\Delta = 0$, the system is unconstrained and naturally in a paramagnetic state, while at $\Delta = \pi$, the only allowed state (up to global symmetry) is the Néel state. Between these extremes, for any $\Delta < \Delta_{\mathrm{max}}$, long-ranged order is prohibited by an extension of the Mermin-Wagner theorem to constrained systems [14,15]. The system instead undergoes a KT transition at $\Delta_{\mathrm{KT}} \approx 0.435\pi$ [16], into a phase with quasilong-ranged (QLR) order, with algebraically decaying correlations. Note that the model has no inherent notion of energy or temperature. Instead, Eq. (1) separates states into two classes—allowed and disallowed—without endowing them either with dynamics or with a notion of (high and low) energy. Thus, nontrivial correlations are of entropic origin, i.e., a form of "order by disorder" (OBD) familiar from the nematic ordering of Onsager's hard rods [17] and its descendants, including a recurrent appearance in frustrated magnetic systems.

It is well known that the KT transition can be understood as an unbinding transition of topological defects, which on the square lattice are vortices, see Fig. 1(b). Defect unbinding is indeed the mechanism behind the equilibrium transition in our model, but within the QLRO phase, these vortices become incompatible with Eq. (1) for $\Delta > \pi/2$. This is shown most easily by realizing that on a bipartite graph such as the square lattice, any exclusion model as defined by Eq. (1) maps on an inclusion model defined by

$$\tilde{\phi}_{ij} < \Delta_{\mathrm{incl}} \;\; \forall \langle ij \rangle \in \mathcal{L}, \tag{2}$$

where the spins on one of the two sublattices are flipped:

$$\tilde{\mathbf{S}}_j = \begin{cases} \mathbf{S}_j & \text{if } j \text{ in sublattice } A \\ -\mathbf{S}_j & \text{if } j \text{ in sublattice } B, \end{cases} \tag{3}$$

and $\Delta_{\mathrm{incl}} = \pi - \Delta$. An antiferromagnetic vortex then maps onto a regular ferromagnetic vortex. Such a vortex however must have a core [11], which is a single plaquette with a winding of 2π. Since there are only four sites around a plaquette, this is only possible if $\Delta_{\mathrm{incl}} > 2\pi/4 = \pi/2$, which implies $\Delta < \pi/2$ in the exclusion model.

Jamming hardcore spins. As a first step toward studying our model far from equilibrium, we define a notion of compression, which here will mean an increase of the exclusion angle Δ while simultaneously evolving the state under some local dynamics. An analogous protocol for hard disks was implemented by Lubachesvky and Stillinger [13]. In this work, the radii of the disks were increased during a molecular dynamics simulation while keeping the volume fixed. When the compression rate was slow with respect to the time scale set by the molecular dynamics, the final state was approximately close packed. In contrast, when the radii were increased very fast, the system ended up "jammed" in a polycrystalline state (to be contrasted with "maximally random jammed" states [18]), at a density well below close packing.

The Lubachevsky-Stillinger (LS) algorithm is straightforwardly adapted to and implemented for hardcore spins, the most subtle point being the choice of dynamics. Arguably, the closest analog to the molecular dynamics studied by LS is given by continuous-time "Hamiltonian" dynamics. For hardcore spins, however, such dynamics are not ergodic even at infinitesimal exclusion angles since they preserve the local vorticity on each plaquette [12] (see also Refs. [19,20] therein). Because of this, in the main text, we focus on a different kind, that is discrete-time, stochastic Monte-Carlo dynamics. In each time step, a single Monte-Carlo move is performed. Each such move consists of choosing a random site in the lattice, then choosing a random new configuration

