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## A tentative replica study of the glass transition

Marc Mézard<sup>†§</sup> and Giorgio Parisi<sup>‡||</sup>

<sup>†</sup> Laboratoire de Physique Théorique de l' Ecole Normale Supérieure<sup>¶</sup>, 24 rue Lhomond, 75231 Paris Cedex 05, France

<sup>‡</sup> Dipartimento di Fisica, Università *La Sapienza*, INFN Sezione di Roma I, Piazzale Aldo Moro, Roma 00187, Italy

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**Abstract.** In this paper we propose a method aiming at a quantitative study of the glass transition in a system of interacting particles. In spite of the absence of any quenched disorder, we introduce a replicated version of the hypernetted chain equations. The solution of these equations, for hard or soft spheres, signals a transition to the glass phase at reasonable values of the density, and finds a nice form for the correlations in the glass phase. However, the predicted value of the energy and specific heat in the glass phase are wrong, calling for an improvement of this method.

### 1. Introduction

The long-lasting studies of the glass transition, in spite of recent progress [1], have not yet produced a theory which would be able to derive the low-temperature behaviour of glasses starting from a microscopic Hamiltonian of interacting particles.

It has been proposed in the last years that near this transition real glasses could behave in the same way as some disordered systems which are described by a Hamiltonian with quenched randomness [2–7]. This proposal is supported by the existence of a wide class of mean-field systems, with fixed (non-random) Hamiltonians, which show a typical glassy behaviour [3, 8, 9, 6, 10–14]. Although their Hamiltonian involves only one (or a few) coupling constants, these systems behave as if they were typical samples of a class of systems with quenched randomness (apart from the possible existence of a crystal-like phase [9]).

In this type of approach, one finds that the disordered systems which are relevant for the mean-field study of the glass transition belong to a special category, sometimes called systems with a ‘one step replica symmetry breaking’ because of their peculiar pattern of phase transition in the replica approach [21]. The physical nature of their freezing behaviour displays, in particular, the following striking properties. There are two phase transitions: the usual static transition at low temperature ( $T_C$ ), where the replica symmetry is broken and the specific heat is discontinuous, is preceded by a dynamic transition at a higher temperature ( $T_D$ ), where some time-persistent correlations set in. In the region where  $T < T_D$  the infinite system, quenched from some high-energy configuration, gets trapped into metastable states, such that its energy density is larger than the equilibrium value. Therefore, dynamically the

<sup>§</sup> E-mail address: mezard@physique.ens.fr

<sup>||</sup> E-mail address: parisi@roma1.infn.it

<sup>¶</sup> Unité propre du CNRS, associée à l'École Normale Supérieure et à l'Université de Paris Sud.

metastability appears at  $T_D$  and the thermodynamic transition, which is present at a lower temperature, is not accessible [2, 3, 15–19]. Beyond the mean-field approximation one finds that the equilibration time is no longer divergent at  $T_D$ , but it becomes large in the region  $T_C < T < T_D$ . More precisely, it can be argued that in some spin model the equilibration time diverges as  $\exp(A|T - T_C|^{-\gamma})$ ,  $\gamma = d - 1$  in  $d$  dimensions [4, 5]. This very interesting problem of the rounding of the dynamical transition in finite dimension will not be studied here, we shall stay at a mean-field level.

In this paper we present a progress report on an analytical study of the glass transition for a real three-dimensional model of interacting particles, within a static approach. In section 2 we show how to introduce the replica method in spite of the absence of randomness. In section 3 we write down the hypernetted chain equations for the replicated theory, and the numerical solution of these equations is given in section 4. The last part contains some discussion and perspectives.

## 2. Breaking the replica symmetry

### 2.1. Generalities

We consider a system of  $N$  interacting particles in a volume  $V$ . We study the infinite volume limit in which  $N \rightarrow \infty$  at fixed  $\rho \equiv N/V$ . The Hamiltonian is given by:

$$H\{x\} = \sum_{i < k} U(x_i - x_k). \quad (1)$$

We will consider two forms of the potential among particles. The hard-sphere case where  $U(x) = \infty$  for  $r \equiv |x| < 1$  and  $U(x) = 0$  for  $r > 1$ , and a soft-sphere case  $U(x) = r^{-12}$ .

In both cases, if the system is cooled from high to low temperature fast enough (or alternatively if the density is increased), crystallization is inhibited and the system undergoes a glass transition. For hard spheres this transition is known to occur at a density around  $\rho \simeq 1.15$  independently from the temperature, while the crystallization would occur for an equilibrium system at a density around  $\rho \simeq 0.95$ . In the case of soft spheres, the thermodynamic quantities are functions of the dimensionless density  $\gamma \equiv \rho T^{-1/4}$  and the glass transition is located around  $\gamma \simeq 1.6$ , while the freezing value of  $\gamma$  is around  $\gamma \simeq 1.15$  [20].

