The growing correlation length observed in supercooled liquids as their temperature is lowered has been studied with the aid of a single occupancy cell model. This model becomes more accurate as the density of the system is increased. One of its advantages is that it permits a simple mapping to a spin system and the effective spin Hamiltonian is easily obtained for smooth interparticle potentials. For a binary liquid mixture the effective spin Hamiltonian is in the universality class of the Ising spin glass in a field. No phase transition at finite temperatures is therefore expected and the correlation length will stay finite right down to zero temperature. For binary mixtures of hard disks and spheres we were not able to obtain the effective spin Hamiltonian analytically, but have done simulations to obtain its form. It again is in the universality class of the Ising spin glass in a field. However, in this case the effective field can be shown to go to zero at the density of maximum packing in the model, (which is close to that of random close packing), which means that the correlation length will diverge as the density approaches its maximum. The exponent $\nu$ describing the divergence is related in $d$ dimensions to the Ising spin glass domain wall energy exponent $\theta$ via $\nu = 2/(d - 2)$. 

I. INTRODUCTION

One of the key concepts which has emerged in the last few years in the field of glasses is that of a growing correlation length scale $\xi$ \cite{1-5}. There are now many ways of defining and obtaining such a length scale: point-to-set \cite{2}, patches \cite{6}, dynamics \cite{1, 4} etc. When it becomes large, they are probably all proportional to each other, as they are basically just a measure of the size of the cooperatively re-arranging regions in the liquid \cite{4}. Simulations show that $\xi$ increases as the temperature decreases, or in the case of hard sphere and hard disk systems, as their density is increased. In this paper we report on our attempts to understand this growth, particularly in the context of hard disk systems in two dimensions but also for particles interacting with realistic potentials in any dimension.

The leading theory for the growth of the correlation length has been that of the Random First-Order Transition (RFOT) theory \cite{7-9}. In this theory the growth is driven by the decreasing configurational entropy or complexity \cite{10, 11} of the supercooled liquid as its temperature is decreased towards $T_K$, the Kauzmann temperature \cite{12}. In hard spheres there is a packing fraction $\phi_K$ at which the complexity apparently goes to zero, at least in the mean-field calculations of Refs. \cite{10, 11}. At this density the correlation length diverges to infinity. However, there are arguments that RFOT theory must be incorrect for systems in any finite dimension \cite{13}.

In this paper we shall try to understand the growth of the length scale $\xi$ not on the basis of RFOT theory but from lessons which have been learnt from studying in finite dimensions the same $p$-spin models which inspired the RFOT theory. In Refs. \cite{13, 15} it has been shown that these models behave at low temperatures rather like an Ising spin glass in a field \cite{16}. Furthermore the correlation length grows as the temperature is decreased but saturates to a finite value at $T = 0$. It has also been argued that real glasses as well as $p$-spin models behave like Ising spin glasses in a field \cite{17}. This approach involved extensive use of the replica trick and is quite non-intuitive. It is one of the purposes of this paper to explain why, say, a binary mixture of hard spheres at high densi-
ties will have features in common with Ising spin glasses in the presence of a field, but without the aid of the heavy machinery of replicas.

To this end, we introduce in Sec. II the Single Occupancy Cell (SOC) model [18, 19]. In two dimensions it is a model in which the centers of the hard disks are each constrained to stay forever within a plaquette of a square lattice grid as in Fig. 1. (The generalization of this to higher dimensions is simple: in $d = 3$ one would use spheres whose centers are confined within the primitive cell of the simple cubic lattice). As the area of the disks is increased, the partition function of this constrained model becomes ever closer to that of the unconstrained model. This model with disks of the same size is not a glass: in fact it undergoes an Ising-like phase transition [20] to a state which is one of the two differently orientated slightly disordered crystal lattices shown in Fig. 3. In order to investigate glassy behavior we introduce in Sec. III a variant of the SOC model. This has two species of particles, A and B, present in equal numbers but randomly distributed over the plaquettes as indicated in Fig. 2.

Fig. 2 also shows that the SOC model can be regarded as a spin model. An effective spin Hamiltonian is derived in Sec. IV for particles A and B which interact with a smooth potential $V(r)$, e.g. the Lennard-Jones potential. For such potentials it is possible to calculate analytically a good leading order effective spin Hamiltonian. The Hamiltonian is very familiar in the field of random magnetic systems; its vector spins have $d$ components and interact with a $d$-component vector random field. The spin interactions are a mixture of exchange and pseudo-dipolar couplings and there are also single ion anisotropy terms. Because it is so well understood we shall just briefly outline in Sec. V the phases which can exist for the effective spin Hamiltonian. There are choices for the interatomic potentials for which the spin Hamiltonian is in the universality class of the Ising spin glass in a field and it this choice which is appropriate if one is interested in the properties of supercooled liquids or glasses [17].

The Ising spin glass in a field does not have a phase transition in dimensions $d \leq 6$ [22, 23], but the correlation length can become large as the temperature is reduced, provided the ratio $h/J$ of the standard deviation $h$ of the random field to the standard deviation $J$ of the spin-spin coupling is small. In fact, we believe that for hard disks and spheres within the SOC model this ratio becomes zero as the packing fraction (density) approaches its maximum possible value $\phi_{\text{max}}$. The SOC model should therefore show features usually associated with ideal glass behavior in this limit. Much of the paper is devoted to investigating this intriguing possibility.

Our analytical approach to the derivation of an effective spin Hamiltonian does not extend to non-continuous potentials such as that appropriate to hard disks or spheres. In order to study them we have had to resort to simulations of the SOC model, in particular, event driven
molecular dynamics. The details of this are described in Sec. VII.

We used the Lubachevsky-Stillinger (LS) algorithm in Sec. VII to find some of the jammed states of the SOC model for hard disks. Its jammed states are similar to those of the unconstrained model. At the densest packing possible, \( \phi_{\text{max}} \), the state is jammed. We obtain an estimate of \( \phi_{\text{max}} \) from the largest value of the packing fraction \( \phi_j \) of the jammed states which we have found in small systems, for which there is a chance that the LS algorithm might actually find the densest state. It is actually very hard to do good simulations in the region of most interest, that is when \( \phi \to \phi_{\text{max}} \), because the constraints introduced by the cell walls makes the dynamics even slower than that of the unconstrained system. In two dimensions, \( \phi_{\text{max}} \) turns out to be very close to estimates of the glass close packing density \( \phi_G \), which is sometimes identified with the random close packing density \( \phi_{\text{rcp}} \).

We study in Sec. VIII and Sec. IX correlation functions of the hard disk system in order to determine the variance of the random field \( h^2 \) and the variance of the spin-spin couplings \( J^2 \). The physical reason for the presence of a random field is also elucidated in Sec. VIII. The form of the effective Hamiltonian is very similar to that obtained for smooth potentials in Sec. IV that is, it is a mixture of exchange and pseudo-dipolar couplings. Unfortunately because of the difficulties associated with the long relaxation times as \( \phi \to \phi_{\text{max}} \) we cannot get good numerical estimates of how \( h \) and \( J \) vary with packing fraction in that limit. Fortunately we can provide an argument in Sec. XI that shows \( h/J \sim (1 - \phi/\phi_{\text{max}}) \) as \( \phi \to \phi_{\text{max}} \).

