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Ludovic Berthier[1], Hugo Jacquin[2] and Francesco Zamponi[3]

[1] Laboratoire des Colloïdes, Verres et Nanomatériaux, UMR CNRS 5587, Université Montpellier 2, 34095 Montpellier, France
[2] Laboratoire Matière et Systèmes Complexes, UMR CNRS 7057, Université Paris Diderot—Paris 7, 10 rue Alice Domon et Léonie Duquet, 75205 Paris cedex 13, France
[3] Laboratoire de Physique Théorique, École Normale Supérieure, 24 Rue Lhomond, 75231 Paris Cedex 05, France
E-mail: berthier@lcvn.univ-montp2.fr, hugo.jacquin@univ-paris-diderot.fr and francesco.zamponi@lpt.ens.fr

Abstract. When materials such as foams or emulsions are compressed, they display solid behaviour above the so-called 'jamming' transition. Because compression is done out of equilibrium in the absence of thermal fluctuations, jamming appears as a new kind of a nonequilibrium phase transition. In this proceedings paper, we suggest that tools from equilibrium statistical mechanics can in fact be used to describe many specific features of the jamming transition. Our strategy is to introduce thermal fluctuations and use statistical mechanics to describe the complex phase behaviour of systems of soft repulsive particles, before sending the temperature to zero at the end of the calculation. We show that currently available implementations of standard tools such as integral equations, mode-coupling theory, or replica calculations all break down at low temperature and large density, but we suggest that new analytical schemes can be developed to provide a fully microscopic, quantitative description of the jamming transition.

Contents

From the point of view of statistical mechanics, the jamming transition observed by compressing random packings of soft repulsive particles in the absence of thermal fluctuations is an intriguing phenomenon [1]. It is a phase transition, in the sense that the mechanical response of the system changes abruptly at a critical density [2]. It is also a critical phenomenon, since several scaling laws and diverging length scales have been described on both sides of the transition [3, 4]. Finally, it is a nonequilibrium phenomenon because the transition occurs in samples prepared out of equilibrium in the absence of any relevant thermal fluctuations, and it is thus not possible to describe jamming without stating precisely the protocol used to prepare the system [5]. Yet, quite remarkably, many features of the jamming transition appear to be protocol-independent.

Given the central role played by far from equilibrium critical phenomena in statistical mechanics [6], jamming is thus a very active field of research and attracts the attention of the statistical mechanics community [1, 7]. In this conference paper, we mainly discuss the problem of the jamming transition from the point of view of statistical mechanics. We review recently published work on the subject, and expand it in some places. We also discuss the philosophy and provide the first new results of our on-going effort to develop a new analytical approach to the problem [8].

This paper is organized as follows. In section 1, we give a short account of the properties of the jamming transition that theory should explain and reproduce. In section 2 we briefly review the main theoretical approaches and explain the basic ideas behind our approach. In section 3 we show how liquid state theory fares, and explain why it fails at low temperature. In section 4, we treat the fluid–glass transition of harmonic spheres using both mode-coupling theory and replica calculations, where new results are presented. We present our conclusions in section 5.
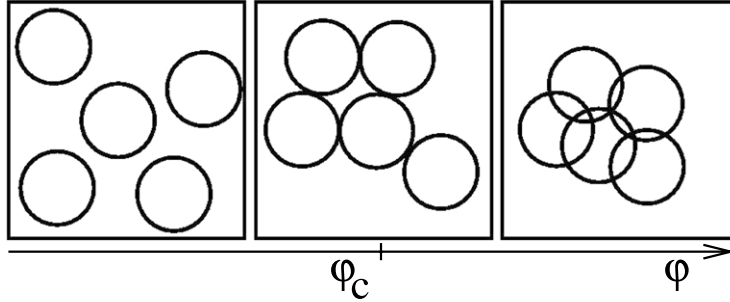
Figure 1. Packings of soft repulsive spheres at $T = 0$ undergo a nonequilibrium jamming transition at a critical packing fraction φ_c. The mechanical properties change from fluid to solid across φ_c. Energy, pressure, and mechanical moduli increase continuously from zero above φ_c, while the number of contacts per particle jumps discontinuously to a finite value at φ_c.