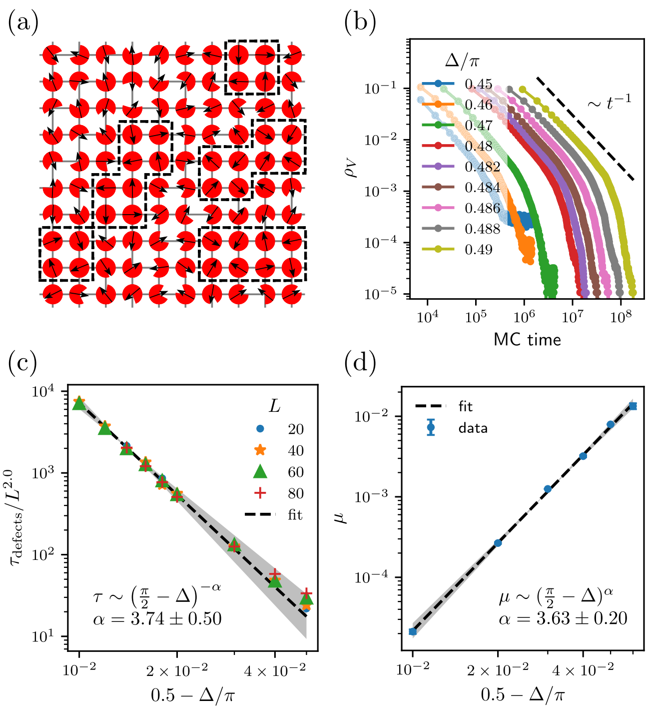

FIG. 2. (a) State at $\Delta = \Delta_J$, frozen vortex cores are enclosed by dashed lines. (b) Vortex density ρ_V of far-from-equilibrium states relaxing toward equilibrium at different exclusion angles Δ, for $L = 60$. (c) Doubly algebraic behavior of relaxation time scale fitted from long-time tail of ρ_V as $\Delta \to \Delta_J$. (d) Vanishing defect mobility as $\Delta \to \Delta_J$.

for the spin on the site and accepting the move if and only if the new configuration is allowed by Eq. (1). A similar technique was previously applied in the compression of hard spheres in Ref. [21].

The compression protocol then proceeds as follows. Starting from a random state at $\Delta = 0$, one alternates N_{rattle} Monte Carlo sweeps (with one sweep consisting of N Monte Carlo moves) and an increase of the exclusion angle by δ, where the increment δ is chosen as large as possible without invalidating the current state. Fast compression in this context then means large δ/N_{rattle}. The protocol terminates if the increment δ repeatedly falls below a threshold value.

On an $L = 40$ square lattice, we run the LS compression protocol for hardcore spins with different values of N_{rattle} to see whether jamming dynamics is observed. Out of 100 runs with $N_{\text{rattle}} = 100$, all runs terminate at $\Delta_{\max} = \pi$; that is, they reach the Néel state which is our analog to close packing. In contrast, for $N_{\text{rattle}} = 1$ all runs terminate at $\Delta_J = \pi/2$. For $N_{\text{rattle}} = 10$, runs fall into two classes, with 16 terminating at Δ_J and the rest at $\Delta_{\max}$. The "jammed" states at Δ_J have a finite ordered moment, which increases with N_{rattle} but is always lower than the equilibrium expectation value [12]. To illustrate that the arresting dynamics here is indeed explained by our abovementioned mechanism, in Fig. 2(a) we show a state at Δ_J for $L = 10$ and indicate the frozen vortex cores by dashed black boxes. These vortex cores are completely frozen under local dynamics since the constituent spins enclose an angle of exactly $\pi/2$.

Relaxation dynamics. To corroborate the picture of defect freezing as the mechanism for the failure of nonadiabatic compression beyond Δ_J in our model, we study relaxation dynamics toward equilibrium close to this point in more detail. Generally speaking, one expects such a freezing to appear in conjunction with a diverging relaxation time scale.