One can use the droplet theory of spin glasses to determine the growth of the correlation length \( \xi \) from the ratio of \( h/J \). According to the droplet picture, the correlation length \( \xi \) can be estimated by equating the energy that can be gained from flipping the spins in a region of size \( \xi \) in the random field, \( h\xi^{d/2} \), to the domain wall energy cost of doing this, \( J\xi^\theta \), so
\[
\xi \sim \left( \frac{J}{h} \right)^{\frac{2}{d\theta}}, \tag{1}
\]
which reduces for \( h/J \sim (1 - \phi/\phi_{\text{max}}) \) to
\[
\xi \sim \frac{1}{(1 - \phi/\phi_{\text{max}})\nu}, \quad \nu = \frac{2}{d - 2\theta}, \tag{2}
\]
\( \theta \) is the domain-wall exponent for Ising spin glasses in zero field. For \( d = 2 \), \( \theta \approx -0.287 \) so \( \nu \approx 0.78 \) while for \( d = 3 \), \( \theta \approx 0.24 \) and \( \nu \approx 0.79 \). Behavior of a power law kind is also expected in RFOT at a packing fraction \( \phi_K \), the value of \( \nu \) in that approach is dependent on whether or not "wetting" effects are considered necessary, but the wetting form \( \nu = 2/d \) is not very different from that of Eq. (2) in two and three dimensions due to the fact that in these dimensions \( \theta \) is small. However, in our approach, we have not seen any evidence for the ideal glass transition at \( \phi_K \). For us the divergence of the correlation length is associated with glass close packing and jamming.

Finally in Sec. XII we discuss the key question: which features of supercooled liquids and glasses can the SOC model be expected to describe correctly? It is argued that the SOC model should be good for understanding some of the phenomena which exist on time scales less than the alpha relaxation time, as the caging of the particles on time scales less than the alpha relaxation time is mimicked by the trapping of the particles in the cells in the SOC model. The dynamical correlation length is extracted from the properties of correlations at the alpha timescale so we expect that the SOC model should at least give \( \nu \) correctly.

II. THE SINGLE OCCUPANCY CELL MODEL

Cell occupancy models have a long history in the study of phase transitions in fluids and liquids. In the past, they have been used to calculate the equation of state of hard spheres at high density or to place bounds on derivatives of the free energy or entropy. The system is divided into cells of a chosen geometry and a constraint is applied which fixes the number of particle centers found in each cell. We focus on the single occupancy cell (SOC) model, where each cell can contain at most one particle. We work in two dimensions, although the model is easily generalized to higher dimensions. Fig. 1 shows a hard disk fluid with a single cell occupancy constraint using square cells. The constraints mean that disk centers interact only with cell walls and disk surfaces interact only with other disk surfaces.

We note that it might be possible to realize the SOC system experimentally, at least in two dimensions. The square cells could be produced by a wire grid, and a post could be attached at the center of each disk so that while the circumference of the disk can pass under the wire grid, the post at the center cannot.

SOC models are useful to us because they make the introduction of a spin representation of the problem straightforward. A disadvantage of using the cell constraint is that at low packing fractions the behaviour of the system deviates significantly from the behaviour of the unconstrained system. At low packing fractions most of the collisions will be between disks and cell walls, so the cell geometry dominates. As the packing fraction is increased, more collisions occur between disks and close to jamming, almost all collisions will be between disks. The closer the packing fraction is to \( \phi_{\text{max}} \), the better an approximation the constrained model becomes to the unconstrained model as the cell walls no longer dominate the dynamics.

Another peculiarity of SOC models is the appearance of singularities in thermodynamic properties. This occurs because of how the constraints limit the size of clusters that can form. Without constraints, it is possible to find
all particles forming a single cluster at all packing fractions. This is not possible in the constrained system. As shown by Hoover and Alder for a one-dimensional hard rod SOC model, it is only possible to form clusters of a certain size above a certain packing fraction. For example at very low packing fractions, the constraints mean that clusters can only contain at most two particles. As the packing fraction is increased clusters can contain three then four particles. At the packing fractions where it becomes possible for larger clusters to form, the partition function changes its analytic form and this means that discontinuities appear in thermodynamic quantities such as $\partial^2 P/\partial V^2$. These packing fractions get closer together approaching $\phi_{\text{max}}$, and the discontinuities decrease in size, meaning that the shortcomings become less important. We expect similar behavior in two dimensions, but as each disk has more nearest neighbors the effect will be smaller. In any case, it has not been noticeable in our simulation results.

The model with disks of the same size, as in Fig. 1, is not a glass. Without constraints the largest possible value of the packing fraction $\phi$ occurs when a triangular lattice with all disks touching their neighbors is formed; so $\phi_{\text{max}} = \pi/2\sqrt{3} \approx 0.9069$. In the SOC version of the model, the constraints mean an exact triangular lattice cannot form, so we find $\phi_{\text{max}} \approx 0.88$. When $\phi = \phi_c \approx 0.77$ there is a phase transition to a slightly disordered crystal which is orientated in one of two possible directions as in Fig. 3. The critical exponents of this transition are expected to be those of the two-dimensional Ising model because of this two-fold degeneracy of the orientation of the slightly disordered crystal lattices.

III. SINGLE OCCUPANCY CELL MODELS FOR MODELLING GLASSES

To make a glassy model, we introduce two different sizes of disk. The binary disk system consists of hard disks of two species (A and B), where the SOC constraints have been applied, as in Fig. 2. The species of disk have different radii $\sigma_A$ and $\sigma_B$, where the size ratio $R_{AB} = \sigma_A/\sigma_B$ is held fixed as the packing fraction is altered. The packing fraction is given by

$$\phi = \pi(\sigma_A^2 + \sigma_B^2)/2,$$

where the side of the square plaquette has been taken to be of unit length. We set $R_{AB} = 1.0/1.4$ - this is a well explored choice. There are equal numbers of each species ($N_A = N_B = N/2$), and each cell contains a disk of species A or B with equal probability.

When $R_{AB} \to 1$, the system undergoes crystallization to one of the two disordered crystal states shown in Fig. 3, but with substitutional disorder. Disks of species A and B will be distributed at random throughout the defected crystal.

For $R_{AB} = 1.0/1.4$ without constraints, the densest state is a phase separated crystal where the two species form separate triangular crystals. Although this state is very stable, it takes such a long time to form that it is rarely reproduced in simulations. This makes the system a good model glass former. Recent work has shown that phase separation may be achieved on simulational time scales in some three dimensional binary systems. It may be that some nascent phase separation could be driving behaviour normally identified as glassy (slow dynamics, dynamic heterogeneity and growing correlation lengths). For an example, see Ref. 36.

With the introduction of the single occupancy constraints, phase separation can no longer occur as fixing the species of the disk in each cell fixes the local composition of the hard disk fluid. We chose to distribute the species across the cells with equal probabilities. This mimics what would happen if a well mixed fluid at low
packing fraction was rapidly ‘quenched’ to a higher packing fraction without allowing the disks to phase separate. As phase separation is prevented by the cell constraints, this means that glassy behavior can be investigated in a fully equilibrated model: there are no concerns that if one runs the simulation for longer there will eventually be phase separation.

IV. THE SPIN HAMILTONIAN

Our main reason for studying the SOC model is that it makes mapping to a spin system easy. This is acheived by drawing a vector from the center of each cell to the center of the disk that occupies that cell. The cells are labelled $i$, where $i = 1, 2, \ldots, N$ and the spin $\hat{s}_i$ is defined as

$$\vec{x}_i = \vec{R}_i + \hat{s}_i,$$  

(4)

where $\vec{x}_i$ is the position vector of the disk in cell $i$ and $\vec{R}_i$ is the position vector of the center of cell $i$. This mapping is illustrated in Figs. 2 and 4.