1. Jamming as a nonequilibrium phase transition

In a pioneering study, Durian showed that jamming could fruitfully be studied in computer simulations using simple models of soft repulsive spheres, and he introduced a model of harmonic spheres interacting through the simple pair potential [2]

$$V(r) = \epsilon \left(1 - \frac{r}{\sigma}\right)^2 \theta \left(1 - \frac{r}{\sigma}\right), \tag{1}$$

where σ represents the particle diameter, ϵ is an energy scale, and $\theta(x)$ is the Heaviside function. Thus particles repel each other harmonically when they overlap, but ignore each other otherwise. In Durian's original work, the potential was meant to describe the physics of wet foams, but this 'bubble' model is in fact so generic that it could equally be applied to the physics of soft colloids (such as dense microgels [9]) or emulsions [10]. Therefore, ϵ can be interpreted as a parameter accounting for the elasticity of the soft particles, be they soft bubbles, colloids or droplets. In the absence of thermal fluctuations or external forcing, the unique control parameter for the phase behaviour of the model of harmonic spheres is the number density, $\rho = N/V$, for a system composed of N particles enclosed in a volume V. Equivalently, one can use the 'packing fraction', $\varphi = \pi \sigma^3 \rho / 6$, although this name only strictly makes sense when particles do not overlap at low enough density. Indeed, because particles are soft, φ is not bounded.

In figure 1 we summarize schematically the main features of the jamming transition that have been discovered, mostly through numerical observations [1]. Simulations have revealed the existence of a critical packing fraction, φ_c, below which the packings have no overlap. In this phase, the energy, pressure and number of contacts between particles are zero. Above φ_c, pressure, energy, number of contacts, bulk and shear moduli are non-zero. The linear (elastic) response of the system to deformation changes abruptly at the transition: below φ_c, small deformations can be imposed without any energy cost, while above φ_c, an arbitrarily small deformation causes an increase in energy.

Interestingly, almost all these quantities increase continuously from zero across φ_c and vary algebraically with the distance to the transition, $\varphi - \varphi_c$. A notable exception is the number of contacts, which, as suggested by figure 1, jumps discontinuously to a finite value

at φ_c given by $z_c = 2d$, where d is the space dimensionality. The critical z_c corresponds to the 'isostatic' value, i.e. the minimal value for the system to be rigid [11]. At φ_c the system is therefore marginally solid, with vanishing shear and bulk moduli. Moreover, the pair correlation $g(r)$ of systems at φ_c is very different from both amorphous glasses or dense liquids, and presents a number of singular behaviours, from a diverging contribution at the interparticle distance $r = \sigma$ [12, 13], to large-distance anomalies [14] reflected in a peculiar low-wavevector behaviour of the isothermal compressibility [15].

Finally, the nonequilibrium nature of the transition is clear from the fact that thermal fluctuations are actually irrelevant for the features described above. This implies that 'crossing' the transition by 'compressing' the system is not a uniquely defined procedure [16]. It is thus crucial to also specify how this is done in practice, in particular how averages at each density are performed, that is, how different configurations at the same density are sampled. In an equilibrium setting, this is not necessary as configurations are sampled with their associated Boltzmann weights. Two well-studied procedures to study the jamming transition are the following. First, rapid compressions of hard sphere systems simulated by molecular dynamics [17] produce jammed configurations in the limit of infinite pressure [18, 19]. Note that in this procedure thermal fluctuations play a role since thermal equilibrium can be reached at low enough density. Note also that the jammed phase cannot be accessed since particles cannot overlap. A second and very different procedure consists of studying systems of soft repulsive spheres, as in equation (1), directly at $T = 0$ using energy minimization methods [3]. In both cases, sampling and averages are performed by repeating the compression or minimization protocol from a different set of initial conditions. A critical volume fraction φ_c with the properties described above is generically found for any of these protocols. At present, there is numerical evidence that if the exact value of φ_c is protocol dependent, the critical properties are not [20].

2. On the theory of the jamming transition

At the theoretical level, there is at present no accepted framework to understand and account for all the features of the jamming transition that we have described, which mostly stem from very detailed numerical observations [1]. Thus, if the physics and the main features of the transition are well described [7], the theory is by comparison less advanced. An elegant scaling theory, which identifies a divergent length scale and relates various observed scaling laws or critical exponents, has been elaborated [4, 7]. Additionally, several distinct statistical frameworks have also been developed [21]–[23], using in particular the idea that a statistical ensemble (the 'Edwards ensemble' [24] or a 'force ensemble' [25]) distinct from the Gibbs ensemble must be introduced to study the jamming transition. A detailed account of these approaches is beyond the scope of this short paper and we refer the reader to the recent reviews [1, 7] for further references.

Here, we shall argue that the three main characteristics discussed above, namely the existence of a fluid–solid jamming phase transition, its associated critical properties, and its nonequilibrium nature can in principle all be accurately computed within the standard framework of equilibrium statistical mechanics, starting from the sole knowledge of the interaction between the particles in equation (1). The general strategy we propose is to study the statistical mechanics of a system of harmonic spheres in the presence of thermal

fluctuations. If this procedure is properly implemented, then we expect that a sharp phase transition with the above characteristics will occur at a critical volume fraction in the limit of $T \to 0$.

