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Comment on "Packing hyperspheres in high-dimensional Euclidean spaces"

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It is shown that the numerical results of Skoge *et al.* [Phys. Rev. E **74**, 041127 (2006)] are in very good agreement with the theoretical predictions of Parisi and Zamponi [J. Stat. Mech.: Theory Exp. (2006) P03017].

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In a recent paper [1] Skoge *et al.* presented new accurate numerical data on amorphous packings of hard spheres in space dimension $d>3$. It was shown (see, e.g., Fig. 4 in [1]) that, on compressing the low-density liquid at a constant rate γ, the pressure of the system follows the equilibrium pressure of the liquid up to some density (often called the glass transition density) above which the pressure starts to increase faster than in equilibrium, and diverges on approaching a value of density $\phi_J(\gamma)$, which is called the jamming density (here and in the following by "density" we mean the packing fraction, defined as $\phi = v_d(\sigma/2)\rho$, where ρ is the number density of spheres, $v_d(r)$ the volume of a d-dimensional hypersphere of radius r, and σ the diameter of one sphere). Crystallization seems to be strongly suppressed by kinetic effects in dimension $d>3$ and can then be neglected in the following discussion. Values of $\phi_J(\gamma)$ have been accurately measured in [1] as a function of γ. On the contrary, $\phi_g(\gamma)$ is not precisely determined as long as $\gamma>0$: the glass transition is smeared and happens in a crossover region $[\phi_g^-(\gamma), \phi_g^+(\gamma)]$. However, the amplitude of the crossover interval seems to decrease for $\gamma \to 0$ (see again Fig. 4 in [1], and see [2] for a recent theoretical discussion of these effects).

Recently, a theory of the glass transition of hard spheres, that can be applied in any space dimension d, was developed [3,4]. The basic idea is that the phenomenology observed at finite γ is due to an underlying thermodynamic glass transition [5–7]: i.e., that in the limit $\gamma \to 0$, $\phi_g^\pm(\gamma) \to \phi_K$, the Kauzmann density, at which an equilibrium phase transition to a glass phase happens. This is an idealized picture that neglects metastability effects due to the presence of the crystal: the consequences of this approximation might be important but cannot be discussed here; see [4] for a detailed discussion. However, as it seems that crystallization is negligible in $d>3$, a comparison between the theory and the data of [1] is possible. In the equilibrium glass phase, the pressure increases faster than in the liquid phase (i.e., the compressibility is smaller), and diverges at a value of density $\phi_{RCP} = \lim_{\gamma \to 0} \phi_J(\gamma)$ which we call the random close packing (RCP) density. This is the definition of random close packing that can be given within our theory. However it is affected by the metastability effects related to the presence of the crystal; see [4,8] for a discussion. In particular, in [8] the notion of the random close packing density has been criticized and an alternative notion of maximally random jammed (MRJ) packings has been proposed (see below).

Our theory is based on standard liquid theory and on the replica trick: it takes as input the equation of state of the liquid phase (in practice one has to choose an expression that describes well the liquid at low density and extrapolate to higher density), and gives as output (i) the Kauzmann density ϕ_K; (ii) the random close packing density ϕ_{RCP}; (iii) the equation of state in the glass phase; (iv) some properties of the pair correlation function in the glass phase, e.g., its shape close to contact; (v) the equation of state of the metastable glass states that are reached for $\gamma>0$ and their contribution to the entropy (the configurational entropy or complexity); see [3] for all the technical details. One of the most interesting predictions of the theory is that $2^d \phi_{RCP} \sim d \log d$ for large d. As far as I know, this scaling was proposed in [3] for the first time. The aim of this comment is to show that the results of [1] are fully compatible with this prediction.

With this aim, an expression for the equation of state of the liquid in $d>3$ is needed as input to the theory. The simplest choice is a generalization of the celebrated Carnahan-Starling equation of state to $d>3$ [9]:

$$Y(\phi) = \frac{1-\alpha\phi}{(1-\phi)^d},$$

$$\alpha = d - 2^{d-1}(B_3/b^2), \tag{1}$$

where $Y(\phi) = g(\sigma^+)$ is the value of the radial distribution function at contact, and b and B_3 are the second and third virial coefficients, whose exact expression is known [9]. The entropy of the liquid $S(\phi)$ is obtained by integrating the exact expression

$$\phi \frac{dS}{d\phi} = -\frac{\beta P}{\rho} = -1 - b\rho Y(\phi). \tag{2}$$

Given $S(\phi)$, the random close packing density is the solution of

$$S(\phi) - d \log\left(\frac{\sqrt{8}}{2^d \phi Y(\phi)}\right) + \frac{d}{2} = 0, \tag{3}$$

while the Kauzmann density is the solution of

$$S(\phi) - d \log\left(\frac{\sqrt{2\pi}}{2^d Q_0 \phi Y(\phi)}\right) = 0, \tag{4}$$

with $Q_0 = 0.638\ldots$ [3]. These equations can be easy solved numerically to get the values of ϕ_{RCP} and ϕ_K for any given value of d. The results are reported in Table I for $d \leq 8$, and compared with ϕ_{MRJ} as reported in [1]. The latter quantity is

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TABLE I. Values of ϕ_K and ϕ_{RCP} from the theory (only values for $d \leqslant 8$ are reported for brevity; values for $d \geqslant 8$ are in Fig. 1) compared with the available measured values of ϕ_{MRJ} [1]. The last column gives the value of ϕ_{RCP} extrapolated from the data of [1] (see text).