The system may now be analyzed as if it were a spin system. Unlike the particles, the spins are equivalent and all details of the interaction between them are found in the terms and couplings of the spin Hamiltonian. If we write $\hat{s}_i = (x_i, y_i)$, which is appropriate for $d = 2$, then in the usual XY model $|\hat{s}_i| = 1$, but in the SOC spin model, $x_i$ and $y_i$ take values which keep the disk in the $i$th plaquette.

Let us suppose that the particles in the cells interact with each other through the potential $V(r)$, where $r$ is the interparticle separation. The hard disk problem is a special case of this potential where $V(r) = \infty$ if $r$ is less than the sum of the radii of the two disks and is otherwise zero. If we have a binary mixture of two types of particles A and B, $V(r)$ will be a shorthand for $V_{ij}(r)$, where $i$ and $j$ encode the species of the interacting particles. We shall now proceed to derive the effective Hamiltonian in terms of the spin variables $\hat{s}_i$.

Using the notation in Fig. 1, the distance $r$ between a particle in cell $i$ and one in cell $j$ is

$$r = |\vec{x}_i - \vec{x}_j| = |\vec{R}_i + \hat{s}_i - \vec{R}_j - \hat{s}_j|. \tag{5}$$

To second order in the spin variables,

$$V(r) = V(R) + V'(R) \vec{R} \cdot (\hat{s}_i - \hat{s}_j)/R + \frac{V''(R) - V'(R)/R}{2} (\vec{R} \cdot (\hat{s}_i - \hat{s}_j))^2 / (2R^2) + \frac{V'(R)}{R} |\hat{s}_i - \hat{s}_j|^2 / (2R) + \cdots, \tag{6}$$

where $R = |\vec{R}_i - \vec{R}_j| = R_{ij}$.

The partition function $Z$ of the SOC model is

$$Z = \int \prod_{i=1}^{N} dx_i dy_i \exp[-\beta \mathcal{H}], \tag{7}$$

where the integration over $x_i, y_i$ covers the area of the $i$th plaquette. The Hamiltonian $\mathcal{H}$ is, to second order in the spin displacements, of the form (up to constants)

$$\mathcal{H} = -\sum_{i,\mu} h_i^\mu \hat{s}_i^\mu - \frac{1}{2} \sum_{i,\mu,\nu} D_{ij}^{\mu\nu} \hat{s}_i^\mu \hat{s}_j^\nu + \cdots, \tag{8}$$

where the sums over $\mu$ and $\nu$ run from 1 to 2 and in $d = 2$, $\hat{s}_i = (x_i, y_i)$. The fields $h_i^\mu$ are given by

$$h_i^\mu = \sum_{j \neq i} V'(R_{ij}) R_{ij}^\mu / R_{ij}. \tag{9}$$

If all the particles are identical, the “field” term $h_i^\mu$ is identically zero. However, if we have a binary mixture of two types of particles A and B such that $V_{AA}, V_{BB}$, and $V_{AB}$ all differ, then the field term $h_i^\mu$ is non-zero and time-reversal invariance is broken.

We can calculate the average of $h_i^\mu$ when the average is taken over the various possibilities allowed by the selected disk distribution. We will consider just nearest-neighbor interactions to illustrate how the calculations can proceed, and the case $\nu = x$. Only the sites to the right and left of the site $i$ contribute to the sum in Eq. (9). At each of these sites there can be an A or a B disk (with equal probability) and at the site $i$ there is an equal probability of the disk being A or B. Summing over the various possibilities one finds $\overline{h_i^\mu} = 0$. The distribution of the random field components is such that $\overline{h_i^\mu h_i^\nu} = h^2 \delta_{\mu\nu}$, where

$$h^2 = \frac{1}{4} [(V'_{AA} - V'_{AB})^2 + (V'_{BB} - V'_{AB})^2]. \tag{10}$$

The various derivative are calculated at the nearest-neighbor distance. Note that if $V_{AA} = V_{BB} = V_{AB}$, then $h = 0$, as expected.
The quadratic term in Eq. (8) takes the form for $i \neq j$

$$H_{eff}(\vec{s}_i, \vec{s}_j) = -\frac{V'(R_{ij})}{R_{ij}} \times \left[ \vec{s}_i \cdot \vec{s}_j - \left( 1 - \frac{R_{ij}V''(R_{ij})}{V'(R_{ij})} \right) (\vec{R}_{ij} \cdot \vec{s}_i)(\vec{R}_{ij} \cdot \vec{s}_j) \right], \quad (11)$$

where the unit vector $\vec{R}_{ij}$ is $R_{ij}/R_{ij}$. Note if the interaction $V(r) = -A/r^n$, Eq. (11) reduces to

$$H_{eff}(\vec{s}_i, \vec{s}_j) = -\frac{nA}{R_{ij}^{n+2}} \left[ \vec{s}_i \cdot \vec{s}_j - (n + 2)(R_{ij} \cdot \vec{s}_i)(\vec{R}_{ij} \cdot \vec{s}_j) \right]$$

which for $n = 1$ is the familiar dipole-dipole coupling interaction. For other non-power law potentials $H_{eff}(\vec{s}_i, \vec{s}_j)$ can be regarded as a mixture of the exchange interaction with pseudo-dipolar couplings.

When $i \neq j$, $D_{ij}^{\mu
u}$ is of the form

$$D_{ij}^{\mu
u} = \left[ A_{ij} \delta_{\mu\nu} - B_{ij} \vec{R}_{ij} \vec{R}_{ij} \right], \quad (12)$$

where

$$A_{ij} = -\frac{V'(R_{ij})}{R_{ij}}, \quad (13)$$

and

$$B_{ij} = \frac{V'(R_{ij})}{R_{ij}} (1 - \frac{R_{ij}V''(R_{ij})}{V'(R_{ij})}). \quad (14)$$

For $i = j$ there are single-ion anisotropy terms with coefficients

$$D_{ii}^{\mu
u} = -\sum_{j \neq i} D_{ij}^{\mu\nu}. \quad (15)$$

For smooth potentials like the Lennard-Jones potential, the $h_i^{\mu}$ and $D_{ij}^{\mu\nu}$ can therefore be directly calculated. The configurational average and variance of $D_{ij}^{\mu\nu}$ due to the quenched random distribution of A or B particles in the plaquettes can be obtained by the method used to obtain Eq. (10); the expressions are complicated.

The only approximation which arises from the use of the Hamiltonian in Eq. (8) is the truncation to second order in $s_i^{\mu}$. The hope is that this truncation does not alter the “universality class” associated with the phase transitions of the spin system. Of course, further terms could be included if required.

When Eq. (15) is used to fix the single-site terms, the Hamiltonian will still have in its quadratic terms the translational invariance of Eq. (8). Similarly if

$$h_i^{\mu} = \sum_{j \neq i} C_{ij} \hat{R}_{ij}^{\mu}, \quad (16)$$

that will ensure translational invariance in the linear term in Eq. (8). The quantities $A_{ij}$, $B_{ij}$, and $C_{ij}$ thus specify an effective spin Hamiltonian for our problem.

In Fig. 5 the positions are shown of the plaquettes whose associated disk can interact with the disk in the central plaquette when the packing fraction is high. The number of such disks is surprisingly large; 20. At smaller packing fractions the number is reduced to 8. (In three dimensions the number at large packing fractions is 80). Now for the blue disk to interact with the disk in plaquette 1, the disks in 2, 5, 6, and 10 must be occupying only a restricted portion of their plaquettes. A complicated many-spin set of terms in the effective spin Hamiltonian is needed to describe this feature. It is clear that keeping for example only nearest-neighbor spin-spin interactions does not contain the physics of the increase in the effective number of interacting spins as the packing fraction increases. Truncating the effective Hamiltonian to just binary spin interactions may also fail to capture the properties successfully modelled by $p$-spin models such as the dynamic transition. In this paper, our main concern is the behavior of glasses at temperatures below the dynamic transition temperature or at densities above $\phi_d$, the packing fraction associated with the (avoided) dynamic transition (see Sec. XIII) and binary spin interactions are quite sufficient to capture the Ising spin glass behavior which prevails there. An investigation as to whether the considerable range of the spin interactions can explain the utility of mean-field ideas in glasses is being carried out.