The main conceptual difficulty to be faced has actually a physical origin, and deep consequences. In the relevant regime, the system is in fact characterized by the existence of a large number of amorphous metastable states separated by large free energy barriers [5]. This means that the system gets naturally dynamically arrested in nonequilibrium glassy states, and that the free energy landscape is quite complex. This implies first that the above mentioned dynamical protocols to probe the jamming transition are naturally affected by the glass transition [5, 19]. Second, this means that statistical mechanics treatments must accurately take the complexity of the phase space into account—or will necessarily fail. A theoretical framework to handle this complexity was developed in [26] and applied in the context of particle systems in [27]–[29]. It was also more recently implemented in [19] for hard spheres.

The aim of the present work is to show that, although the approach is conceptually simple and direct, there remain purely technical difficulties, since previous implementations of these ideas are not very accurate in the limit of interest to describe the jamming transition, where temperature is low and density is large. In a separate work [8], we describe our on-going efforts to circumvent these technical difficulties to try and yield a predictive, quantitative, microscopic approach to the jamming transition.

3. Statistical mechanics of harmonic spheres: fluid phase

3.1. Integral equations

Our first step is to start investigating the behaviour of repulsive harmonic spheres in a regime where temperature is large. In the absence of attractive forces, the system is thus in a fluid phase, where correlations between particles are small.

In this regime, it is enough to treat the system using tools developed to study the statistical mechanics of the liquid state, such as integral equations [30]. These are typically closure relations yielding the pair correlation function of the fluid,

$$g(r) = \frac{1}{\rho N} \left\langle \sum_{i \neq j} \delta(|\mathbf{r} - \mathbf{r}_{ij}|) \right\rangle, \tag{2}$$

where brackets denote a thermal average.

In [31] we studied the potential (1) using one particular closure relation, the Hyper-Netted Chain (HNC) approximation. In this approximation,

$$g(r) = \exp[-\beta V(r) + g(r) - 1 - c(r)], \tag{3}$$

where $\beta = 1/T$, $c(r)$ is the direct correlation function defined through the Ornstein–Zernike equation:

$$g(r) - 1 = c(r) + \rho \int \mathrm{d}\mathbf{r}' \, c(|\mathbf{r} - \mathbf{r}'|)[g(r') - 1]. \tag{4}$$

By numerical integration of equation (3), one can get $g(r)$, and thus study the thermodynamic behaviour of the model for any state point (φ, T).
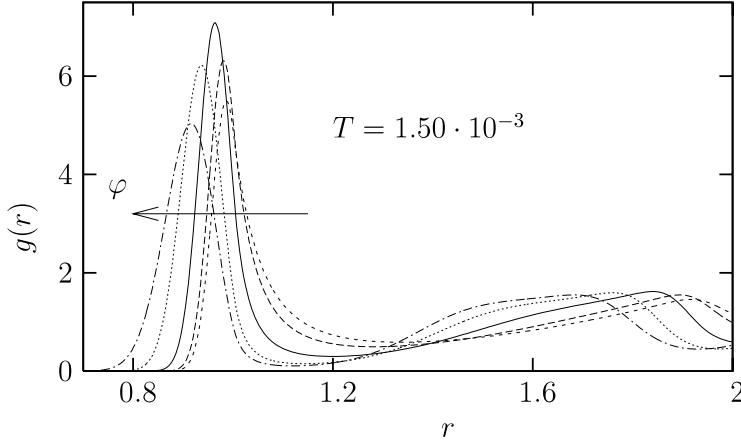
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Figure 2. Nonmonotonic evolution of the pair correlation function when volume fraction is increased at constant temperature in the fluid phase, as predicted using the HNC approximation [31], a simple integral equation frequently used in liquid state theory. Volume fractions are $\varphi = 0.600, 0.663, 0.777, 0.900$, and 1.00 (from right to left).

Not surprisingly, no phase transition is detected by compressing the system at constant temperature within such an approach, even when temperature is small. In fact, it can easily be shown that the ground state energy density,

$$e_{\text{gs}}(\varphi) = \lim_{T \to 0} e(T, \varphi) \tag{5}$$

remains zero at all φ, since the energy density vanishes as $e(T, \varphi) \sim T^{3/2}$, a result which is clearly inconsistent with the sketch in figure 1. Simultaneously, the pair correlation function remains smooth and shows none of the jamming singularities described in the introduction in the range where the jamming transition is found numerically. As we argue below, this is not an artefact of the specific approximation employed, but is likely a generic feature of the integral equations developed for liquids.