d	ϕ_K (theory)	ϕ_{RCP} (theory)	ϕ_{MRJ} [1]	ϕ_{RCP} (extrapolated)
3	0.6175	0.6836	0.64	
4	0.4319	0.4869	0.46	0.473
5	0.2894	0.3307	0.31	
6	0.1883	0.2182	0.20	
7	0.1194	0.1402		
8	0.0739	0.0877		

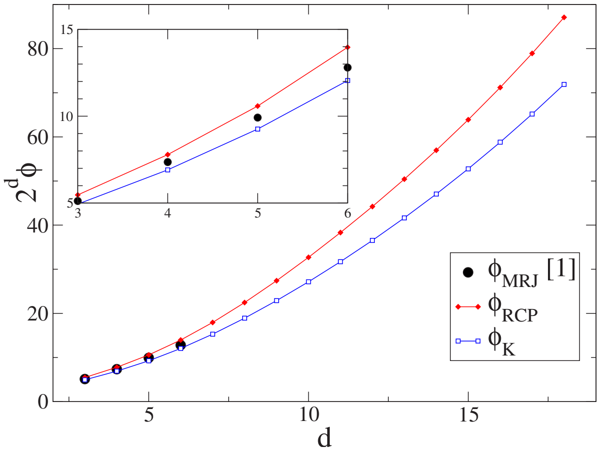

FIG. 1. (Color online) Plot of ϕ_K [open squares, obtained by solving Eq. (4)], ϕ_{RCP} [full diamonds, Eq. (3)], and ϕ_{MRJ} (full circles, numerical estimate of [1]) as a function of the dimension. Both ϕ_K and ϕ_{RCP} scale as $2^d\phi \sim d \log d$ for large d, while their distance scales as $2^d[\phi_{RCP} - \phi_K] \sim d$. In the inset the same plot for $3 \leqslant d \leqslant 6$ (compare with Fig. 6 in [1]).

the density of the maximally random (according to some measure of "order") collectively jammed packings of the system (see [8] for the precise definition); it is estimated in [1] by the jamming density $\phi_J(\gamma)$ for finite but small γ (see Sec. IV in [1] for a detailed discussion). As $\phi_J(\gamma)$ is expected to increase on decreasing γ and $\phi_{RCP} = \lim_{\gamma \to 0} \phi_J(\gamma)$, it follows that ϕ_{MRJ}, as estimated in [1], should be strictly lower than ϕ_{RCP}, but close to it, consistently with the data in Table I. A plot of ϕ_K and ϕ_{RCP} for d up to 19 is reported in Fig. 1. Note that it has been suggested in [1] that $2^d \phi_{MRJ} \sim c_1 + c_2 d$; this scaling is not in contradiction with $2^d \phi_K, 2^d \phi_{RCP} \sim d \log d$ because ϕ_{MRJ} does not need to be bigger than ϕ_K, even if this seems to be the case for $d \leqslant 6$.

The very nice data for $d=4$ reported in Fig. 4 of [1] allow for a more precise comparison of the numerical and theoretical results: the value of $\phi_J(\gamma)$ is reported for five different values of $\gamma = 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}$. A standard procedure to extrapolate to $\gamma \to 0$ is to fit the data to a Vogel-Fulcher law:

$$\gamma(\phi_J) = \gamma_0 10^{-D/(\phi_{RCP} - \phi_J)} \Leftrightarrow \phi_J(\gamma) = \phi_{RCP} + \frac{D}{\log_{10}[\gamma/\gamma_0]}.$$

Such extrapolations are often ambiguous; however, the fit is good and gives $\phi_{RCP} = 0.473$, $D = 0.03$, $\gamma_0 = 0.45$. The final result for ϕ_{RCP} differs by $\sim 10\%$ from the theoretical value (see Table I). This is a very good result given the ambiguities that are present both in the numerical data (numerical error and extrapolation) and in the theory (the choice of a particular expression for the equation of state of the liquid that is not exact; see [10] for recent contributions). Note that a similar extrapolation is not possible in $d=3$ due to crystallization, and for $d > 4$ due to lack of numerical data. Hopefully, new data for $d > 4$ will allow for a similar comparison also in this case. Note also that the value of $\phi_K \sim 0.43$ we obtain in $d=4$ seems to agree very well with the extrapolation of $\phi_g(\gamma)$ (defined roughly as the point where the curves leave the liquid equation of state) to $\gamma = 0$ in Fig. 4 of [1].

A more accurate comparison of the theory with the numerical data is possible: for instance, the theory gives a prediction for the glass equation of state that is close to the measured pressure in the glass branch for very small γ, e.g., $\gamma = 10^{-7}$ in Fig. 4 of [1]; it also predicts that the amorphous packings are isostatic, i.e., the average number of contacts per sphere is $z = 2d$, in any dimension d, and this seems to be confirmed by the numerical data. Other properties of the packings such as the shape of the correlation function $g(r)$ close to contact are predicted to be independent of the dimension. Unfortunately we are still not able to give a prediction for the splitting of the second peak of $g(r)$, which seems to be strongly suppressed in $d > 3$. We hope that future work will address this and many other open questions [4]. The data reported in [1] provide a very good test of the theories aiming to understand the behavior of hard spheres in large space dimension [3,11–13] and strongly call for further developments.

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