Exact theory of dense amorphous hard spheres in high dimension I. The free energy

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Abstract. We consider the theory of the glass transition and jamming of hard spheres in the large space dimension limit. Previous investigations were based on the assumption that the probability distribution within a ‘cage’ is Gaussian, which is not fully consistent with numerical results. Here we perform a replica calculation without making any assumption on the cage shape. We show that thermodynamic functions turn out to be exact within the Gaussian ansatz—provided one allows for arbitrary replica symmetry breaking—and indeed agree well with numerical results. The actual structure function (the so-called non-ergodic parameter) is not Gaussian, an apparent paradox which we discuss. In this paper we focus on the free energy, future papers will present the results for the structure functions and a detailed comparison with numerical results.

Keywords: cavity and replica method, disordered systems (theory), structural glasses (theory)
1. Introduction

Hard spheres in the limit of large spatial dimensions provide us with an opportunity for an analytic solution covering many aspects of the liquid and glass physics [1]–[4]. The reason why this limit is solvable is geometric: consider three spheres A, B and C, with AB and BC in contact, respectively. What are the chances that A and C will themselves also be in contact? In high dimensions, vanishingly small. This led to the realization [1] that all terms in the virial expansion above the second could be neglected in high dimensions, as they involve geometrically heavily suppressed ‘coincidences’, leaving one with only the
two first terms of the series for the entropy

\[ S[\rho(x)] = \int d^d x \rho(x)[1 - \log \rho(x)] + \frac{1}{2} \int d^d x \, d^d y \, \rho(x) \rho(y) f(x - y). \]  

(1)

Here \( f(x) = e^{-v(x)} - 1 = -\theta(D - |x|) \) is the Mayer function of the hard sphere potential \( v(x) \), which is infinite for \( |x| < D \) and zero otherwise. \( D \) is therefore the sphere diameter. For the liquid phase, one has \( \rho(x) = \rho \), a constant, and the above expression gives the liquid entropy; non-uniform phases are described by solutions of the stationarity equation \( \partial S/\partial \rho(x) = 0 \) that are not constant\(^5\). The liquid phase stays metastable at higher densities when one expects the thermodynamics to be dominated by a modulated, crystalline phase, which is however only known in small dimensions [5].

Even neglecting the crystalline phase, one expects that, at some density, there is the possibility of a thermodynamic glass transition into a phase where one or several spatially-dependent nonperiodic solutions dominate. The conceptual (and practical) method to neglect the crystalline phase and uncover a possible liquid–glass transition was proposed years ago [6, 7]: one studies the system perturbed by a spatially random external field—whose function is to kill the crystal and select one of many amorphous solutions. One in fact computes the average over the ‘pinning’ field realizations, and then continues the solution to zero field intensity. This program has been followed for the hard sphere case [8] (see [9] for the state of the art). The inclusion of a random field brings about the problem of treating quenched averages, and this has been done using replica methods (i.e. introducing \( m \) copies of the same system). One ends up with a truncated virial expansion [9]

\[ S[\rho(\bar{x})] = \int d\bar{x} \rho(\bar{x})[1 - \log \rho(\bar{x})] + \frac{1}{2} \int d\bar{x} \, d\bar{y} \rho(\bar{x}) \rho(\bar{y}) f(\bar{x} - \bar{y}) \]  

(2)

where now the density \( \rho(\bar{x}) \) is a function of \( m \) coordinates in \( d \) dimensions \( \bar{x} = \{x_a\} = \{x_1, \ldots, x_m\} \), and one has then to analytically continue over \( m \) from integer values of \( m \) to non-integer ones. The stationary points of equation (2) satisfy the equation

\[ \log \rho(\bar{x}) = \int d\bar{y} \rho(\bar{y}) f(\bar{x} - \bar{y}). \]  

(3)

This equation has also a probabilistic meaning, as discussed in [10]. Indeed the same equation appears in the study of a hard sphere model on the Bethe lattice [11].

Even though equation (3) is (morally) exact in large dimensions, in order for it to be useful we need an expression for \( \rho \) that contains \( m \) explicitly and allows one to continue the results for real \( m \). An approach to do this is to propose a ‘Gaussian ansatz’ for \( \rho(\bar{x}) \) [8, 9]:

\[ \rho(\bar{x}) = \frac{\rho m^{-d/2}}{(2\pi A)^{(m-1)d/2}} \exp \left( -\frac{1}{2mA} \sum_{a<b}^{1,m} (x_a - x_b)^2 \right) \]  

(4)

and to extremize (2) with respect to the parameters in (4). Having to content oneself with the Gaussian ansatz might seem somewhat disappointing: we have paid the price of going to unphysically high dimensions in order to have an exact answer, and now we do not even have this.

\(^5\) This statement is exact at low densities. At higher densities equation (1) would have corrections, however these corrections are exponentially small in the density region we consider in this paper [3, 4].

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The purpose of this paper is that of obtaining the exact solution of (3) in the high-dimensional limit without assumptions. We find that the Gaussian ansatz turns out to be, in a sense, exact: it gives for large dimensions the exact values for the thermodynamic quantities. The reason, whose consequences we shall develop below, can be seen as follows:

A generic replica problem is written in terms of the order parameter \( \rho(\bar{x}) \), or, alternatively, of the tensors \( \langle x_a x_b \rangle, \langle x_a x_b x_c \rangle, \langle x_a x_b x_c x_d \rangle \ldots \) The solution involves an ansatz for replica tensors of all degrees, which makes the problem analytically hard. However, in our case, the \( x_a \) are vectors in \( d \)-dimensional space, and we are looking for a solution that is statistically translationally invariant and isotropic. The only possibility with these properties is that \( \rho(\bar{x}) \) depends exclusively on the \( |x_a - x_b|^2 = q_{aa} + q_{bb} - 2q_{ab} \), where we have introduced the scalar products \( q_{ab} = x_a \cdot x_b \). All \( d \)-dimensional integrals may be expressed as low-dimensional integrals in terms of the \( q_{ab} \), with volume factors, a simple generalization of spherical coordinates. As we shall see, the dimensionality appears explicitly, and the limit of large \( d \) may be taken in a straightforward way, by saddle point evaluation of the integrals.

It will turn out, however, that the ‘cage shape’ is not Gaussian, as already observed in simulations [12], but may be calculated exactly for large \( d \) within this framework. The fact that the Gaussian approximation gives the correct result for thermodynamic functions but by itself does not give the right cage shape may be understood with a simple example. Consider a single particle in a \( d \)-dimensional spherical potential \( V \), which for convenience we write as \( \beta V = d U(|x|^2/d) \). Let us denote \( q \equiv r^2 = |x|^2 \). Clearly, the exact Gibbs distribution is

\[
\rho(q) = \frac{e^{-d U(q/d)}}{\mathcal{N}_o} \quad \text{with} \quad \mathcal{N}_o = \frac{1}{2} \int dq q^{(d-2)/2} e^{-d U(q/d)}. \tag{5}
\]

The entropy \( S = -\int dx \rho \ln \rho \) is easily evaluated and gives:

\[
S = -\int dq q^{(d-2)/2} \frac{e^{-d U(q/d)}}{\mathcal{N}_o} \left\{ -d U(q/d) - \ln \mathcal{N}_o \right\}. \tag{6}
\]