At low density the system is in the liquid phase, and the correlations of the positions of the particles can be described by the two-point correlations:

$$g(x - y) \equiv 1 + h(x - y) \equiv \frac{1}{\rho^2} \sum_{i \neq j} \langle \delta(x_i - x) \delta(x_j - y) \rangle \quad (2)$$

where the correlation  $h$  goes to zero at large distances.

### 2.2. The replicated equilibrium theory

Let us consider  $n$  replicas of the same system, with  $n$  a positive integer to start with. The position of the particle number  $j$  in the replica  $a$  is  $x_j^a$ , and the total energy is given by:

$$H_n\{x\} = \sum_a H\{x^a\} + \epsilon \sum_{a \neq b} \sum_{i,k} \phi_{ab}(x_i^a - x_k^b). \quad (3)$$

This energy is the sum of two terms: one is the usual pair interaction between any two particles within the same replica. To this we have added a new pair interaction  $\phi_{a,b}$  between

the particles in different replicas. The detailed form of this potential is irrelevant to our approach. We shall just assume that it is short range in space (in order for the corresponding energy to be extensive), that it is attractive, and that its strength  $\epsilon$  is small.

Basically we are interested in the limit  $\epsilon \rightarrow 0$  (taken after the thermodynamic limit). If the positions of the particles with different replica indices remain correlated in this limit, replica symmetry is said to be spontaneously broken. This criterion (with  $n \rightarrow 0$ ) is known to provide a reliable identification of the existence of an equilibrium glass phase in disordered systems like spin glasses [22] or directed polymers in random media [23]. It is also useful in the present case, in spite of the absence of disorder, as we now argue.

### 2.3. The glass phase and its replica counterpart

We propose the following picture of the glass phase. There are many equilibrium states, which we label by an index  $\alpha$  (modulo rotations and translations). These states are identified by the local density  $\langle \hat{\rho}(x) \rangle_\alpha \equiv \rho_\alpha(x)$  which depends on  $x$  in each state. In this paper we denote by  $\hat{\rho}(x)$  the density operator  $\sum_j \delta(x - x_j)$ , and the brackets stand for thermal expectation values. This situation will clearly lead to a replica symmetry-breaking effect of the type described in the previous section, due to the possibility for different replicas to be frozen in the same state.

It is in general difficult to have access to each individual state density  $\rho_\alpha$  directly. The quantities which can be computed are averaged over the equilibrium states, each of them,  $\alpha$ , being weighted by its corresponding weight  $w_\alpha$  in the Boltzmann measure<sup>†</sup>. Since the one-point average  $\sum_\alpha w_\alpha \rho_\alpha(x) = \rho$  is uniform, we need to study the two-point correlations like:

$$\begin{aligned} \tilde{g}(x, y) &= \frac{1}{\rho^2} \sum_\alpha w_\alpha \sum_{i \neq j} \langle \delta(x_i - x) \delta(x_j - y) \rangle_\alpha \\ g_1(x, y) &= \frac{1}{\rho^2 \sum_\alpha w_\alpha^2} \sum_\alpha w_\alpha^2 \sum_{i \neq j} \langle \delta(x_i - x) \rangle_\alpha \langle \delta(x_j - y) \rangle_\alpha. \end{aligned} \quad (4)$$

As for the densities in two different states,  $\alpha \neq \beta$ , we assume that they are generically uncorrelated. For a given number of particles,  $N$ , the weights  $w_\alpha$  are deterministic quantities (there is no disorder in this problem). However, we expect that they may strongly depend on  $N$ , since they are sensitive to very small (non extensive) changes in the relative free energy of the states. It is then convenient to introduce a probability distribution for the weights,  $P[w]$ , describing the fluctuations of the weights when we vary  $N$  inside a small window around  $\bar{N}$ , in the large  $\bar{N}$  limit. We shall use the notation:

$$w_k \equiv \overline{\sum_\alpha w_\alpha^k} \equiv \int dw P(w) w^k. \quad (5)$$

What is the translation of this situation in terms of the replicated system of the previous section? We clearly need that, for small  $\epsilon$ , the replica correlation verify:

$$\frac{1}{n(n-1)} \sum_{a \neq b} \sum_{i \neq j} \langle \delta(x_i^a - x) \delta(x_j^b - y) \rangle = \rho^2 (w_2 g_1(x, y) + 1 - w_2). \quad (6)$$

<sup>†</sup> At this stage we assume that the crystalline states do not contribute. The equilibrium situation that we study is only a quasiequilibrium one reached dynamically, where these crystalline states do not appear.