Although a sharp jamming transition is not found, there is an interesting feature which emerges from the study of integral equations, as shown in figure 2. Upon compression at constant temperature, the evolution of the first and second peaks in the pair correlation function shows two distinct regimes, depending on the value of the volume fraction. For $\varphi < \varphi^{\star}(T)$, the position of the first peak of $g(r)$ shifts to smaller distances, reflecting the fact that particles get closer to each other. The height of the peak increases and structural order increases in the fluid. For $\varphi > \varphi^{\star}$, the position of the peak continues to shift to smaller r, but the height of the peak now decreases with φ. Thus, the fluid becomes more disordered as density is increased, an 'anomalous' behaviour not seen in simple liquids.

This density anomaly is actually well known in the context of the physics of ultrasoft particles [32, 33], i.e. particles interacting with a pair potential that remains finite when particles fully overlap, as in equation (1) where $V(r = 0) = \epsilon$, but it is interesting to rephrase its physical explanation in the context of jamming [31], where the crossover $\varphi^{\star}$ plays the role of a 'soft jamming' [34] or a 'thermal vestige' [9] of the jamming transition. It is therefore also particularly interesting in the context of the question asked in our title, since the physics behind the density anomaly is a competition between energy and
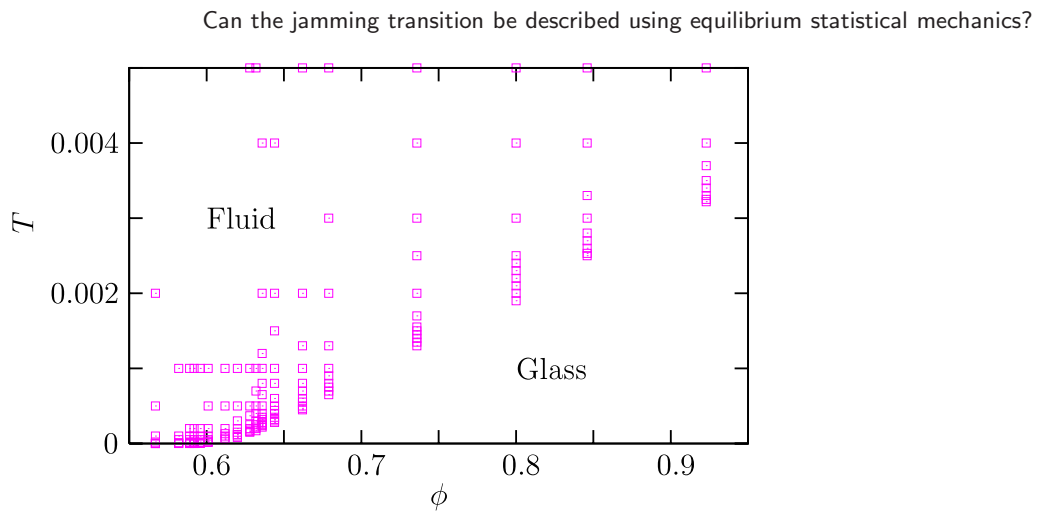
Figure 3. Numerical phase diagram for a binary mixture of harmonic spheres [36]. The symbols correspond to 'fluid' state points where thermal equilibrium can be reached using molecular dynamics simulations. In the 'glass' phase with no symbols, the relaxation time has become too large to be numerically determined, the system is effectively a nonergodic glass. Note that the jamming transition at $T = 0$ and $\varphi = \varphi_c$ cannot be accessed at thermal equilibrium. Fluids do not jam, only glasses do.

entropy to minimize the free energy at thermal equilibrium. Briefly, the anomaly stems from the increasing difficulty, and thus the increasing entropic cost, to find states with little overlap, and thus with little energy, when φ becomes large. Above $\varphi^\star$, the system thus prefers instead to expend some finite energy to allow particle overlaps, which can be done in many different ways and thus makes the structure of the fluid less ordered.

As shown in figure 1, the jamming transition corresponds to an extreme case of the crossover observed at finite temperature, namely a transition between a low-φ phase, where numerous states with no overlap can be found, and a large-φ phase, where states without overlap only exist with a vanishing probability. This suggests theories of the liquid state fail to describe a sharp jamming transition because they do not accurately describe this competition at very low temperatures and large densities, as we confirm in section 3.2.