For large dimension \( d \), the integrals for \( \mathcal{N}_o \) and for \( S \) are dominated by the saddle point \( q^* \) which maximizes \( \frac{1}{2} \ln q - U(q/d) \). The entropy is then, to leading order in \( d \):

\[
S = -d U(q^*/d) - \ln \mathcal{N}_o \sim -d U(q^*/d) + d U(q^*/d) + \frac{d}{2} \ln q^* = \frac{d}{2} \ln q^*. \tag{7}
\]

Suppose instead that we had done this calculation approximately, proposing a variational Gaussian distribution \( \rho_G = e^{-|x^2/(2A)|}/\mathcal{N}_G \). The same calculation as before gives for the entropy:

\[
S_G = -\int dx \rho_G \ln \rho_G \sim \frac{d}{2} \ln q_A \tag{8}
\]

where \( q_A \) maximizes \( \frac{1}{2} \ln q - q/(2d A) \). We now have to fix the parameter \( A \) by minimizing the free energy:

\[
-\beta F = \int dx \left[ -\beta V - \ln \rho_G \right] \rho_G \sim -d U(q_A/d) + \frac{d}{2} \ln q_A. \tag{9}
\]

The minimum is clearly attained by \( q_A = q^* \), by definition of \( q^* \). All in all, we have to choose the value of \( A \) such that \( q_A = q^* \), the ‘true’ saddle point. Entropy and free energy
give, for this value, the correct results $S_G = S$ and $F_G = F$. We note that the only purpose of the Gaussian ansatz at this stage is to fix the correct value of $q^*$ that dominates all integrals, a purely geometric feature: indeed, any other ansatz (e.g. a delta function) would have given the correct result by a similar argument. This is akin to the equivalence of different thermodynamic ensembles in infinite dimensional space.

If in the same example we are interested in the radial ‘cage’ function $\rho(r)$, the result will be Gaussian if we use $\rho_G$, while it will generically have tails $\sim e^{-dU}$ that are not Gaussian in the exact case. In other words, the tails of the ‘cage’ distribution are large deviation functions with (large) parameter $d$. They could also be computed in the Gaussian approximation by evaluating the free energy as a function of the intensity $h$ of an additional potential $hx$: as usual, large deviations control the thermodynamics in presence of an external field.

This paper is organized as follows: in section 2 we write the replicated van der Waals entropy in coordinates corresponding to the scalar products, as described above. Sections 3 and 4 are devoted to the calculation of the Jacobians of these changes of coordinates, which will play the role of the term $r^{d-1}$ of polar coordinates in the example above. (We need two Jacobians, corresponding to integrations in spaces of $m$ vectors $\{x_a\}$, and to $2m$ vectors $\{x_a, y_a\}$—as required by the Mayer function—in terms of the corresponding scalar products.) In section 5 we compute the Mayer function in terms of these coordinates. Thus, we obtain a complete expression (section 6) for the entropy, in terms of low-dimensional integrals, with the dimension $d$ appearing as a parameter. In sections 7 and 8 we do the analog of the previous paragraph: we compute the thermodynamic functions using the Gaussian ansatz and the exact solution taking saddle points that become exact as $d \to \infty$. Both results coincide, thus validating the Gaussian ansatz.

## 2. The replicated van der Waals entropy

The starting point of our calculation is the free energy of a replicated liquid, where each atom is replaced by a ‘molecule’ made by one atom per each of the $m$ replicas [8, 9]. We denote by $\vec{x} = \{x_1, \ldots, x_m\}$ the coordinate of such a molecule, each $x_a$ being a vector in $d$-dimensional space. We assume that in the glass phase the molecule is well defined, the typical distance between atoms in a molecule being of order $\sqrt{A}$, which is small at the glass transition [9]. Note that this is a non-trivial assumption: molecules might dissociate, especially close to the glass transition, and lose their identity. However, we will show self-consistently in the end that this is not the case, at least for $d \to \infty$. Taking into account this effect in finite dimensions might be a non-trivial task.

The liquid state is described by a single copy of the system, $m = 1$, with uniform density $\rho$. When $d \to \infty$, its entropy (per particle) is given by equation (1) for $\rho(x) = \rho$, which corresponds to the van der Waals mean field equation:

$$s_{\text{liq}} = \frac{S[\rho]}{N} = 1 - \log \rho + \frac{\rho V_d D^d}{2} = 1 - \log \rho + 2^{d-1}\varphi. \quad (10)$$

Here $V_d$ is the volume of a sphere of unit radius in $d$ dimensions, and $D$ is the sphere diameter, and we introduced the \textit{packing fraction} $\varphi = \rho V_d (D/2)^d$. It has been shown in [1, 3, 4] that equation (10) is exact in the limit $d \to \infty$, provided $2^d \varphi$ does not grow.
exponentially with $d$. If this is the case, the other virial corrections are exponentially suppressed in $d$.

In the replicated liquid, atoms within a molecule can overlap, while atoms of different replicas belonging to different molecules have the normal hard sphere interaction. If $\sqrt{A} \ll D$, the molecule–molecule interaction is similar to the normal hard sphere interaction and one can repeat the analysis of [3]. The replicated liquid with integer $m \geq 1$ can thus be described in terms of a replicated van der Waals entropy given by equation (2) (see [9, 13]), where $\rho(\vec{x})$ is the single molecule density, normalized to $V^{-1} \int d\vec{x} \rho(\vec{x}) = \rho$, where $V$ is the system volume, and $f(\vec{x} - \vec{y})$ is the replicated Mayer function that describes the molecule–molecule interaction:

$$f(\vec{x} - \vec{y}) = -1 + \prod_{a=1}^{m} \theta(|x_a - y_a| - D).$$  \hfill (11)

We wish to make use of the homogeneity of the molecular liquid, which implies that we have to consider a generic translationally and rotationally invariant form of $\rho(\vec{x})$. Let us start with translational invariance. We can perform a change of variables, $m$ is the system volume, and $\rho$ have to consider a generic translationally and rotationally invariant form of $\rho$.

$$D_v \sum_{a=1}^{m} \theta(|x_a - y_a| - D).$$  \hfill (12)

and translational invariance implies that $\rho(\vec{x})$ does not depend on $X$. We obtain

$$S[\rho(\vec{u})] = V \int D\vec{u} \rho(\vec{u})[1 - \log \rho(\vec{u})] + \frac{V}{2} \int D\vec{u} D\vec{v} \rho(\vec{u}) \rho(\vec{v}) \hat{f}(\vec{u} - \vec{v}),$$

$$\hat{f}(\vec{u} - \vec{v}) = \int dX f(X + \vec{u} - \vec{v}),$$

where $X + \vec{u}$ means adding $X$ to each component of $\vec{u}$.