While the LS protocol suffices to demonstrate the presence of jamming dynamics in hardcore spins, it is limited in that it allows only moderate compression speeds, resulting in partial equilibration, evidenced by a finite ordered moment of the final states. Because of this, we implement a second kind of compression protocol, originally developed by Xu *et al.* [22], which utilizes a softened constraint to compress faster and hence avoid partial equilibration. This is done by introducing an energy functional

$$V(\phi_{ij}, \Delta) = \begin{cases} \frac{1}{2}(1 - \phi_{ij}/\Delta)^2 & \text{for } \phi_{ij} < \Delta \\ 0 & \text{for } \phi_{ij} \geqslant \Delta \end{cases} \tag{4}$$

which is zero if Eq. (1) is fulfilled, and introduces a quadratic energy penalty if neighboring hardcore spins overlap. The introduction of the soft constraint enables us to use much larger increments δ. This is because one does not have to choose δ such that the current state of the system stays valid, but instead one can choose it such that a conjugate gradient minimization step after the increment recovers a state with zero energy.

The softcore compression protocol consistently yields far-from-equilibrium states with an ordered moment close to zero. We prepare such states at a range of exclusion angles Δ close to Δ_J and show their defect density as a function of Monte Carlo time in Fig. 2(b). As expected from scaling arguments [23], it decays diffusively initially, but at long times, this behavior gives way to an exponential decay with a characteristic relaxation time τ_{defects}. This relaxation time as a function of exclusion angle Δ is shown in Fig. 2(c), for a range of different system sizes. Evidently, the data is consistent with a doubly algebraic behavior:

$$\tau \sim L^z(\Delta_J - \Delta)^{-\alpha} \tag{5}$$

with $z = 2$ and $\alpha = 3.74 \pm 0.50$. These two power laws are conceptually quite distinct. The divergence of the relaxation times with system size $\tau \sim L^z$ owes its existence to universal long-wavelength physics of phase-ordering kinetics under local dynamics and consequently, its value $z = 2$ [24] is quite robust. In contrast, the divergence of relaxation time as a function of exclusion angle is related to the defect mobility μ. It is measured by preparing two isolated vortices in an otherwise paramagnetic state. Their distance then follows the time dependence $D(t) = \sqrt{D_0 - \mu t}$, from which μ can be determined by a linear fit. As shown in Fig. 2(d), it vanishes as a power law as $\Delta \to \Delta_J$ with, for a given local dynamics, roughly the same exponent α as the relaxation time. However, this exponent can be readily varied by changing the rules of the dynamical evolution even locally. For example, results from studying phase ordering kinetics under Hamiltonian dynamics plus tunneling are consistent with Eq. (5), with $z = 2$ but $\alpha = 1.87 \pm 0.02$ [12].

Triangular lattice. Finally, we compare the simple picture of the square lattice model to that on the triangular lattice.

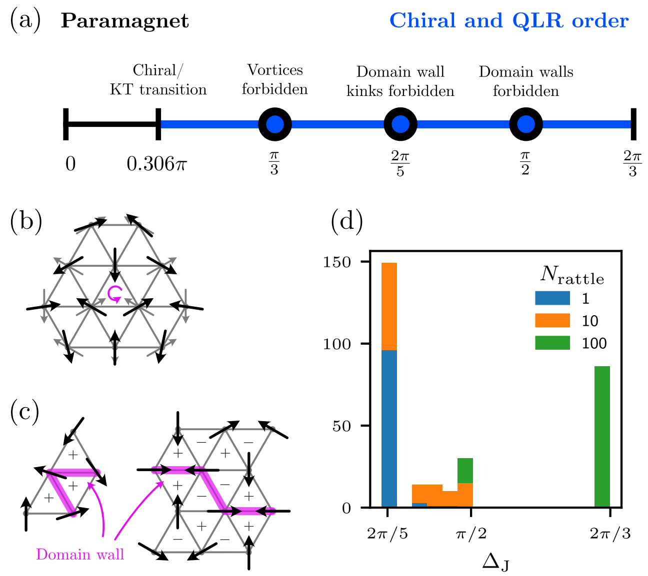

FIG. 3. (a) Equilibrium phase diagram of the model on the triangular lattice. (b) A vortex on the triangular lattice. (c) Domain walls of chirality both with a kink (left) and without any kinks (right). (d) Distribution of jamming angles Δ_J as a function of compression speed for $L = 42$; lower N_{rattle} implies faster compression.