For hard disks and spheres the potential $V(r)$ is infinite when $r$ is such that they overlap, and zero otherwise. Such a potential makes $V'(r)$ zero except at the contact distance where it is infinite. As a consequence the expansion used in Eq. (6) is not useful. For hard disks
and spheres we shall still use quantities like $h^\mu_i$ and $D_{ij}^{\mu\nu}$, but instead of deriving them from the potential we will obtain their values as fitting parameters chosen to reproduce measured correlations (like $\langle s^\mu_i \rangle$ or $\langle x_i \rangle$ etc.) rather in the spirit of Ref. [39]. This is done in Sec. IX.

We have already noted that when $R_{AB} \to 1$, the system will undergo crystallization to one of the two disordered crystal states in Fig. 3 but with substitutional disorder. The disks of species $A$ and $B$ will be distributed at random throughout the defected crystal. However, when $R_{AB}$ is close to 1 there will be effectively random fields arising from the small differences in the A and B particles. We suspect that this changes the transition to the disordered crystalline state to that of the random-field Ising universality class. We shall suppose from now on that $R_{AB}$ is sufficiently different from unity that this crystal-like transition no longer arises and that only glass ordering behavior (i.e. spin-glass ordering in the spin mapping) need be considered.

V. SPIN GLASS BEHAVIOR

In this section we shall discuss the properties of a spin Hamiltonian like that in Eq. (8). For any smooth potential, the $h^\mu_i$ and $D_{ij}^{\mu\nu}$ can be directly calculated from the potential. These expressions will be renormalized by the effects of multi-spin interactions neglected in Eq. (8), but hopefully they provide a good first approximation. For hard spheres or disks they are parameters obtained by fitting to the measured correlation functions (see Sec. IX).

For the binary SOC model, the $D_{ij}^{\mu\nu}$ between sites $i$ and $j$ will depend on whether the particles in the plaquettes are $A$ or $B$ particles. As the particles can never escape from their cells, there is quenched disorder present. One can obtain the probability distribution function of the $h^\mu_i$ and $D_{ij}^{\mu\nu}$ and obtain their mean and variance. Rather than do this, (which is rather cumbersome and uninformative), we will just outline some of the possibilities which might arise. What actually happens for a given set of potentials $V_{AA}, V_{AB}, V_{BB}$ requires explicit calculations and simulations and the number of possible phases is large. To limit the discussion it is useful to recall the underlying system: disks (or spheres) whose centers are trapped in the squares (cubes) of a square (simple cubic) lattice. Ferromagnetic ordering in the spin system would correspond to a crystallization of the disk centers into a square lattice of the same periodicity as that of the plaquettes. This will not happen if one uses an appropriate binary mixture for modelling glasses and so we will discount the possibility of a transition to a ferromagnetic state and just concentrate on situations which are spin-glass like, i.e. those where the standard deviation of the couplings $D_{ij}^{\mu\nu}$ dominates their mean values. We will therefore not be discussing the type of ordering shown in Fig. 3 (for the monatomic system) where there is clear crystal order present: Glass behavior is not associated with any kind of long-range crystalline order.

The spins in the system are $d$-component spins so that one might have thought that any spin glass phase in this system would be in the universality class of the $d$-component vector spin glass. However, it was shown a long time ago [40] that in the presence of pseudo-dipolar-like terms, the transition to the spin glass phase is changed from one in the $d$-vector spin glass universality class to one in the Ising spin glass universality class.

The random field terms $h^\mu_i$ have a dramatic effect on the nature of the spin glass. At mean-field level and for dimensions $d > 6$ a $d$-component random field present in a $d$-component vector spin glass produces a phase transition—the de Almeida-Thouless transition [21]—which is in the same universality class as an Ising model in a field [22, 21]. The presence of the pseudo-dipolar terms just reinforces the Ising nature of this transition. For $d \leq 6$ the spin glass transition is removed by the presence of the random field [22, 23].

The spin-glass correlation length, which is equivalent to the point-to-set length scale, can still become large for $d \leq 6$ if the ratio $h/J$ is small. ($J$ is a measure of the standard deviation associated with the $D_{ij}^{\mu\nu}$). According to the droplet picture [25–27] the correlation length $\xi$ depends on this ratio as in Eq. (1). This is the correlation length appropriate to $T = 0$. As a function of temperature the correlation length is small at high temperatures and grows to this value in the limit when $T \to 0$. We expect that $\xi$ might become large for real fragile glasses at low temperatures. However, on this picture $\xi$ will never become infinite unless $h/J$ goes to zero. We suspect that this never happens for smooth potentials. In other words, for such potentials no diverging length scale is expected in $d \leq 6$.

Note that if we had used the mean-field approximation to determine the properties of the spin system, we would have found a phase transition, the de Almeida-Thouless transition, at a finite temperature provided the ratio $h/J$ is not too large. We would have then been tempted to identify this transition with the ideal glass transition. However, it is our belief that the AT transition does not occur for dimensions $d \leq 6$ [22, 23].

One might further wonder whether the multi-spin “p-spin” interactions which were alluded to in the discussion of Fig. 6 might make a transition to a one-step replica symmetry broken state possible. We have neglected them in our discussion. This is the scenario envisaged in the RPFOT and is the origin of the ideal glass transition. We do not think such a transition can exist outside the mean-field approximation, that is, in finite dimensions, where the one step replica symmetry broken state is unstable against the thermal excitation of large droplets [12].

For binary mixtures of hard spheres and disks, a mechanism might exist to drive the ratio $h/J$ to zero. In the SOC model there is a maximum packing fraction for hard disks or spheres. For our binary mixture of hard disks, this value is estimated in Sec. VII. Its value $\phi_{\text{max}}$ is very similar to $\phi_{\text{crp}}$ of the unconstrained model and in both
models at these densities, the pressure is infinite. We shall present numerical evidence and arguments in Sec. IX that the ratio $h/J \sim (1 - \phi/\phi_{\text{max}})$, so that in our version of the SOC model, the correlation length $\xi$ diverges to infinity according to Eq. (1). In other words there are features of a glass transition in the hard disk SOC model as $\phi \to \phi_{\text{max}}$, in that there is a diverging correlation length in spin–glass-like correlation functions. The rest of this paper is devoted to the study of this behavior.

To acquire data to determine $\phi_{\text{max}}$ and to obtain estimates of $h$ and $J$, it is necessary to perform simulations of the SOC hard disk system. In the next section, our simulation methods for hard disks are outlined.

VI. EVENT DRIVEN MOLECULAR DYNAMICS AND THE LUBACHEVSKY-STILLINGER ALGORITHM

To simulate the hard disk system, we use event driven molecular dynamics following the method described by Lubachevsky [44]. This is an efficient way to perform simulations of hard disk systems. We will not describe the method in full here, but the basic principle involved is to keep a list of the next collision each particle will be involved in ordered by time. Time is moved forward by jumping to the collision that occurs next, and then recalculating the list in light of the new velocities and positions the colliding particles now have. The speed of the simulation is further boosted by the fact the cell constraints restrict the particles that can possibly collide.