Next we consider rotational invariance, which implies that $\rho(\vec{u})$ and $\hat{f}(\vec{u})$ are functions of $q_{ab} = u_a \cdot u_b$ only. Let us define the following quantities:

$$q_{ab} = u_a \cdot u_b \quad p_{ab} = u_a \cdot v_b \quad r_{ab} = u_a \cdot \bar{v}_b.$$  \hfill (14)

Note that translational invariance implies that $\sum_{a=1}^{m} q_{ab} = \sum_{b=1}^{m} q_{ab} = 0$ for all rows and columns. Denoting $d\hat{q} = \prod_{a \leq q}^{m} d\hat{q}_{ab}$, we have

$$S[\rho(\hat{q})]/V = \int D\hat{u} \rho(\hat{q})[1 - \log \rho(\hat{q})] + \frac{1}{2} \int D\hat{u} D\hat{v} \rho(\hat{q}) \rho(\hat{p}) \hat{f}(\hat{q} + \hat{p} - \hat{r} - \hat{r}^T)$$

$$= \int d\hat{q} J(\hat{q}) \rho(\hat{q})[1 - \log \rho(\hat{q})] + \frac{1}{2} \int d\hat{q} d\hat{p} d\hat{r} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{q}) \rho(\hat{p})$$

$$\times \hat{f}(\hat{q} + \hat{p} - \hat{r} - \hat{r}^T).$$  \hfill (15)

Here we introduced two Jacobians $J(\hat{q})$ and $K(\hat{q}, \hat{p}, \hat{r})$ that describe the change of variables from $\vec{u}$ to $\hat{q}$, and from $(\vec{u}, \vec{v})$ to $(\hat{q}, \hat{p}, \hat{r})$ respectively. We compute them in the next sections. Before doing that, note that translational and rotational invariances imply that the integrals are reduced from $\sim m$ variables $\vec{u}$ to $\sim m(m - 1)/2$ variables $\hat{q}$. This is crucial because now the number of integration variables does not grow with $d$ and we can use saddle point methods when $d \to \infty$.  

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3. The Jacobian \( J \)

3.1. Definition

The Jacobian \( J(\hat{q}) \) is defined as:

\[
J(\hat{q}) = \int D\hat{u} \prod_{a \leq b}^{1,m} \delta(q_{ab} - u_a \cdot u_b) = m^d \int d\hat{u} \delta \left( \sum_{a=1}^{m} u_a \right) \prod_{a \leq b}^{1,m} \delta(q_{ab} - u_a \cdot u_b),
\]

where the second line is obtained easily by manipulating the delta functions.

The delta functions take into account translational invariance. The last term instead takes into account rotational invariance, and it can be shown that

\[
\int d\hat{u}_1 \cdots d\hat{u}_{m-1} \prod_{a \leq b}^{1,m-1} \delta(q_{ab} - u_a \cdot u_b) = C_{m,d} e^{(1/2)(d-m) \log \det \hat{q}^{m,m}},
\]

where \( \hat{q}^{a,b} \) is the \((m-1) \times (m-1)\) matrix that is obtained by removing from \( \hat{q} \) the \( a \)th row and the \( b \)th column. In fact, equation (17) can be thought as a change of variables from a \( d \times (m-1) \) matrix \( \hat{U} = \{u_1, \ldots, u_{m-1}\} \) whose columns are the coordinates of the vectors \( u_1 \cdots u_{m-1} \), to the \((m-1) \times (m-1)\) matrix \( \hat{q}^{m,m} = \hat{U}^T \hat{U} \). The corresponding Jacobian is given by equation (17), see [14].

Using this, we get the final result:

\[
J(\hat{q}) = m^d C_{m,d} \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} q_{ab} \right) e^{(1/2)(d-m) \log \det \hat{q}^{m,m}},
\]

Note that this form of \( J \) is consistent with the fact that the choice of the \( m \)th row and column in (16) is arbitrary: we could have chosen any other row and column. But because the matrix \( \hat{q} \) has the property that the rows and columns add up to zero, it has the property that \( \det \hat{q}^{a,b} = \det \hat{q}^{m,m} \) for any \( a, b \).

The normalization constant is

\[
C_{m,d} = 2^{1-m} \prod_{k=d-m+2}^{d} \Omega_k,
\]

\[
\Omega_d = \frac{2^n d/2}{\Gamma(d/2)}, \quad \text{(the } d \text{-dimensional solid angle)}
\]

as we show in section 3.2.

3.2. Calculation of the normalization constant

Here we compute the normalization constant \( C_{m,d} \). First we note that one can compute it directly for \( m = 2 \) and \( m = 3 \), using polar and bi-polar coordinates respectively:

\[
C_{2,d} = \frac{\Omega_d}{2}, \quad C_{3,d} = \frac{\Omega_d \Omega_{d-1}}{4}.
\]

This already hints strongly at the form (19).
Next we perform an asymptotic computation for large \( d \) at fixed \( m \). For this, we write (dropping for convenience the superscript \((m,m)\) on the matrix \( \hat{q} \) that here we consider here to be a generic \((m-1) \times (m-1)\) matrix):

\[
(2\pi)^{d(m-1)/2} = \int du_1 \cdots du_{m-1} e^{-(1/2)\sum_{a=1}^{m-1} q_{aa}} = \int d\hat{q} \int du_1 \cdots du_{m-1} e^{-(1/2)\sum_{a=1}^{m-1} q_{aa}} \prod_{a \leq b} \delta(q_{ab} - u_a \cdot u_b) = C_{m,d} \int d\hat{q} e^{(1/2)(d-m)\log det \hat{q} - (1/2)\sum_{a=1}^{m-1} q_{aa}}. \tag{21}
\]

The latter integral can be evaluated by a saddle point. Using \( \frac{d}{dq_{ab}} \log det \hat{q} = (\hat{q}^{-1})_{ab} \), the stationary equation reads:

\[-I + (d - m)\hat{q}^{-1} = 0, \quad \hat{q} = (d - m)I. \tag{22}\]

Next we expand

\[\hat{q} = (d - m)I + \hat{t}\]

and we obtain, truncating the expansion in \( \hat{t} \) at quadratic order:

\[
(2\pi)^{d(m-1)/2} = C_{m,d} \int d\hat{t} \times e^{\frac{1}{2}(d-m)\left\{ (d-m)\log(d-m) + \text{Tr}[(\hat{\hat{t}}/2(d-m) - \hat{\hat{t}}^2/2(d-m)^2 + \cdots)] - (1/2)\sum_{a=1}^{m-1} t_{aa} - (1/2)(d-m)(m-1) \right\}} \int d\hat{t} e^{-(1/2)(d-m)(m-1)\frac{1}{2} \sum_{a \leq b} r_{ab}} \times e^{-(1/2)(d-m)^2/2} = C_{m,d}(d - m)^{(d-m)(m-1)/2}e^{-(1/2)(d-m)(m-1)\frac{1}{2} \sum_{a \leq b} r_{ab}} \times e^{-(1/2)(d-m)^2/2} \sqrt{2\pi(d - m)^{m(m-1)/2}}. \tag{24}\]

We therefore get

\[C_{m,d} = 2^{-(1/4)(m-1)(2+m-2d)} \times e^{\frac{1}{2}(d-m)(m-1)\pi - (1/4)(m-1)(m-2d)(d - m)^{(1/4)m(m-1)-(1/2)d(m-1)}}. \tag{25}\]

It is easy to show that the limit for \( d \to \infty \) of this expression divided by equation (19) is given by 1.

### 4. The Jacobian \( K \)

#### 4.1. Definition

The Jacobian \( K(\hat{q}, \hat{p}, \hat{r}) \) is defined as:

\[
K(\hat{q}, \hat{p}, \hat{r}) = \int \mathcal{D}\hat{u} \mathcal{D}\hat{v} \prod_{a \leq b}^{1,m} \delta(q_{ab} - u_a \cdot u_b) \prod_{a \leq b}^{1,m} \delta(p_{ab} - v_a \cdot v_b) \prod_{a,b}^{1,m} \delta(r_{ab} - u_a \cdot v_b) = m^{2d} \int d\hat{u} d\hat{v} \delta \left( \sum_{a=1}^{m} u_a \right) \delta \left( \sum_{a=1}^{m} v_a \right) \prod_{a \leq b}^{1,m} \delta(q_{ab} - u_a \cdot u_b)
\]
where the last line is obtained easily by manipulating the delta functions.