3.2. Numerical simulations

Why does liquid state theory fail to account for the jamming transition? A direct answer is provided by numerical studies of the finite temperature behaviour of the model (1). In [35, 36], the dynamics of harmonic spheres was studied using molecular dynamics simulations. In figure 3, we report in the (φ, T) plane the state points for which thermal equilibrium could be reached, and the typical relaxation time measured with sufficient precision during the course of the numerical study. Numerical simulations thus indicate that it becomes increasingly difficult to reach equilibrium in the regime where density is large and temperature low, see figure 3. In the 'glass' phase, structural relaxation does not occur during the timescale allowed by the numerical experiment, and the system is essentially frozen in a very long-lived metastable state. For practical purposes, it has all

the characteristics of a glass [37], i.e. an amorphous (liquid-like) structure, which does not relax (solid-like) on the observation timescale.

Therefore, simulations teach us that the free energy landscape of the system of harmonic spheres becomes very complicated in the glass regime [5]. It is this complexity which is responsible for the breakdown of liquid state theory, which cannot be used to explore the glass phase.

In figure 3 we also note that, along the $T = 0$ axis, equilibration cannot easily be achieved above $\varphi \approx 0.60$, while most numerical determinations of φ_c are much above this value, in the range $\varphi_c \approx 0.64$–0.66. Thus, we conclude that even if one introduces thermal fluctuations into the game, the jamming transition cannot be crossed at thermal equilibrium because the glass transition intervenes first, whatever path in the (φ, T) plane is followed, compressions or quenches. Therefore, the jamming transition can only be observed by compressing glasses—not fluids.

The unavoidable conclusion is that a theory of the glass state is needed, instead of a theory of the liquid state, as we describe in section 4.

4. Statistical mechanics of harmonic spheres: glass phase

Although the theoretical literature of the glass transition is vast [37], there are not very many microscopic quantitative approaches, i.e. capable of formulating quantitative predictions starting from the knowledge of the interaction between the particles, as we attempt to do here. The mode-coupling theory of the glass transition and the replica approach to the glass phase are the two examples we discuss in this section. For both approaches, new results are presented.

4.1. Mode-coupling theory

The mode-coupling theory of the glass transition was developed in the mid-80s [38]. It is built using tools first developed to describe the structure and dynamics of liquids, and, in its initial formulation, uses the formalism of projection operators to derive a closed set of dynamical equations of motion for time correlation functions of supercooled liquids. In its common implementation, mode-coupling theory can thus be seen as a 'black box' which is fed by structural information on the fluid (the two-point static structure factor of density fluctuations), and provides as an outcome the time dependence of density–density autocorrelation functions at any wavevector.

This short description shows that mode-coupling theory is in principle able to describe the features revealed by the numerical results shown in figure 3. Indeed we present in figure 4 results from the analytical study of the phase diagram of harmonic spheres. The low density part of these results was presented in [39], where technical details can be found. In that work, a detailed analysis of the dynamic scaling properties near the fluid–glass transition occurring near $T = 0$ was presented. In [40] a similar theoretical analysis was performed for an interaction potential very close to the harmonic potential studied here, where the harmonic exponent 2 in equation (1) is changed to 5/2, the so-called Hertzian sphere potential, yielding results qualitatively similar to those presented in figure 4.

Importantly, the results of the mode-coupling analysis shown in figure 4 confirm the propensity of the harmonic sphere system to form a glass at large density and low
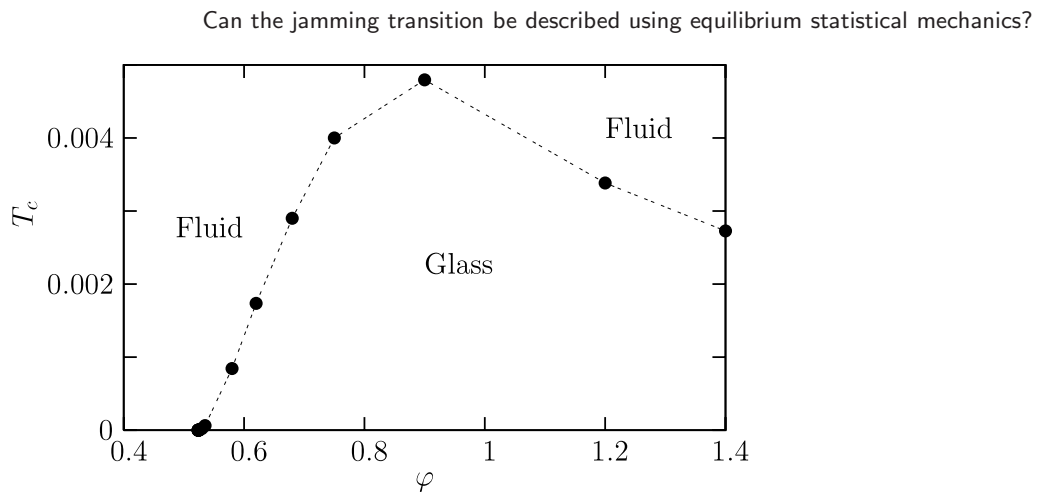
Figure 4. Dynamical phase diagram for harmonic spheres derived from mode-coupling theory [39] confirms the propensity of harmonic spheres to undergo a glass transition at low temperatures. The reentrant glass line at large φ is a dynamical counterpart of the density anomaly shown in figure 2.

temperature. However, the mode-coupling results are quantitatively not very accurate, as is well known after two decades of mode-coupling studies in the field of the glass transition [37, 38].