We generate configurations at a particular packing fraction by first placing particles randomly in each cell in such a way that each cell is equally likely to contain a particle of either species. The particles start with zero radius (so there is no possibility of overlap) and at time $t$ have radius $r_i(t) = \Gamma_i t$ where the $i$ denotes the species of the particle in question. The growth rate $\Gamma_i$ is set to be small to allow the disks to remain in equilibrium as the simulation progresses. We use $\Gamma \sim 10^{-4}$. Each disk is given a random velocity so that $\langle |v_i| \rangle = 1$.

The disks are allowed to collide and grow until the system reaches the desired packing fraction. Then the disk radii are set to be constant and measurements may be made.

To generate jammed states, we make use of the Lubachesky-Stillinger algorithm [24]. We begin the simulation as described above, but in this case the growth rate of the disks is not set to zero at any time. As the simulation proceeds, collisions (events) become separated by smaller and smaller time intervals and the simulation will become slower. If $\delta t_{DD}$ is the time between disk-disk collisions, $1/\delta t_{DD} \to \infty$ as the simulation proceeds. This is equivalent to a divergence in the pressure. The Lubachesky-Stillinger algorithm works by choosing a value of $\delta t_{DD}$ below which collisions are close enough together that the system has effectively jammed. Here we use $\delta t_{DD} = 10^{-8}$ with $\langle |v_i| \rangle = 1$. Repeating the simulation yields a range of jammed configurations, with a distribution of jammed packing fractions $\phi_J$.

VII. DETERMINING THE MAXIMUM PACKING FRACTION IN THE SOC BINARY MODEL

In this section we shall estimate the largest packing fraction $\phi_{\text{max}}$ for our binary hard disk system. It is as $\phi \to \phi_{\text{max}}$ that we expect the correlation length to diverge, so $\phi_{\text{max}}$ is like the critical temperature of the system.

As already discussed, at low packing fractions the behavior of the constrained fluid is very different from that of the unconstrained fluid, becoming closer to it as the packing fraction is increased. At some packing fraction the system will jam. In a jammed state for the unconstrained system, the disks are held in place by their neighbors, (except for a few rattlers), where $z = 2d$ – the so-called isotatic condition [15]. In the SOC model a disk can be jammed when its center is pinned against a plaquette wall.

Jammed states were obtained for a range of system sizes using the Lubachesky-Stillinger algorithm [24] described in Sec. VI. A plot of the values of $\phi_J$ values for the binary hard disk system can be seen in Fig. 6. The plot does not show the complete range of jammed states possible in the $L \times L$, but a subset obtained from several runs of the algorithm.

There is a fall from $\phi_{\text{max}} \approx 0.855$, when $L = 5$, then $\phi_{\text{max}}(L)$ settles around $\phi = 0.835$ before falling off slightly when $L > 30$. This fall off is due to inefficiencies in the simulation for generating jammed states of the highest packing densities. The value $\phi_{\text{max}} \approx 0.835$ is quite close to the value of the packing fraction at which unconstrained binary disk systems of this type jam, $\phi_J \approx 0.84$, using the protocol studied in Ref. [33]. In other words, it is close to the numbers quoted for “random close packing” in two dimensional systems.

The most significant change from the unconstrained binary fluid is the presence of a well-defined maximum jamming density $\phi_{\text{max}}$. In the unconstrained fluid when a jammed configuration has been acquired, one can always imagine creating a denser state by rearranging a few of the particles into a region with more local crystalline order. This will create a small amount of free volume which will allow further arrangements to be made. If this programme is continued, the final point is a completely crystalline configuration. A continuum of states at packing fractions between $\phi_J$ and $\phi_{\text{crystal}}$ can be constructed by this method (although there is no guarantee that they will be stable). This makes defining a densest non-crystalline state problematic. However, since the cell constraints do not allow the composition of the fluid to be altered, this programme cannot be followed in the SOC model and there is indeed a well-defined maximum density. This maximum density will depend on the par-
particular realization of the distribution of large and small disks over the cells, but it is probably a self-averaging quantity.

In the unconstrained model each protocol for producing jammed states produces states with a characteristic value of \( \phi_J \) as \( N \to \infty \). The Lubachevsky-Stillinger algorithm used in this paper produces, in the SOC model, states of a characteristic \( \phi_J \), which will not in general include the states at \( \phi_{\text{max}} \), except possibly at small values of \( N \). Within the SOC, different protocols will also produce different values for \( \phi_J \). Protocols which produce jammed states whose \( \phi_J \) is close to \( \phi_{\text{max}} \) are producing jammed states closer to those in the unconstrained model. As a consequence, we are expecting that for the densest jammed states, nearly all the disks will be touching 4 other disks in the jammed state and very few, if any, will be jammed because their center is touching a plaquette wall. In principle, but probably not in practice, one could obtain estimates of \( \phi_{\text{max}} \) by calculating the pressure \( P \) in a fully equilibrated system and determining \( \phi_{\text{max}} \) by fitting to

\[
\frac{PV}{N k_B T} = \frac{d\phi}{\phi_{\text{max}}(1 - \phi/\phi_{\text{max})}},
\]

which becomes exact as \( \phi \to \phi_{\text{max}} \). The problem with using this procedure is that it is very hard to equilibrate the system at packing fractions close to \( \phi_{\text{max}} \).

The cell constraints affect the dynamics of the system. This is a key concern as it affects how quickly the system can be equilibrated and hence the quality of simulations which can be done. The system is clearly glassy - simulations performed on systems with packing fractions above \( \phi = 0.75 \) become noticeably slow, while approaching the maximum packing fraction of around \( \phi \approx 0.835 \) makes good measurements extremely hard. The presence of the cell constraints makes the dynamics even slower than that of the unconstrained system.

Imagine a binary fluid at high packing fraction, focusing on one single disk. At any given time there will be a variety of moves the disk will be able to make. Most will be short and rapid (the typical behavior of a caged particle), but some may be part of large rearrangements that will allow the structure of the fluid to relax and change. It is reasonable to assume that the cell constraints will block a lot of these movements (simply because the walls of the cell will intercept the paths the disk wants to take), and they are more likely to interfere with the longer paths. Thus with the cell constraints in place, it is expected that the dynamics of the system will become slower. Lots of local rattling will be allowed, but the system will have to wait for longer before large, cooperative movements that allow structural rearrangements take place.

VIII. ORIGIN OF THE RANDOM FIELD FOR HARD DISKS

We have already remarked that when all the particles are identical the field term \( h_i \) in Eq. (8) is zero. For binary mixtures it is non-zero and this makes the expectation of the local magnetization \( \langle s_i^z \rangle \) also non-zero. This is easily understood from Fig. 7.

Zero local magnetisation means that a disk spends its time symmetrically distributed over its cell. With this in mind it is easy to see why the local magnetization is finite at all \( \phi \) in the binary system. When the packing fraction is very low the disks rattle backwards and forwards in their cells, rarely colliding with each other. The finite local magnetization is caused by having disks of different sizes on either side of the central disk. Say there is a large disk to the right, and a small disk to the left (as shown in Fig. 7). The neighboring disks will intrude into the cell. When their sizes are different they can intrude by different amounts. In the case just described the central disk will spend more time on the left hand side of the cell as there is more free volume there. As the packing fraction is increased, there is more intrusion by the neighboring disks and the deviation from the center of the cell becomes larger. This means that the local magnetization gets larger. This suggests that there should be three different types of behavior for the local magnetization: large disk to the left and small disk to the right \( \langle s_i^z \rangle > 0 \), large disk to the right and small disk to the left \( \langle s_i^z \rangle < 0 \) and lastly disks of the same size on each side \( \langle s_i^z \rangle \sim 0 \). In Fig. 8 the components of the local magnetisation split into these three groups. At higher packing fractions, the groups blur into one due to interactions between increasing numbers of disks, and the components are randomly distributed about zero.