We can define again a matrix $\hat{U} = \{u_1, \ldots, u_{m-1}, v_1, \ldots, v_{m-1}\}$ of size $d \times 2(m-1)$ and a matrix $\hat{Q} = \hat{U}^T \hat{U}$ of size $2(m-1) \times 2(m-1)$, such that

$$\hat{Q} = \begin{bmatrix} \hat{q}^{m,m} & \hat{p}^{m,m} \\ \hat{r}^{m,m} & \hat{r}^{m,m} \end{bmatrix}$$

is obtained from the matrices $\hat{q}, \hat{p}, \hat{r}$ from which the $m$th row and column have been removed.

Clearly we can write, using equation (17) and calling $U_a$ the columns of the matrix $\hat{U}$:

$$\int du_1 \cdots du_{m-1} dv_1 \cdots dv_{m-1} \prod_{a \leq b}^{1,m-1} \delta(q_{ab} - u_a \cdot u_b)$$

$$\times \prod_{a \leq b}^{1,m-1} \delta(p_{ab} - v_a \cdot v_b) \prod_{a,b}^{1,m-1} \delta(r_{ab} - u_a \cdot v_b)$$

$$= \int dU_1 \cdots dU_{2(m-1)} \prod_{a \leq b}^{1,2(m-1)} \delta(Q_{ab} - U_a \cdot U_b)$$

$$= C_{2m-1,d} e^{(1/2)(d-2m+1)} \log \det \hat{Q}.$$  \hspace{1cm} (28)

Using this, we get the final result:

$$K(\hat{q}, \hat{p}, \hat{r}) = m^{2d} C_{2m-1,d} e^{(1/2)(d-2m+1)} \log \det \hat{Q} \prod_{a=1}^m \delta \left( \sum_{b=1}^m q_{ab} \right) \prod_{a=1}^m \delta \left( \sum_{b=1}^m p_{ab} \right)$$

$$\times \delta \left( r_{mm} - \sum_{a,b} r_{ab} \right) \prod_{a=1}^{m-1} \delta \left( \sum_{b=1}^{m-1} r_{ab} \right) \prod_{a,b}^{m-1} \delta \left( \sum_{b=1}^{m-1} r_{ab} \right).$$  \hspace{1cm} (29)
5. The replicated Mayer function $\tilde{f}$

5.1. General expression

We now investigate the replicated Mayer function $\tilde{f}(\bar{u})$, which is defined as

$$\tilde{f}(\bar{u}) = \int dX \left\{ -1 + \prod_{a=1}^{m} \theta(|X + u_a| - D) \right\} = -\int dX \theta(D - \min_a |X + u_a|).$$

(30)

The $u_a$ are $m$ vectors in $d$ dimensions. In the following we assume that $d > m$. A remark that will be useful in the following is that when all $u_a = 0$, then $\tilde{f} = -V_d D^d$, while when the distance between each pair $|u_a - u_b| > D$, we have $\tilde{f} = -m V_d D^d$.

We define $X_\|$ as the part of $X$ that lies in the hyperplane defined by the $u_a$ and $X_\perp$ the orthogonal part. Then, recalling that $\Omega_d$ is the $d$-dimensional solid angle and $V_d = \Omega_d/d$,

$$\tilde{f}(\bar{u}) = -\int dX \theta(D - \min_a |X + u_a|) = -\int dX \theta(D^2 - \min_a |X + u_a|^2)$$

$$= -\int d^m X_\| d^{d-m} X_\perp \theta(D^2 - \min_a \{|X_\| + u_a|^2 + |X_\perp|^2\})$$

$$= -\Omega_{d-m} \int d^m X_\| \int_0^\infty dx \ x^{d-m-1} \theta(D^2 - x^2 - \min_a |X_\| + u_a|^2)$$

$$= -\Omega_{d-m} \int d^m X_\| \int_0^{\sqrt{D^2 - \min_a |X_\| + u_a|^2}} dx \ x^{d-m-1}$$

$$= -V_{d-m} \int d^m X_\| \ (D^2 - \min_a |X_\| + u_a|^2)^{(d-m)/2} \theta(D^2 - \min_a |X_\| + u_a|^2)$$

$$= -V_{d-m} \int d^m X_\| \Theta_{d-m}(D^2 - \min_a |X_\| + u_a|^2)$$

(31)

where we defined the function

$$\Theta_{d-m}(x) = x^{(d-m)/2} \theta(x).$$

(32)

While the above formula is always valid as long as $d > m$, for large $d$ the last integral is dominated by the points where $\min_a |X_\| + u_a| = 0$, which means that $X_\| = -u_a$ for some $a$ (each value of $a$ defines a different saddle point). Observing that $\tilde{f} = -V_d D^d$ when $u_a = 0 \ \forall a$, we can also write:

$$\tilde{f}(\bar{u}) = -V_d D^d \frac{\int d^m X_\| \Theta_{d-m}(D^2 - \min_a |X_\| + u_a|^2)}{\int d^m X_\| \Theta_{d-m}(D^2 - |X_\|^2)}.$$  

(33)

5.2. Evaluation of $\tilde{f}$ for $d \to \infty$

Let us consider first the case where the vectors $u_a$ are very large. In this case, if we write $X_\| = -u_a + \varepsilon$, for small $\varepsilon$ the minimum $\min_a |X_\| + u_a|$ will still be assumed in the same...
value of $a$ as for $\varepsilon = 0$, hence $\min_a |X_\parallel + u_a| = |\varepsilon|$. Then we get

$$
\tilde{f}(\tilde{u}) \sim -V_{d-m} \sum_{a=1}^{m} \int d^m \varepsilon \left( D^2 - |\varepsilon|^2 \right)^{(d-m)/2} \theta(D - |\varepsilon|) \\
\sim -m V_{d-m} \Omega_m \int_0^D d\varepsilon \, e^{m-1} \left( D^2 - \varepsilon^2 \right)^{(d-m)/2} \\
\sim -m V_{d=m} \Omega_m D^d \frac{\Gamma((d-m+2)/2) \Gamma(m/2)}{d \Gamma(d/2)} = -m V_d D^d
$$

(34)

which implies that $\tilde{f}(\tilde{u})$ is a constant exactly equal to minus the volume of $m$ hyperspheres, $-m \times V_d D^d$. Note that the integral over $\varepsilon$ is dominated by a saddle point at $\varepsilon \sim 1/\sqrt{d}$, as can be easily checked. On the other hand, in the limit $|u_a| = 0$ for all $a$, we trivially obtain $\tilde{f}(\tilde{u}) = -V_d D^d$, the volume of one hypersphere.

Therefore, the region where $\tilde{f}$ has a non-trivial dependence on the $u_a$ is where the $u_a$ have a length proportional to $1/\sqrt{d}$. We can define $u_a = x_a D/\sqrt{d-m}$ and $X_\parallel = \varepsilon D/\sqrt{d-m}$, and we can write from equation (33):

$$
\tilde{f}(\tilde{u}) = -V_d D^d \\
\times \frac{\int d^m \varepsilon \left( 1 - (\min_a |\varepsilon + x_a|^2)/(d - m) \right)^{(d-m)/2} \theta \left( 1 - (\min_a |\varepsilon + x_a|^2)/(d - m) \right)}{\int d^m \varepsilon \left( 1 - |\varepsilon|^2/(d - m) \right)^{(d-m)/2} \theta \left( 1 - |\varepsilon|^2/(d - m) \right)} \\
\sim -V_d D^d \frac{\int d^m \varepsilon \, e^{-(1/2) \min_a |\varepsilon + x_a|^2}}{\int d^m \varepsilon \, e^{-(1/2)|\varepsilon|^2}}
$$

(35)

which is still of the order of $V_d D^d$ times a non-exponential factor that depends on the $u_a$.