Although quantitative agreement is not found between theory and simulations, mode-coupling theory makes one striking prediction for the phase behaviour shown in figure 4. Theory predicts the existence of a temperature regime where the fluid of harmonic spheres becomes a solid glass upon compression at constant temperature. Strikingly, upon compressing the glass further, there exists a second critical volume fraction above which the glass is melted and becomes a flowing fluid. Such a glass melting at high density is typically not observed in standard models of liquids, and is the direct result of the particle softness [40]. We in fact already provided an explanation for this behaviour when we discussed the physics of the density anomaly in section 3.1 and figure 2. The reentrant glass transition predicted theoretically in figure 4 had not been observed in [35, 36], because the range of volume fractions studied numerically was too narrow, but it was recently observed for a system of Hertzian spheres in [40].

Now, although the mode-coupling equations can in principle be used to describe the (nonergodic) dynamics in the glass phase, it needs as input the static structure of the fluid, which is the very problem we posed ourselves at the beginning of the paper. Thus, although this approach is useful in determining the existence and location of the glass phase in the system, it cannot be employed to describe the thermodynamic behaviour and structural evolution deep into the glass phase. To do so, we must turn to the thermodynamic replica approach.

4.2. Thermodynamic replica approach

4.2.1. The replica method. The replica approach to the glass transition [26]–[29] can be seen as a modern and more systematic implementation of the self-consistent phonon theory developed long ago by Wolynes and co-workers [41]. The goal is to properly evaluate the thermodynamics of the glass phase, by carefully taking into account the existence

and proliferation of long-lived metastable states which are indeed responsible for the breakdown of liquid state approaches at low temperatures, as described in section 3.

To account for the effect of metastable states, the partition function is decomposed into the respective contributions of inter-and intra-states free energies,

$$Z = \int \mathrm{d}f \, \mathrm{e}^{-N\beta(f - T\Sigma(f))}, \tag{6}$$

such that $\mathcal{N}(f) = \exp[N\Sigma(f)]$ represents the number of metastable states with free energy f, and $\Sigma(f)$ is called 'complexity'. This decomposition can be seen as a generalization of the one based on the concept of inherent structures developed earlier by Goldstein [42] and Stillinger and Weber [43].

The replica approach is a computational tool devised to derive analytically the complexity of the system as it approaches the glass transition, and the thermodynamic properties of the system deep in the glass phase [26, 29]. It is based on the introduction of an effective temperature $T_{\mathrm{eff}} = T/m$ conjugated to the free energy f in equation (6), in the same way as temperature is conjugated to energy in standard computations. If m is an integer, it can be interpreted as the number of replicas of the original system [26]. A careful analysis shows that one is then able to deduce the thermodynamics of the glass from the thermodynamics of a m-times replicated liquid, with m being analytically continued to non-integer values. To compute the properties of the glass, one must then study the properties of an effective liquid that is a 'mixture' of m copies of the original system [27, 29]. We refer to [19, 44] for extensive reviews of a technique whose advantages and shortcomings, successes and failures, are by now well established.

As briefly mentioned in the introduction, this step is of course crucial to understand the physics of the glass transition, but it is equally fundamental to properly describe the jamming transition which lies deep in the glass phase. The numerical protocols devised to study the jamming transition indeed all rely on a dynamical exploration of the ground state properties of the system at $T = 0$ found either using gradient descent methods (which indeed produce inherent structures [43]), or rapid compressions. Given the topology of the phase diagram in figure 3, both rapid quenches and fast compressions hit the glass transition at some point, and from that point these numerical procedures in fact follow the zero temperature properties of long-lived metastable states across the jamming transition. The thermodynamic replica method, centred around the properties of these states, appears therefore very well suited to describe the jamming transition in soft repulsive systems.

As discussed at length in the glass literature [37, 44], the decomposition in equation (6) relies on the existence of infinitely long-lived states, such that a thermodynamic calculation makes sense. This is a typical mean-field assumption, because in finite dimensions metastable states only have a finite lifetime (which of course becomes extremely large in the glass phase), and this makes the thermodynamic replica approach prone to criticism.