In the spin interpretation, a finite local magnetization randomly distributed about zero implies the presence of a local random field \( h_i \) interacting with each spin through a term of the form \( -\sum_i h_i s_i \). The expectation value of the total magnetization \( \langle M \rangle = 0 \), where \( M = \sum_i s_i/N \).
for all packing fractions. This suggests that the \( h_i^\mu \) must be evenly distributed around zero. The source of the random nature of the field is the random distribution of the species of disk over the cells, since this affects the local magnetization at all packing fractions through the mechanism described above. This field will be discussed again in the following sections.

**IX. SPIN-SPIN CORRELATIONS**

We now study correlations of the form \( \langle s_i^\nu s_j^\mu \rangle \) where \( i \) and \( j \) index the lattice sites and \( \nu \) and \( \mu \) label the \( x \) and \( y \) components of the spins. For a spin in cell \( i \), we can calculate \( \langle s_i^x s_j^x \rangle \), \( \langle s_i^y s_j^y \rangle \), \( \langle s_i^x s_j^y \rangle \) and \( \langle s_i^y s_j^x \rangle \) for nearest neighbors (the spins north, south, east and west of spin \( i \)) and next-nearest neighbors (the spins northeast, south-east, south-west and north-west of the spin \( i \)). We are interested in using these correlations as a guide to the effective interaction between the hard disks.

Our studies suggest that the effective spin interactions follow closely the form expected in Sec. IV: the effective spin Hamiltonian is well-approximated by Eqs. (8) and (12).

There are many different local environments a disk can experience. We have therefore studied the average of these correlations, defined as follows. We have calculated for each site \( i \) its spin’s correlation with its neighbors at \( i + \delta \), where \( \delta \) is a label running over the N,W,E,S nearest neighbors and NW, SW, SE, and NE next-nearest neighbors (i.e. we calculate \( \langle s_i^\nu s_{i+\delta}^\mu \rangle \)). The site averages of these correlation functions were also calculated and the results are shown in Figs. [9] and [10] for \( N = 256 \). In principle there is no need to do an average over disk realizations as the site averages are self-averaging quantities.

There are some notable features visible in these Figures. The correlations are seen to grow as the packing fraction increases, suggesting that the coupling between spins increases in strength with packing fraction. Studying Fig. [9] the strongest correlations are seen to be those with the East and West spins for \( \langle s_i^x s_j^x \rangle \) and with the North and South spins for \( \langle s_i^y s_j^x \rangle \). It makes sense that (for
It is always non-zero even at small packing fractions.

fraction is increased towards its maximum possible value. It can be seen that the overlap increases as the packing of the amorphous or glass order in the system. In Fig. 11, the quenched disorder in the system (here the species of the central spin). Studying Fig. 10, it is clear that for the overlap measured for a spin glass in a field is finite at all values of the temperature, growing larger as \( T \rightarrow 0 \). This happens because the (random) fields bias the orientations of the spins.

**X. EFFECTIVE SPIN HAMILTONIAN FOR HARD DISKS**

We will try to understand the correlations studied in Sec. IX with the aid of an effective Hamiltonian like that in Eqs. (8) and (12), but for simplicity we ignore all couplings except those between nearest neighbors. This is a poor approximation at large packing fractions, but is better for low packing fractions. We will also work to lowest non-trivial order for each quantity studied.

A weak coupling expansion can be made which allows fitting of \( A_{ij} \) and \( B_{ij} \) from the simulation results. Unfortunately, as this is a weak coupling approximation (i.e. it is valid when \( A_{ij} \) and \( B_{ij} \) are small) it cannot be used to accurately measure them in the region of most interest, \( \phi \rightarrow \phi_{\text{max}} \), as there they become large.

The correlation \( \langle s^x_i s^x_j \rangle \) is calculated using:

\[
\langle s^x_i s^x_j \rangle = \frac{1}{Z} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} s^x_i s^x_j e^{-\beta H_{\text{eff}}} \prod_k d^2 s_k, \tag{19}
\]

where the spins components \( s^x_k \) are integrated over the kth cell, which has unit side length. The partition function is

\[
Z = \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} e^{-\beta H_{\text{eff}}} \prod_k d^2 s_k. \tag{20}
\]

The integrals can be performed by first Taylor expanding the exponential, and then integrating to give the correlation in terms of \( A_{ij} \), and \( B_{ij} \) and some simpler averages.
measurements to determine $\beta A_{ij}$ (nearest-neighbor pair). The values of $\beta A_{ij}$

On performing the Taylor expansion we find

$$\langle s_i^\mu s_j^\nu \rangle \approx \frac{1}{Z} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} s_i^\mu s_j^\nu \sum_{\langle i,j \rangle} \beta D_{\mu \nu}^0 s_i^\mu s_j^\nu \prod_k d^2 s_k,$$

and performing the integration yields

$$\langle s_i^\mu s_j^\nu \rangle \approx \beta \left[ A_{ij} \delta_{\mu \nu} - B_{ij} \frac{R_i^0 R_j^0}{|\vec{R}_{ij}|^2} \right] \langle (s_i^\mu)^2 \rangle \langle (s_j^\nu)^2 \rangle. \quad (21)$$

To the order we are working $\langle (s_i^\mu)^2 \rangle = \langle (s_i^\nu)^2 \rangle \approx 1/12$.

Because we have measured $\langle s_i^\mu s_j^\nu \rangle$ we can use these measurements to determine $\beta A_{ij}$ and $\beta B_{ij}$ for each bond (nearest-neighbor pair). The values of $\beta A_{ij}$ and $\beta B_{ij}$ have a distribution, with a mean and a standard deviation. The standard deviation is important as it is the randomness of the effective couplings which is encoded in the standard deviation which can be the cause of spin glass behavior if it is sufficiently large compared to the means of the couplings. In Fig. 12 we have plotted the averages of $\beta A_{ij}$ and $\beta B_{ij}$ as a function of the packing fraction $\phi$.

Using the same approximation for the effective Hamiltonian we can determine the variance of the random field $\bar{h}_i$ from our results for $q$.

$$\langle h_i^\mu \rangle \approx \frac{1}{Z} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} s_i^\mu e^{-\beta H_{eff}} \prod_k d^2 s_k,$$

and expanding

$$\langle h_i^\mu \rangle \approx \frac{1}{Z} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} s_i^\mu (1 - \beta H_{eff}) \prod_k d^2 s_k$$

$$\approx \beta h_i^\mu \langle (s_i^\mu)^2 \rangle. \quad (23)$$

Again one can replace $\langle (s_i^\mu)^2 \rangle$ by 1/12.

Thus the variance $\langle h^2 \rangle$, defined as

$$\langle h^2 \rangle = \frac{1}{N} \sum_i \beta h_i^\mu \langle (h_i^\mu)^2 \rangle \approx \frac{144}{N} \sum_i \langle (s_i^\mu)^2 \rangle = 72q. \quad (24)$$

Eq. (24) shows that the variance of the random field will increase with packing fraction just like $q$ does, at least when $q$ is small, (see Fig. 11). The equation will not hold at high packing fractions, where we actually expect $\langle h^2 \rangle$ to diverge but $q$ must always remain less than $1/2$.

This inequality arises because $q$ cannot exceed the value it would have if all the disks were simultaneously at the corners of plaquettes).