Its phase diagram, Fig. 3(a), also has a paramagnetic phase including $\Delta = 0$, with a single (up to global symmetries) three-sublattice ordered state at $\Delta = 2\pi/3$; this comes in two chiralities that are not related by global rotation but instead by exchange of two sublattices. In between, chiral and quasilong-range order develop either simultaneously or at two separate transitions [25,26] in proximity to $\Delta \approx 0.306\pi$ [12] (see also Refs. [27–31] therein).

The properties of topological defects, and in particular their preclusion upon increasing Δ, remain central to the jamming phenomenology. These are richer than in the square lattice case. Vortices, as shown in Fig. 3(b), become forbidden at a single packing fraction $\Delta = \pi/3$. In contrast, domain walls have internal structure (their shape) and become incompatible with the hardcore constraint over a range of exclusion angles. First, kinks in domain walls, shown on the left of Fig. 3(c) become forbidden at $\Delta = 2\pi/5$ while at $\Delta = \pi/2$, *any* domain wall becomes incompatible with Eq. (1) [12].

In Fig. 3(d) we show a histogram of the angle at which compression of random initial states using the LS protocol at different N_{rattle} terminates. On the square lattice, such a histogram is strictly bimodal with two narrow peaks at $\Delta_{\mathrm{J}} = \pi/2$ and $\Delta_{\max} = \pi$. In contrast, on the triangular lattice, for intermediate compression speed $N_{\mathrm{rattle}} = 10$, we see a continuous distribution between $\Delta = 2\pi/5$ with a pronounced peak at $\Delta = \pi/2$. This can be understood by considering the same mechanism as on the square lattice: fast compression (that is small N_{rattle}) fails because it arrives with a finite density of topological defects at a point where these become incompatible with Eq. (1). Now if there are multiple kinds of defects in the system, these can have different relaxation time scales and hence lead to a more complex dependence of the jamming angle on compression speed.

In this picture, it is somewhat surprising that in Fig. 3(d) there is no peak at $\Delta = \pi/3$, where vortices become forbidden. This is just a consequence of the fact that vortices are only well defined in the presence of chiral order, whereas we start from random initial states that are neither chirally nor QLR ordered and have no well-defined vortex density to begin with. A random initial state will however have a well defined and large domain wall density, which leads to the failure of fast compression (jamming) at $\Delta_{\mathrm{J}} = 2\pi/5$, which is where kinked domain walls become forbidden. At intermediate speeds, the system is then able to partially equilibrate and reach zero domain-wall-kink density, but still has smooth domain walls, leading to jamming at $\Delta_{\mathrm{J}} = \pi/2$. Between these two points, in the range $2\pi/5 < \Delta < \pi/2$, there exist a multitude of local clusters with long but finite relaxation times, leading to jamming of protocols with intermediate compression speeds.

An important, qualitative difference to the square lattice model is that on the triangular lattice the only *vanishing* defect mobility in the model is that of domain walls at $\Delta = \pi/2$. Still, we observe a failure of the compression protocols at other points, where different defects become forbidden without a concomitant freezing. This is not unexpected since a long but finite relaxation time of such defects might still bring compression to a halt. In the language of granular materials, such freezing is *fragile* in that rattling of a jammed state might unjam it.

Conclusion. In summary, we have provided a detailed phenomenology and comprehensive understanding of arresting dynamics in hardcore spin models, uncovering an intricate interplay of lattice geometry, ordering and defects, and the dynamics at long and short wavelengths. Particularly noteworthy from a conceptual perspective is the role played by the (in)ability to anneal defects under purely local dynamics. This fundamentally accounts for the phenomenon in this *lattice* model, with considerable added richness as a result of the variability and multiplicity of defects and their configurations. In addition to lending this model intrinsic interest on its own, the central role of defects to the (slow) dynamics resonates with a possibility previously formulated for the case of the glass transition [9].

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