Approaching the jamming transition, though, the lifetime of the states indeed diverges, so that we expect the mean-field approximation to behave better upon approaching the jamming point than it does around the glass transition [19]. We conclude therefore that thermodynamic replica calculations offer a promising theoretical framework to study the ground state properties of harmonic sphere glasses.

In sections 4.2.2 and 4.2.3, we present two attempts to apply the replica approach to harmonic spheres near jamming. Although partially unsuccessful, these new results
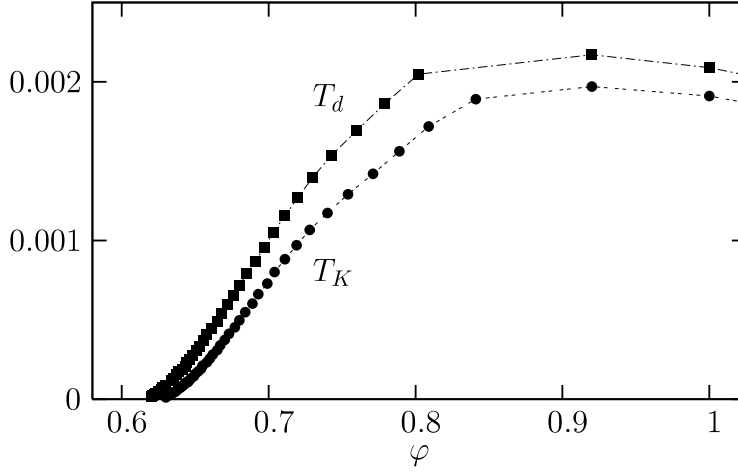
Figure 5. Thermodynamic, $T_K(\varphi)$, and dynamic, $T_d(\varphi)$, glass lines determined from solving the replicated HNC approximation are in good qualitative agreement with both simulations, figure 3, and mode-coupling results, figure 4.

nevertheless provide useful guidance into the difficulties to be faced in properly describing the jamming transition.

4.2.2. First attempt: replicated Hyper-Netted Chain (HNC). In practice, the thermodynamics of the replicated liquid has to be computed using some liquid theory approximation. The simplest of these approximations is the replicated HNC theory developed in [27]. It leads to a set of coupled equations for the diagonal and off-diagonal replica correlation functions, whose solution allows one in principle to determine the full phase diagram of the system. However, it has been checked in the case of hard spheres that this approximation is correct in the liquid phase, while it fails badly in the glass phase and in particular close to jamming [27]. The origin of this failure has been discussed in [19, section IV], where the replicated HNC equations are presented in full detail.

Therefore, this approximation can only be used to determine the glass transition lines $T_K(\varphi)$ and $T_d(\varphi)$ for harmonic spheres. Within mean-field theory, the former represents the thermodynamic glass transition where the complexity vanishes, while the second represents the dynamic glass transition marked by the appearance of metastable states (it is closely related, in principle, to the mode-coupling singularity discussed above).

These new results are shown in figure 5. The curves have the expected shape and suggest, once again, the existence of a glass phase at low temperatures and large density, as seen in computer simulations, see figure 3. In particular, $T_d(\varphi)$ has the same qualitative behaviour of the mode-coupling transition temperature in figure 4, suggesting that the reentrant glass transition scenario should be a robust feature of this system [40]. Note also, that the ratio $(T_d - T_K)/T_K$ is often (inversely) correlated to the kinetic fragility of glassforming systems. Then, one prediction of the replicated HNC approach is that this ratio decreases on increasing density above $\varphi \sim 0.6$, which is consistent with the numerical observation that the liquid becomes more fragile when φ increases [35, 36].
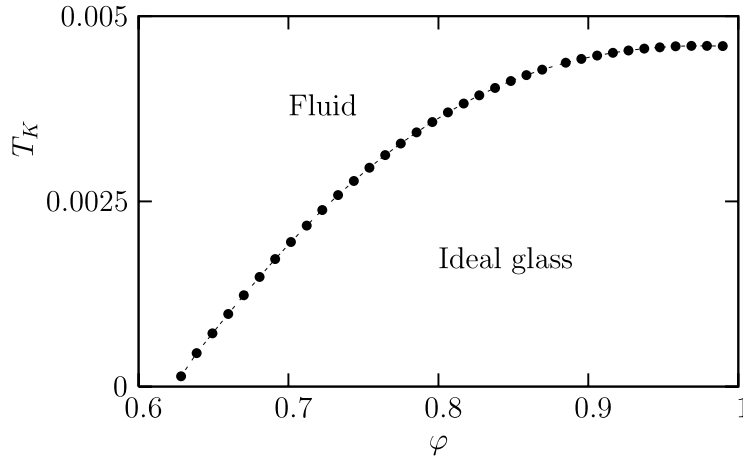
Figure 6. The ideal glass transition line, $T_K(\varphi)$, determined using the first order small cage expansion of the replica approach. Note that no transition is found below $T_K \sim 1.4 \times 10^{-4}$, and the $T \to 0$ limit cannot be studied.