**XI. THE CORRELATION LENGTHS**

The quantity of most interest is the spin glass correlation length as it should be the glass correlation length. We shall determine it via the spin-glass susceptibility. First the cumulant $\chi_{ij}^{\mu \nu} = \langle s_i^\mu s_j^\nu \rangle - \langle s_i^\mu \rangle \langle s_j^\nu \rangle$ is obtained. This measures fluctuations in the correlations between the $\mu$ and $\nu$ components of the spins $i$ and $j$. The spin glass wave-vector dependent susceptibility is

$$\chi_{SG}(\vec{k}) = \frac{1}{N} \sum_{\mu,\nu, i,j} [\chi_{ij}^{\mu \nu} (2)]_{av} \exp(ik.\vec{R}_{ij}), \quad (25)$$

where $\vec{R}_{ij}$ is the vector connecting lattice sites $i$ and $j$. From $\chi_{SG}(\vec{k})$ the spin glass correlation length $\xi_{SG}$ can be calculated using the formula

$$\xi_{SG} = \frac{1}{N} \sum_{\mu,\nu, i,j} \left[ \frac{\chi_{SG}^{\mu \nu}(0)}{\chi_{SG}(\vec{k}_{min})} - 1 \right]^{1/2}, \quad (26)$$

where $\vec{k}_{min}$ is the minimum non-zero wave-vector $\vec{k}_{min} = (2\pi/L, 0)$.

Additionally, a ferromagnetic correlation length can be calculated and compared to the spin glass length to see which kind of correlations are dominating the system. A ferromagnetic wave-vector dependent susceptibility is defined:

$$\chi_{F}(\vec{k}) = \frac{1}{N} \sum_{\mu,\nu, i,j} \langle (s_i^\mu)^2 \rangle_{av} \exp(ik.\vec{R}_{ij}). \quad (27)$$

This is similar to the spin glass susceptibility, but $\chi_{ij}^{\mu \nu}$ is not squared. From this, a ferromagnetic length scale $\xi_{F}$ can be calculated:

$$\xi_{F} = \frac{1}{N} \sum_{\mu,\nu, i,j} \left[ \frac{\chi_{F}^{\mu \nu}(0)}{\chi_{F}(\vec{k}_{min})} - 1 \right]^{1/2}. \quad (28)$$
for the system to equilibrate and the susceptibility to reach its correct level.

XII. SCALING OF THE EFFECTIVE COUPLINGS NEAR $\phi_{\text{max}}$

As $\phi \to \phi_{\text{max}}$ it is just not possible to equilibrate the system. Furthermore even if we could measure the correlations in this limit, we would not be able to determine $h_{ij}^\mu$ and $D_{ij}^{\mu \nu}$ by the procedure of Sec. [X which relied on the validity of the weak-coupling approximation, which fails as $\phi \to \phi_{\text{max}}$. Our numerical studies only tell us that $h_{ij}^\mu$ and $D_{ij}^{\mu \nu}$ are increasing with packing fraction. In this Section we present a simple argument that in the limit $\phi \to \phi_{\text{max}}$ their dependence on packing fraction is as

$$\beta h_{ij}^\mu \sim 1/(1 - \phi/\phi_{\text{max}})$$

and that

$$\beta D_{ij}^{\mu \nu} \sim 1/(1 - \phi/\phi_{\text{max}})^2.$$  

The total phase space of a finite system of hard disks or spheres is fractured into a number of regions (“blocked states”) which are mutually inaccessible. As the density is pushed up there are fewer and fewer blocked states [11]. Eventually as the packing fraction reaches the maximum for the system there is only one blocked state left. This can be compressed to a jammed state at $\phi_{\text{max}}$. The pressure diverges to infinity according to Eq. (17). We can use this observation to deduce how $h_{ij}^\mu$ and $D_{ij}^{\mu \nu}$ in the effective spin Hamiltonian of Eq. (8) must vary as $\phi \to \phi_{\text{max}}$ so as to recover the exact expression for the pressure of the hard sphere or hard disk gas in Eq. (17). Our argument is just a variant of the procedure of Salsburg and Wood [30].

The jammed state at $\phi_{\text{max}}$ will be isotactic to a high degree of approximation. That is, each disk or sphere will be touching $z = 2d$ neighbors. Only a few (if any) will be jammed by virtue of their centers touching a plaquette wall and we will assume this does not occur for the state at $\phi_{\text{max}}$. In Sec. [XIII a variation of the SOC model based on Voronoi cells is outlined where this will certainly be true. A finite number of disks touching the plaquette wall would not in any case affect the argument. Then in the spin mapping, such a jammed state should be a minimum of the Hamiltonian in Eq. (8). Suppose this minimum occurs at values of $s_i^\mu = S_i^\mu$. The Hamiltonian at its minimum,

$$\beta H_{\text{min}} = -1/2 \sum_{i,j} (\beta h_{ij}^\mu) F_{ij}^{\mu \nu}(\beta h_{ij}^\nu),$$

is just a constant, independent of $\phi$ with the above scalings of $h_{ij}^\mu$ and $D_{ij}^{\mu \nu}$. (Here $F_{ij}^{\mu \nu}$ is the matrix whose inverse is $\beta D_{ij}^{\mu \nu}$.) This expression for $\beta H_{\text{min}}$ in the partition function defined by Eq. (7) would not then give

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**FIG. 13:** (Color online) Spin glass correlation length (in red) and ferromagnetic correlation length (in green) for the spin system derived from the binary hard disk fluid. Calculated for a system with $N = 256$ disks.
a contribution to the pressure. The pressure is actually determined by the contribution from the vicinity of the jammed state at \( \phi_{\text{max}} \). To evaluate this contribution to \( Z \) let us write \( s_i^\mu = S_i^\mu + (1 - \phi/\phi_{\text{max}}) f_i^\mu \). Because we are expanding about a minimum, the integrals over the \( f_i^\mu \) are Gaussian quadratic forms in the \( f_i^\mu \) which do not depend on \( (1 - \phi/\phi_{\text{max}}) \), with our assumed scalings of \( D_{ij}^{\mu\nu} \). They give a contribution to the partition function

\[
Z \approx (1 - \phi/\phi_{\text{max}})^d N,
\]

via the terms which come from the changes in the integration variable from \( s_i^\mu \) to \( f_i^\mu \). This yields Eq. (17) for the pressure. This result is just a consequence of the scaling assumed for \( h_i^\mu \) and \( D_{ij}^{\mu\nu} \) with \( (1 - \phi/\phi_{\text{max}}) \).

Note that according to this argument, both the mean and the standard deviation of the couplings, (which we generically label \( \beta J_0 \) and \( \beta J \) respectively, without distinguishing the labels \( \mu \) and \( \nu \)), will scale in the same way, viz as \( 1/(1 - \phi/\phi_{\text{max}})^2 \). \( \beta h \) will scale as \( 1/(1 - \phi/\phi_{\text{max}}) \).

Inserting these expressions for \( \beta h_i \) and \( \beta J_i \) into Eq. (1) we recover Eqs. (2) for the correlation length. For hard disk systems and hard sphere systems we are therefore predicting that there is an actual divergence of the correlation length as \( \phi \rightarrow \phi_{\text{max}} \). The circumstances where this behavior might be relevant to the unconstrained system are discussed below.

**XIII. DISCUSSION**

In a supercooled liquid, a particle is caged on time scales less than the alpha relaxation \( \tau_\alpha \). On longer time scales it can diffuse anywhere in the system. In the SOC model, each particle is caged forever in the cell into which it was first inserted.