We therefore conclude that $\tilde{f}(\tilde{u})$ has the following scaling form when $d \to \infty$:

$$
\tilde{f}(\tilde{u}) = -V_d D^d F \left( \frac{\sqrt{d-m}}{D} \tilde{u} \right),
$$

(36)

where

$$
F(\bar{x}) = \frac{\int d^m \varepsilon \, e^{-(1/2) \min_a |\varepsilon + x_a|^2}}{\int d^m \varepsilon \, e^{-(1/2)|\varepsilon|^2}} = \int \frac{d^m \varepsilon}{\sqrt{2\pi}} e^{-(1/2) \min_a |\varepsilon + x_a|^2}.
$$

(37)

Note that when all $x_a = 0$, $F = 1$ as it should; and when each distance $|x_a - x_b| \to \infty$, $F \to m$.

6. Rotationally and translationally invariant expression of the replicated van der Waals entropy

6.1. Exact expression of the entropy

Before proceeding, let us collect here the results obtained up to this point. We wrote the replicated van der Waals entropy, taking into account explicitly rotational and
translational invariance, as follows:

\[ S[\rho(\hat{q})]/V = \int d\hat{q} J(\hat{q}) \rho(\hat{q}) [1 - \log \rho(\hat{q})] \]

\[ + \frac{1}{2} \int d\hat{q} d\hat{p} d\hat{r} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{p}) \rho(\hat{p}) \hat{f}(\hat{q} + \hat{p} - \hat{r}^T) \]  

(38)

where

\[ J(\hat{q}) = m^d C_{m,d} \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} q_{ab} \right) e^{(1/2)(d-m) \log \det q^{m,m}} \]  

(39)

(here \(\hat{q}^{m,m}\) is obtained by removing the \(m\)th row and column from \(\hat{q}\) and

\[ K(\hat{q}, \hat{p}, \hat{r}) = m^{2d} C_{2m-1,d} e^{(1/2)(d-2m+1) \log \det \hat{Q}} \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} q_{ab} \right) \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} p_{ab} \right) \]

\[ \times \delta \left( r_{mm} - \sum_{a,b}^{1,m-1} r_{ab} \right) \prod_{a=1}^{m-1} \delta \left( \sum_{b=1}^{m} r_{ab} \right) \prod_{b=1}^{m-1} \delta \left( \sum_{a=1}^{m} r_{ab} \right) \]

(40)

(here \(\hat{Q}\) is obtained from the matrix \(\begin{bmatrix} \hat{q} & \hat{p} \end{bmatrix} \) by removing the \(m\)th and 2\(m\)th rows and columns) and

\[ C_{m,d} = 2^{1-m} \prod_{k=d-m+2}^{d} \Omega_k \sim 2^{-(1/4)(m-1)(2+m-2d)} \]

\[ \times e^{(1/2)(d-m)(m-1)/\pi} (d-m)^{(1/4)m(m-1)-(1/2)d(m-1)}. \]  

(41)

### 6.2. Equation for \(\rho(\hat{q})\)

Remember that \(\rho(\hat{u})\) is normalized by \(V^{-1} \int \int d\hat{x} \rho(\hat{x}) = \int \mathcal{D}\hat{u} \rho(\hat{u}) = \rho\). Starting from equation (38) and differentiating with respect to \(\rho(\hat{q})\), adding a Lagrange multiplier to ensure normalization, we obtain the equation:

\[ J(\hat{q}) \log \rho(\hat{q}) = \int d\hat{r} d\hat{p} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{p}) \hat{f}(\hat{q} + \hat{p} - \hat{r}^T) + \lambda J(\hat{q}). \]  

(42)

Recall now that by definition:

\[ \int d\hat{r} d\hat{p} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{p}) = \int d\hat{p} d\hat{r} \int \mathcal{D}\hat{u} \mathcal{D}\hat{v} \prod_{a=1}^{1,m} \delta(q_{ab} - u_a \cdot u_b) \]

\[ \times \prod_{a=1}^{1,m} \delta(p_{ab} - v_a \cdot v_b) \prod_{a,b}^{1,m} \delta(r_{ab} - u_a \cdot v_b) \rho(\hat{v}) \]

\[ = \int \mathcal{D}\hat{u} \mathcal{D}\hat{v} \prod_{a=1}^{1,m} \delta(q_{ab} - u_a \cdot u_b) \rho(\hat{v}) = \rho J(\hat{q}). \]  

(43)
Therefore we can write the equation for $\rho(\hat{q})$ as follows:

$$
\log \rho(\hat{q}) = \lambda + \rho \int \frac{d\hat{r} d\hat{p} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{p}) \bar{f}(\hat{q} + \hat{p} - \hat{r})}{\int d\hat{r} d\hat{p} K(\hat{q}, \hat{p}, \hat{r}) \rho(\hat{p})},
$$

(44)

where obviously the delta functions involving $\hat{q}$ in the expression of $K$ have to be formally simplified between numerator and denominator. The multiplier $\lambda$ is determined by the normalization condition.

### 7. The Gaussian ansatz

Before moving to the general case, we show here that the computation above gives back exactly the results of [9] if a Gaussian ansatz is made for $\rho(\hat{q})$. Using this Gaussian ansatz, we evaluate equation (38) using the saddle point method. In the next section we will show how this result can be obtained in fully generality.

We observe that because neither $\log \rho(\hat{q})$ nor $\bar{f}(\hat{q})$ are exponential in $d$, the saddle point is only determined by the Jacobians and by $\rho(\hat{q})$ in both terms of equation (38). Therefore, $\hat{r} = \hat{0}$ at the saddle point, and $\hat{q} = \hat{p} = \hat{q}^{sp}$, where $\hat{q}^{sp}$ is the point where the exponential factor in $J(\hat{q}) \rho(\hat{q})$ is maximum. Substituting this saddle point in equation (38), we obtain

$$
S[\rho(\hat{q})]/N \sim 1 - \log \rho(\hat{q}^{sp}) + \frac{\rho}{2} \bar{f}(2\hat{q}^{sp})
$$

$$
= 1 - \log \rho(\hat{q}^{sp}) - 2^{d-1} \varphi \mathcal{F} \left( \frac{d}{D^2} 2 \hat{q}^{sp} \right)
$$

(45)

where the second line is obtained from the first by using equation (36).