4.2.3. Second attempt: the small cage expansion. A more successful approach was later suggested by Mézard and Parisi, based on the physical idea that deep into the glassy phase when the temperature is small, the m replicas of the effective system will undergo small vibrations within each state, suggesting that a perturbative expansion of the free energy in the small cage size, A, can be performed.

With this procedure, the free energy of the replicated system is mapped onto the free energy of a non-replicated system at effective temperature $T_{\text{eff}} = T/m$. The glass phase is found to be described by values of m that are smaller than one, so that the replicated liquid is found, in the small cage expansion, to be equivalent to a non-replicated liquid at higher temperatures. As a result of this purely analytical game, one can finally relate the thermodynamics of a state point of the original system located inside the glass phase, to those of a state point in the liquid phase of the effective system, where liquid state theory, such as HNC, can reliably be applied. This scheme has been successfully applied to Lennard-Jones glasses in [28, 29].

We have studied the system of harmonic spheres using the small cage expansion at first order. From the replicated free energy, one can deduce the locus of the Kauzmann thermodynamic glass transition and all the thermodynamic properties of the glass. We present our results for $T_K(\varphi)$ in figure 6, which is again in qualitative agreement with other schemes described above.

Unfortunately, the small cage expansion, while being well defined in the high density regime, fails in the jamming regime that we are interested in. The reason for this failure is that the non-analyticity at $r = 1$ of the harmonic spheres (which is mandatory for them to behave like hard spheres when $T = 0$) makes the free energy expansion ill-behaved in the limit $T \to 0$ when the density is too small. This can be seen in figure 6, where the glass transition line cannot be followed down to $T_K = 0$, and the transition abruptly disappears at some volume fraction, which is an artefact of the small cage expansion.

For the learned readers, this can be easily seen by looking at the first order expression given in [29]. The first correction to the free energy at small A has the form

$-\beta\Delta F = -12A\beta\varphi(m-1)\int_0^\infty r^2 g(r)\Delta V(r)\,\mathrm{d}r$. We know that $g(r)\sim \mathrm{e}^{-\beta V(r)}$ as $T\to 0$. We then deduce that $-\beta\Delta F \sim 36A\sqrt{\pi\beta}(1-m)/\sqrt{m}$. Since the zeroth order term of $-\beta F$ has a finite limit (the entropy of hard spheres), we conclude that the expansion is not defined in the limit $T\to 0$, because of the $A\sqrt{\beta}$ prefactor, and thus cannot be used to study the approach to the jamming transition from above.

This failure also explains why an alternative free energy expansion was recently developed to study hard spheres [19]. In this approach, a different small cage expansion was performed in powers of $\sqrt{A}$ (instead of A in the Mézard–Parisi scheme), consistent with the observation that the A-expansion is divergent. Using the $\sqrt{A}$ expansion, it was possible to study the jamming transition (pressure, structure) on the hard sphere side [19]. However, this method only applies to hard spheres and it cannot be used to explore the jamming transition of harmonic spheres.

Technically, a full description of the jamming transition thus requires an expansion scheme which is able to describe the crossover between the $\sqrt{A}$ and the $A\sqrt{\beta}$ expansions of the free energy, valid on both sides of the jamming transition. Such a new approximation forms the core of a separate publication [8].

5. Conclusion

In this proceedings paper, we have justified our on-going effort to attack the purely geometric problem of soft sphere packing in three dimensions using the tools of equilibrium statistical mechanics. This philosophy thus suggests to add a temperature axis to the phase diagram and study the statistical mechanics of soft repulsive spheres, the jamming transition being obtained in the limit of $T\to 0$. Adding thermal fluctuations to a situation where hard constraints need to be satisfied is actually a common tool, for instance in combinatorial optimization problems [5, 45].

However, we also showed that adding temperature does not immediately solve the problem, since one quickly realizes that jamming does not occur in a fluid but in the glassy part of the phase diagram where thermal equilibration is not easily reached. Thus, describing jamming requires the development of accurate analytical tools to describe the structure and thermodynamics of soft repulsive glasses, which is a delicate task.

We showed that although conceptually feasible, previously published analytical schemes actually fail near the jamming singularity, suggesting that new theoretical developments are needed to successfully derive a fully microscopic, quantitative theory of the jamming transition. We shall report elsewhere the results of our work in this direction [8].

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