We can measure \( \tau_\alpha \) from the incoherent scattering function:

\[
F(\vec{k}, t) = \frac{1}{N} \sum_i \langle e^{i \vec{k} \cdot [\vec{r}_i(0) - \vec{r}_i(t)]} \rangle.
\]

(33)

However, \( F(\vec{k}, t) \) will never decay to zero in the SOC model – it will fall to a plateau and remain on the plateau for all time. In order to see why that happens consider the root-mean-squared displacement:

\[
\langle r_{\text{MSD}}(t) \rangle = \left\langle \frac{1}{N} \sum_i [\vec{r}_i(t) - \vec{r}_i(0)]^2 \right\rangle.
\]

(34)

For the unconstrained system \( r_{\text{MSD}}(t) \) first steadily increases with time, levels off while the particle is caged and finally grows to infinity. For the system under the SOC the cell walls ensure that \( r_{\text{MSD}}(t) \) will saturate at a value determined by the size of the cell. This in turn ensures that \( F(\vec{k}, t) \) remains non-zero for all time.

This does not mean that the relaxation times of the SOC system are infinite. Consider

\[
C(t) = \frac{1}{N} \sum_i \langle \tilde{s}_i(0) \tilde{s}_i(t) \rangle,
\]

and note that \( \langle \tilde{s}_i(0) \tilde{s}_i(t) \rangle = \langle \tilde{s}_i \rangle \langle \tilde{s}_i \rangle \) as \( t \) goes to infinity, so in this limit \( C(t) \) approaches \( \rho \). The timescale obtained from a study of how long \( C(t) \) takes to reach \( \rho \) would be similar to \( \tau_\alpha \) in the constrained system: the relaxation time \( \tau_\alpha \) comes about because rearrangements on the scale of \( \xi \) in the unconstrained system are needed to relax the cages holding the particles. In the SOC model, rearrangements on the scale of \( \xi \) are also required to allow full relaxation, so the two timescales are similar. We leave the details to future studies.

There is disorder present in structural glasses on the alpha relaxation time scale – their molecules move so little that the local environment of any molecule is effectively disordered. However over periods of many alpha relaxation times, the disorder is averaged out. Given this, the SOC model where quenched disorder is built in, may be appropriate for studying the behavior of the fluid on timescales of order \( \tau_\alpha \). Furthermore it is from data on such timescales that one can obtain estimates of the correlation length \( \xi \). We expect that at least when \( \xi \) is large there is probably little difference between the point-to-set length scale and the dynamic length scale [1].

Estimates of the dynamical length scale \( \xi \) are obtained as follows. The four-point correlation function \( G_4(\vec{r}, t) \) defined as [15]:

\[
G_4(\vec{r}, t) = \langle \rho(0, 0) \rho(0, t) \rho(\vec{r}, 0) \rho(\vec{r}, t) \rangle - \langle \rho(0, 0) \rho(0, t) \rangle \langle \rho(\vec{r}, 0) \rho(\vec{r}, t) \rangle,
\]

(36)

should develop a plateau when the liquid starts to become glassy. The dynamic susceptibility is calculated by integrating \( G_4(\vec{r}, t) \) over volume:

\[
\chi_4(t) = \frac{1}{V} \int G_4(\vec{r}, t) d^d \vec{r}.
\]

(37)

When measured in a glassy system, \( \chi_4(t) \) is observed to grow with time, peaking at times comparable to \( \tau_\alpha \) before decaying. As the temperature is lowered or the packing fraction is increased, the peak moves to longer and longer times (corresponding to the increase in \( \tau_\alpha \)). The dynamic susceptibility can be thought of as a ‘correlation volume’ which reveals the scale of regions which are dynamically correlated [1], providing evidence of a growing correlation length \( \xi \) in glassy systems.

In the binary disk SOC system, quenched disorder is present in the form of the random distribution of disk species over the cells. The growth of \( \chi_{\text{SG}} \) and \( \xi_{\text{SG}} \) reveal the presence of growing amorphous order. Because for the SOC system the quenched disorder persists for all time, not just for timescales up to \( \tau_\alpha \), if \( \chi_4(t) \) were measured in the SOC model it would grow and then saturate at \( \chi_{\text{SG}} \).
It is our belief that SOC models of hard disks and spheres can therefore describe the increase of $\xi$ with packing fraction, at least as regards the value of the exponent $\nu$. We do not expect the value of $\phi_{\text{max}}$ to necessarily coincide with the packing fraction of the divergence in the unconstrained system — after all, $\phi_{\text{max}}$ would be of slightly different value if the cells had not had a square shape or even were of random shape. A way of constructing “random” cells would be to equilibrate the binary disk or sphere system and then use as the cells the Voronoi cells of a single configuration as the cells. Because of this built-in randomness, this same procedure could be used to model the striking glassy features of monodisperse spheres. (For the Voronoi cell version of the SOC model, the argument in Sec. XII is clearly exact [33]. On the other hand, for such cells it would be impossible to carry out the analytical calculations in Sec. IV).

The divergence of $\xi$ as $\phi \to \phi_{\text{max}}$ is likely to be accompanied by a divergence of the relaxation time of the SOC model. Note that such behavior is not that expected of a $G$ point [49]. At a $G$ point $\xi$ and $\tau$ both diverge, but the pressure remains finite. At $\phi_{\text{max}}$ the pressure is infinite, as it is also a jammed state.

Our value for $\phi_{\text{max}}$ is quite close to the estimates of the value of the random close-packing fraction: $\phi_{\text{rcp}} \approx 0.84$ [34]. We think that this similarity is not an accident. Both the packing fractions, $\phi_{\text{max}}$ and $\phi_{\text{rcp}}$, are obtained from situations where the phase space of the hard disks has been curtailed so that the system cannot stray far from its initial state. $\phi_{\text{max}}$ will depend on the choices made for the shape of the cells. It will also depend on how the large and small particles are assigned to the cells. In our work this has been done randomly but one could build into the distribution if desired the local correlations of the unconstrained system. It is also known that the random close packing fraction $\phi_{\text{rcp}}$ is not well-defined: it has a small dependence on the protocol used to determine it [35].

When studying the unconstrained hard sphere or hard disk system, some protocol has to be adopted to see glassy behavior, such as a finite compression rate, and this will result in the pressure going to infinity at some packing fraction less than that of the densest crystalline state. In true equilibrium, the pressure of course remains finite unless the system is at the maximum density of the crystalline state. We believe that the glass state is well-defined provided that the alpha relaxation time $\tau_\alpha$ is such that $1/\tau_\alpha$ is greater than the rate for phase separation and crystallization in the case of binary mixtures, or the time scale for crystal nucleation and growth generally. A finite compression rate should not modify the quasi-equilibrium approach to glasses (like that in this paper) provided that it is small compared to $1/\tau_\alpha$. Since the alpha relaxation time $\tau_\alpha$ is expected to grow with $\xi$ as $\ln \tau_\alpha \sim \xi^{1/2}$ [50], then for a fixed compression rate one can only hope to obtain the growth of $\xi$ up to a compression rate determined value. But within these various constraints we believe the glass problem is well defined and that SOC models are a useful way of studying some aspects of it.

We would expect the SOC model of hard disks or spheres to be most useful at densities above $\phi_d$, the density at which timescales increase rapidly. This density can be quite well-understood with the aid of mode-coupling theory. For hard spheres $\phi_d \approx 0.58$ and for hard disks $\phi_d \approx 0.78$ [11]. In the case of hard disks in the SOC model, timescales were seen to increase very rapidly at a rather similar density. This is because at such densities the timescales are long because they involve collective rearrangements of the disks on a length scale $\xi$ and collisions with the walls of the plaquette are becoming insignificant. Alas, this very rapid increase makes numerical investigations at densities above $\phi_d$ very challenging.

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