#### 7.1. The Gaussian form of $\rho(\bar{u})$ and the entropic term

The Gaussian ansatz has the following form:

$$
\rho(\bar{u}) = \rho m^{-d/2} \left( \frac{2\pi A}{(m-1)d/2} \right)^{d/2} e^{-1/2mA \sum_{a=1}^{m} (u_a - u_b)^2}
$$

$$
\Rightarrow \rho(\hat{q}) = \rho m^{-d/2} \left( \frac{2\pi A}{(m-1)d/2} \right)^{d/2} e^{-1/2mA \left( \sum_{a=1}^{m} q_{aa} - \sum_{a=1}^{m-1} q_{ab} \right)}.
$$

(46)

The first task is to compute the saddle point value of $\hat{q}$ that dominates all the integrals. We have, using the delta functions contained in $J(\hat{q})$, to manipulate the exponential term in $\rho(\hat{q})$:

$$
\rho = \int d\hat{q} J(\hat{q}) \rho(\hat{q}) \propto \int d\hat{q} \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} q_{ab} \right)
$$

$$
\times e^{(1/2)(d-m) \log \det \hat{q}^{m,m} - (1/2A) \left( \sum_{a=1}^{m-1} q_{aa} + \sum_{a=1}^{m-1} q_{ab} \right)}.
$$

(47)

At this point the integral over $q_{am}$ is eliminated by the delta functions and we are left with the $(m-1) \times (m-1)$ matrix $\hat{q}^{m,m}$. The saddle point equation is, for $d \to \infty$ and $a, b = 1, \ldots, m-1$:

$$
(\hat{q}^{-1})^{sp}_{ab} = \frac{1}{dA} (1 + \delta_{ab}).
$$

(48)
The matrix is easily inverted and we obtain
\[ q_{sp}^{ab} = dA \left( \delta_{ab} - \frac{1}{m} \right). \]  
(49)

It is easy to show using the conditions \( \sum_{b=1}^{m} q_{ab} = 0 \) imposed by the delta function that the formula above holds for \( a, b = 1, \ldots, m \). Indeed the saddle point values satisfy
\[ q_{sp}^{ab} = \langle u_a \cdot u_b \rangle \]  
(50)

where the average is over \( \rho(\bar{u}) \) so the same result could be obtained from a direct computation. We get
\[ 1 - \log \rho(\hat{q}^{sp}) = 1 - \log \rho + \frac{d}{2} \log m + \frac{(m-1)d}{2} \log(2\pi A) \]  
(50)

which is the same result that can be obtained by an exact computation, the integrals being Gaussian in this case [9].

7.2. The interaction term

Next, we compute the term involving \( \bar{f} \) in the saddle point. Let us start with the following observation. Because \( \bar{f}(\bar{u}) \) depends only on \( \hat{q} \) thanks to rotational invariance, all values of \( \bar{u} \) that correspond to the same \( \hat{q} \) give the same value of \( \bar{f}(\bar{u}) \). This means that if we want to compute \( \bar{f}(\hat{q}) \), we can do that by choosing our favorite configuration of \( \bar{u} \) that corresponds to the chosen \( \hat{q} \).

Therefore, for the saddle point (49), we can choose any \( u_a^{sp} \) that satisfy the conditions
\[ \sum_{a=1}^{m} u_a^{sp} = 0, \quad u_a^{sp} \cdot u_b^{sp} = q_{sp}^{ab} = dA \left( \delta_{ab} - \frac{1}{m} \right). \]  
(51)

Remember that \( u_a^{sp} \) are d-dimensional vectors. A good choice is \( (u_a^{sp})^b = \sqrt{dA} \delta_{ab} - 1/m \) for their first \( m \) components, \( b = 1, \ldots, m \), and zero for all the other components.

We therefore use this configurations of the \( \bar{u} \) to compute \( \bar{f}(\bar{u}) \). We further define \( \hat{A} \) by \( A = D^2 \hat{A}/d^2 \). Therefore, the corresponding variables \( \bar{x} \) that appear as the arguments of equation (37) in the saddle point equation (45) have to satisfy
\[ x_a^{sp} \cdot x_b^{sp} = \frac{d}{D^2} 2q_{ab}^{sp} \sim 2\hat{A} \left( \delta_{ab} - \frac{1}{m} \right). \]  
(52)

and therefore
\[ (x_a^{sp})^b = \sqrt{2\hat{A}} \left( \delta_{ab} - \frac{1}{m} \right). \]  
(53)

With this choice, a short computation shows that
\[ \min_a \epsilon + x_a^{sp} \right|^2 = \sum_{b=1}^{m} (\epsilon^b)^2 - \frac{2\sqrt{2\hat{A}}}{m} \sum_{b=1}^{m} \epsilon^b + 2\sqrt{2\hat{A}} \min_a \epsilon^a + 2\hat{A} \left( 1 - \frac{1}{m} \right). \]  
(54)

Therefore
\[ \mathcal{F}(\bar{x}^{sp}) = \int \frac{d^m \epsilon}{\sqrt{2\pi}^m} e^{-(1/2) \sum_{a=1}^{m} \epsilon^a + x_a^{sp} \right|^2} = m e^{-\hat{A}(m-1)/m} \int_{-\infty}^{\infty} \frac{d\epsilon}{\sqrt{2\pi}} e^{-(1/2)\epsilon^2 - \sqrt{2\hat{A}} \epsilon ((m-1)/m)} \]  
(54)

\[ \text{doi:10.1088/1742-5468/2012/10/P10012} \]
\[
\times \left( \int_\epsilon^\infty \frac{d\eta}{\sqrt{2\pi}} e^{-(1/2)\eta^2 + (\sqrt{2A/m})\eta} \right)^{m-1}
\]
\[
= m e^{-\hat{A}(m-1)/m} \int_\epsilon^\infty \frac{d\epsilon}{\sqrt{2\pi}} e^{-(1/2)\epsilon^2 - \sqrt{2A} \epsilon ((m-1)/m)} \times \left[ \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\sqrt{2A} - \epsilon}{\sqrt{2m}} \right) \right) \right]^{m-1}
\]
\[
= m \int_\epsilon^\infty \frac{d\epsilon}{\sqrt{2\pi}} e^{-(1/2)\epsilon^2} \left[ \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\sqrt{2A} - \epsilon}{\sqrt{2}} \right) \right) \right]^{m-1}. \tag{55}
\]

It is useful to define
\[
G_m(\hat{A}) = 1 - F(\bar{x}^{\text{sp}}) = 1 - m \int_\epsilon^\infty \frac{d\epsilon}{\sqrt{2\pi}} e^{-(1/2)\epsilon^2} \left[ \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\sqrt{2A} - \epsilon}{\sqrt{2}} \right) \right) \right]^{m-1}. \tag{56}
\]

7.3. The Gaussian result
The final result of the Gaussian computation is therefore, at the leading order for \(d \to \infty\):
\[
S[\rho(\hat{q})]/N = 1 - \log \rho + \frac{d}{2} \log m + \frac{(m-1)d}{2} + \frac{(m-1)d}{2} \log \left( \frac{2\pi D^2 \hat{A}}{d^2} \right)
\]
\[= 2^{d-1} \varphi[1 - G_m(\hat{A})]. \tag{57}
\]

It coincides exactly with the result of [9]; the explicit expression of \(G_m(\hat{A})\) that was given in [9] is different, but it is exactly equivalent to the present one (actually the present one is much easier to compute numerically).

8. The generic 1-step replica symmetry broken saddle point
Finally we analyze the structure of the generic solution for \(\rho(\hat{q})\) in the large \(d\) limit without assuming a Gaussian form for the density function. Like in the Gaussian case, we want to evaluate the integrals in equations (38) and (44) via a saddle point. We will show that we will recover the results coming from the Gaussian case.

8.1. Structure of the saddle point
First we have to derive the saddle point equations. Let us suppose that
\[
\rho(\hat{q}) = e^{-\Omega(\hat{q})}
\]
\[
\omega(\hat{q}^{m,m}) = \Omega \left( q_{ab}, q_{am} = -\sum_{b=1}^{m-1} q_{ab}, q_{mb} = -\sum_{a=1}^{m-1} q_{ab}, q_{mm} = \sum_{a,b}^{1,m-1} q_{ab} \right). \tag{58}
\]

The 1-step replica symmetric breaking (1RSB) solution consists in assuming that \(\Omega(\hat{q})\) has a replica symmetric (RS) structure. Indeed, this corresponds to 1RSB because the present real replica scheme describes what happens inside one of the 1RSB blocks [7]–[9].

\[\text{doi:10.1088/1742-5468/2012/10/P10012}\]
First we want to determine the saddle point value of \( \hat{q} \) that dominates the normalization of \( \rho(\hat{q}) \). We have

\[
\rho = \int \! d\hat{q} J(\hat{q}) \rho(\hat{q}) \propto \int \! d\hat{q} \prod_{a=1}^{m} \delta \left( \sum_{b=1}^{m} q_{ab} \right) e^{(1/2)(d-m) \log \det q^{m,m} - \omega(q^{m,m})}. \tag{59}
\]

Therefore the delta functions allow one to eliminate the \( m \)th row of \( q_{ab} \), and the saddle point equations for the remaining variables \( q_{ab} \), with \( a, b = 1 \cdots m-1 \), are determined by the maximization of the exponential factor for \( d \to \infty \):

\[
\frac{d}{2}(q^{-1}_{ab})^{sp} = \frac{d\omega(\hat{q})}{dq_{ab}} = \frac{d\Omega}{dq_{ab}} + \frac{d\Omega}{dq_{mm}} - \frac{d\Omega}{dq_{am}} - \frac{d\Omega}{dq_{mb}}. \tag{60}
\]

Because \( \Omega(\hat{q}) \) has a RS structure, we have \( d\Omega/dq_{ab} = \Omega_0(\hat{q}) + (d^2/2\Omega_1(\hat{q}))\delta_{ab} \), and

\[
(q^{-1})^{sp}_{ab} = \frac{d}{\Omega_1(\hat{q}^{sp})}(1 + \delta_{ab}), \quad q^{sp}_{ab} = \frac{\Omega_1(\hat{q}^{sp})}{d} \left( \delta_{ab} - \frac{1}{m} \right). \tag{61}
\]

Consider now the integral:

\[
\rho^2 = \int \! d\hat{q} \! d\hat{\rho} \! d\hat{r} K(\hat{q}, \hat{\rho}, \hat{r}) \rho(\hat{q}) \rho(\hat{\rho}). \tag{62}
\]

A very similar procedure leads to the following saddle point equation:

\[
\frac{d}{2} \hat{Q}^{-1} = \frac{d}{2} \left[ \begin{array}{cc} \hat{q}^{m,m} & \hat{p}^{m,m} \\ \hat{p}^{m,m} & \hat{q}^{m,m} \end{array} \right]^{-1} = \left[ \begin{array}{cc} \frac{d^2}{2\Omega_1(\hat{q})} & 0 \\ 0 & \frac{d^2}{2\Omega_1(\hat{p})} \end{array} \right] \left( 1 + \delta_{ab} \right) \tag{63}
\]

whose solution is \( r_{ab} = 0 \) and \( q_{ab} = p_{ab} = q^{sp}_{ab} \), both equal to the solution of equation (61). Finally, we are interested in the integral entering in equation (44), which is the same as the last one but without the condition on \( \hat{q} \). One obtains the same as equation (63) but without the upper left block of the matrix. However, the equation for \( \hat{r} \) is still solved by \( \hat{r} = \hat{0} \), then the equation on \( \hat{\rho} \) decouples from \( \hat{q} \) and leads to the same solution as in equation (61).

We conclude that the integrals in equations (38) and (44) can be evaluated via a saddle point and the result is

\[
S[\rho(\hat{q})]/N \sim 1 - \log \rho(\hat{q}^{sp}) + \rho \frac{d}{2} \bar{f}(2\hat{q}^{sp})
\sim 1 - \log \rho(\hat{q}^{sp}) - 2^{d-1} \varphi \mathcal{F} \left( \frac{d}{D^2} \hat{q}^{sp} \right) \tag{64}
\]

and

\[
\log \rho(\hat{q}) = \lambda + \rho \bar{f}(\hat{q} + \hat{q}^{sp}) = \lambda + 2^d \varphi \mathcal{F} \left( \frac{d}{D^2} (\hat{q} + \hat{q}^{sp}) \right). \tag{65}
\]

Therefore, to conclude the calculation we have to determine \( \hat{q}^{sp} \) and \( \lambda \).

Before proceeding, two remarks are in order. First of all, when the distance between atoms in a molecule is large, the \( q_{ab} \) are large, and \( \mathcal{F} \to m \) as discussed in section 5. Hence
in this limit $\rho(\hat{q}) \sim \exp(-2^d \varphi m)$, and because $2^d \varphi \propto d$ at the glass transition [9], we see that $\rho(\hat{q})$ goes to a very small constant that vanishes exponentially with $d$. Hence, in the $d \to \infty$ limit the molecules are well defined in the glass phase, while for finite $d$ there is an exponentially small probability of dissociation. This guarantees that the molecular liquid is a good description of the glass phase for large $d$. The second remark is that the choice of a given RSB ansatz is self-consistent. We assumed at the beginning a RS structure for $\Omega(\hat{q})$; then we obtained that $\hat{q}^{sp}$ has a RS structure as given in equation (61); and finally that, self-consistently, $\Omega(\hat{q}) = -\log \rho(\hat{q})$ has a RS structure as given by equation (65). We could consider a 1RSB structure for $\Omega(\hat{q})$ (corresponding to a 2RSB computation in the real replica scheme) and we would have obtained self-consistently the same structure for $\hat{q}^{sp}$. Saddle points characterized by many steps of RSB could be needed to describe the metastable states of lower density [15].

### 8.2. Saddle point equation

We now have to solve the saddle point equation (61). We note that, defining $\hat{A}^{sp} = \Omega_1(\hat{q}^{sp})/D^2$, we can rewrite equation (61) as a closed equation for the scalar parameter $\hat{A}^{sp}$:

$$q_{ab}^{sp} = \frac{D^2 \hat{A}^{sp}}{d} \left( \delta_{ab} - \frac{1}{m} \right), \quad \hat{A}^{sp} = \frac{1}{D^2 \Omega_1} \left[ \frac{D^2 \hat{A}^{sp}}{d} \left( \delta_{ab} - \frac{1}{m} \right) \right].$$  

(66)

Furthermore, if we define a function

$$h(\hat{A}) = \Omega \left[ \frac{D^2 \hat{A}}{d} \left( \delta_{ab} - \frac{1}{m} \right) \right],$$  

(67)

then we have

$$\frac{dh}{d\hat{A}}(\hat{A}^{sp}) = \sum_{ab} \frac{d\Omega}{dq_{ab}}(\hat{q}^{sp}) \frac{D^2}{d} \left( \delta_{ab} - \frac{1}{m} \right)$$

$$= \sum_{ab} \left( \Omega_0(\hat{q}^{sp}) + \frac{d^2}{2\Omega_1(\hat{q}^{sp})} \delta_{ab} \right) \frac{D^2}{d} \left( \delta_{ab} - \frac{1}{m} \right)$$

$$= d \frac{D^2}{2\Omega_1(\hat{q}^{sp})} \left( m - 1 \right),$$  

(68)

therefore

$$\Omega_1(\hat{q}^{sp}) = d \frac{D^2 (m - 1)}{2h'(\hat{A}^{sp})},$$  

(69)

and the equation for $\hat{A}^{sp}$ becomes

$$\hat{A}^{sp} = \frac{d (m - 1)}{2h'(\hat{A}^{sp})}. $$  

(70)
The function $h(\hat{A})$ can be computed by using equation (65), which gives $\Omega(\hat{q}) = -\lambda + 2^d \varphi \mathcal{F}((d/D)^2)(\hat{q} + \hat{q}^{sp})$. Then

$$h(\hat{A}) = -\lambda + 2^d \varphi \mathcal{F}\left[(\hat{A} + \hat{A}^{sp}) \left( \delta_{ab} - \frac{1}{m} \right) \right].$$

The computation of this function can be done exactly as we did in the Gaussian case, in section 7.2, and leads to the following result:

$$\mathcal{F}\left[(\hat{A} + \hat{A}^{sp}) \left( \delta_{ab} - \frac{1}{m} \right) \right] = 1 - \mathcal{G}_m[(\hat{A} + \hat{A}^{sp})/2].$$

Therefore

$$h'(\hat{A}^{sp}) = -2^{d-1} \varphi \mathcal{G}'_m(\hat{A}^{sp}),$$

and finally the equation for $\hat{A}^{sp}$ is

$$\hat{A}^{sp} = -\frac{d (m - 1)}{2^d \varphi \mathcal{G}'_m(\hat{A}^{sp})}. \tag{74}$$

It is easy to check that this equation is exactly the same as that obtained by maximization of the Gaussian free entropy equation (57). Therefore, the generic saddle point equation coincides with the Gaussian one.

### 8.3. The computation of $\lambda$

The last ingredient that we need to compute the replicated free entropy in the generic case is the value of $\lambda$. Indeed, combining equations (64) and (65), and recalling that $\mathcal{F}((d/D)^2 \hat{q}^{sp}) = 1 - \mathcal{G}_m(\hat{A}^{sp})$, we obtain

$$\mathcal{S}[\rho(\hat{q})]/N = 1 - \lambda + 2^d \varphi \mathcal{G}_m(\hat{A}^{sp}).$$

The factor $\lambda$ has to be computed by imposing the normalization of $\rho(\hat{q})$:}

$$\rho = \int d\hat{q} J(\hat{q})\rho(\hat{q}) = e^{\lambda m^d} C_{m,d} \int d\hat{q} \prod_{a=1}^m \delta \left( \sum_{b=1}^m q_{ab} \right) e^{(1/2)(d-m) \log \det \hat{q}^{m,m} - 2^d \varphi \mathcal{F}((d/D)^2)(\hat{q} + \hat{q}^{sp})}. \tag{76}$$

It is enough to evaluate the integral at the saddle point level to get the part of $\lambda$ that is proportional to $d$. Corrections to the saddle point give corrections to $\lambda$ that are at most proportional to $\log d$ and will be neglected here. We get from equation (66)

$$\log \det(\hat{q}^{sp})^{m,m} = (m - 1) \log(D^2 \hat{A}^{sp}/d) - \log m. \tag{77}$$

Recalling that from equation (25) we have, neglecting corrections proportional to $\log d$:

$$\log C_{m,d} = \frac{d}{2}(m - 1) \log(2\pi e) - \frac{d}{2}(m - 1) \log d, \tag{78}$$

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and once again that $F((d/D^2)2\hat{q}^s) = 1 - \mathcal{G}_m(\hat{A}^s)$, we obtain the equation for $\lambda$:

$$\log \rho = \lambda + d \log m + \frac{d}{2} (m-1) \log(2\pi e) - \frac{d}{2} (m-1) \log d$$

$$+ \frac{d}{2} [(m-1) \log(D^2 \hat{A}^s/d) - \log m] - 2^d \Phi[1 - \mathcal{G}_m(\hat{A}^s)]$$

$$= \lambda + d \log m + \frac{d}{2} (m-1) + \frac{d}{2} (m-1) \log(2\pi D^2 \hat{A}^s/d^2)$$

$$- 2^d \Phi[1 - \mathcal{G}_m(\hat{A}^s)],$$

where $\log d$ terms are neglected. Plugging this in equation (75) we finally obtain

$$S[\rho(\hat{q})]/N = 1 - \log \rho + \frac{d}{2} \log m + \frac{d}{2} (m-1) + \frac{d}{2} (m-1) \log(2\pi D^2 \hat{A}^s/d^2)$$

$$- 2^{d-1} \Phi[1 - \mathcal{G}_m(\hat{A}^s)],$$

which coincides exactly with the Gaussian result, equation (57).

9. Conclusions

We have derived the large dimensional limit for the statistical mechanics of dense amorphous hard spheres. We have shown that a so-called Gaussian ansatz gives the correct result for the thermodynamic functions. The results previously obtained with such an ansatz are thus validated, at least near the transition where a one-step replica symmetry breaking scheme is expected to suffice. We notice that the same computation would also apply to the Bethe lattice model of [11] in the high coordination and large dimension limit.

There is, however, reason to suspect that the actual exact result has an infinite number of breakings, at least in the limit of high pressure: first of all, the generic situation with systems which have a transition to a one-step solution is to have a further transition to a phase with more—eventually infinite levels of replica symmetry breaking. More physically, we know that hard spheres at large pressure develop many soft vibrational modes [16]–[18] due to isostaticity. This is true not only of the equilibrium states, but also of the metastable ‘J-point’ states. Now, 1RSB equilibrium states have a spectrum with no soft modes—and this is true of all but the very highest metastable states. A full replica symmetry breaking scheme would naturally bring in soft modes, as happens for example in the case of spin glasses. Perhaps the transition into such a phase also brings in isostaticity at high pressure, something the 1RSB solution displays only for the equilibrium states [9]. The study of the stability of the 1RSB solution is under investigation.

As mentioned in the simple example of section 1, the large $d$ calculation we have presented cannot be expected to yield the exact result for the cage distribution, especially its tails. A more detailed calculation, always within this framework and based on equation (65), is possible for the tails of exponentially small probability, both at the glass transition and at jamming. Hopefully such a calculation will be able to reproduce the numerical results of [12], where a large non-Gaussian tail has been detected in the self-part of the van Hove function, which coincides with the cage distribution. It was found that this tail is not reduced on increasing dimension and seems to persist even for $d \to \infty$.
suggesting that it could be described by mean field theory. This will be the subject of a future paper.

To conclude, let us mention that it would be nice to reproduce the results obtained here without using replicas, i.e. by finding directly the amorphous solutions of equation (1). This approach (which is also called density functional theory or DFT) has been pursued in [2], under the assumptions that (i) the density field $\rho(x)$ is the sum of Gaussians centered around amorphous reference positions $R_i$ and (ii) the structure factor of the $R_i$ is the same as those of the liquid. The results of [2] are close but not exactly equivalent to the ones of replica theory. It is likely that hypothesis (i) is not needed thanks to the same mechanism that was exposed in the introductions and is at work in the replica calculation. However, it is less easy to refrain from using hypothesis (ii) in DFT, and it is likely that this hypothesis is false. In fact, the liquid structure becomes akin to the one of the ideal gas when $d \to \infty$, while it is likely that the $R_i$ remain correlated, at least for neighboring particles (as is clear for instance in the jamming limit of infinite pressure). The replica method is indeed designed to integrate over the unknown $R_i$ to get rid of them and avoid hypothesis (ii). Reconciling DFT with the replica method requires a way to solve for the $R_i$, which has yet to be found.

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