A more subtle constraint comes in when one considers higher-order correlations like, for instance, the four-point density correlation function. One needs that

$$\frac{1}{n(n-1)(n-2)(n-3)} \sum'_{a,b,c,d} \sum'_{ijkl} \langle \delta(x_i^a - x) \delta(x_j^b - y) \delta(x_k^c - z) \delta(x_l^d - t) \rangle \quad (7)$$

(the  $\sum'$  means that all the indices which are summed are different one from each other) behaves like  $w_4 g_1(x, y) g_1(z, t)$  when  $x - y = O(1)$ ,  $z - t = O(1)$  and  $x - z \rightarrow \infty$ . This limiting behaviour is different from the factorized form  $(w_2)^2 g_1(x, y) g_1(z, t)$ . This non-factorization of the correlation function is deeply linked to the probability distribution of the variables  $w$ . This crucial ingredient of the description is usually dealt with by using the replica symmetry-breaking formalism. In this formalism, the correlation functions (e.g.  $\sum_{i \neq j} \langle \delta(x_i^a - x) \delta(x_j^b - y) \rangle$ ) are no longer symmetric under the permutation of the replicas, but they have the advantage of being clustering<sup>†</sup>. This formalism provides an automatic bookkeeping of all complications which arise from the existence of many states. If one assumes a given form for replica symmetry breaking, it corresponds to a given form for the probability distribution of the  $w$ . In the simplest case, called one step breaking, one divides the set of  $n$  replicas into  $n/m$  groups of  $m$  replicas and one assumes the following structure of correlation functions:

$$\begin{aligned} \sum_{i \neq j} \langle \delta(x_i^a - x) \delta(x_j^a - y) \rangle &= \rho^2 \tilde{g}(x - y) \\ \sum_{i \neq j} \langle \delta(x_i^a - x) \delta(x_j^b - y) \rangle &= \begin{cases} \rho^2 g_1(x - y) & \text{for } a \neq b \text{ in the same group} \\ \rho^2 & \text{for } a \text{ and } b \text{ in different groups.} \end{cases} \end{aligned} \quad (8)$$

In the physically relevant case where  $m < 1$ , this form of the correlations corresponds to assume that  $w_\alpha = \exp(-\beta f_\alpha) / [\sum_{\alpha'} \exp(-\beta f_{\alpha'})]$  where the  $f_\alpha$  are negative quantities extracted with a probability distribution  $\beta m \exp(\beta m f)$ . Therefore, one gets, for instance  $w_2 = 1 - m$  and the relation (6) is verified. The details of this construction are described extensively in the literature [21].

#### 2.4. From equilibrium computations to dynamical quantities

In the above scheme one finds a free energy which depends on the parameter  $m$ , giving the size of the groups in the one-step replica symmetry-breaking solution. In a static equilibrium approach,  $m$  should be considered as a variational parameter and it is fixed by a stationarity condition of the free energy (in fact the free energy must be maximized—not minimized!—with respect to  $m$ ) [21]. The glass phase is characterized by the existence of a maximum of the free energy at  $m(T) < 1$ , and the glass transition temperature  $T_C$  is obtained when this maximum occurs at  $m(T_C) = 1$ .

This criterion holds in the equilibrium situation. On the other hand, without resorting to a direct dynamical approach, one can perform a static study of the appearance of metastable states which will trap the dynamical evolution of the system. This can be done either by a direct study of the solution of some mean-field equations, like the TAP equations in spin glasses [3, 24, 17], or by a replica approach where the parameter  $m$  is no longer fixed [17, 18]. The accumulated experience, particularly on the study of some types of spin glasses like the  $p$ -spin interaction spin glasses, shows that it is possible to identify the dynamical transition temperature by a ‘so called’ marginality condition [2, 3, 24, 18, 17]. In

<sup>†</sup> We thank Francesco Guerra for discussions on this point.

the replica approach, it has been argued on general grounds that this transition is signalled by the existence of a non-trivial  $g_1(x)$  in the limit  $m \rightarrow 1$  [18, 17].

Within this static approach there is no obvious definition of the energy which is reached dynamically. In the case (like the spherical spin glass with  $p$ -spin interactions) where the equilibrium states of the system can be followed in temperature without a chaotic dependance, then it is possible to compute the energy (or the correlations) of the system at temperature  $T$  by constraining it to have a non zero correlation with a reference system which is equilibrated at the dynamical transition temperature  $T_D$  [17]. This is the procedure which we shall follow hereafter to compute the dynamical energy.

### 3. The replicated hypernetted chain approximation

The programme of the previous section is thus clear. The real difficulty consists in implementing it, i.e. in computing the properties of our replicated system of interacting particles, allowing for replica symmetry breaking. Here we propose a first step in this direction, using the hypernetted chain (HNC) approximation. This is a standard approximation scheme which basically amounts to keeping only a given class of diagrams in the virial expansion [25]. It gives a reasonable account of the liquid phase, and it has also been used for studying the first-order transition to the crystal phase [27]. We will consider here this approximation because it has the advantage of having a simple variational formulation.

In the liquid phase, where the density is constant, the usual HNC equation (for the non-replicated system) can be written as

$$g(x) = \exp(-\beta U(x) + W(x)) \quad (9)$$

where:

$$\begin{aligned} \rho^2 g(x) &= \rho^2(1 + h(x)) = \langle \hat{\rho}(x)\hat{\rho}(0) \rangle - \rho\delta(x) \\ W(x) &\equiv \int \frac{d^d p}{(2\pi)^d} e^{-ipx} \frac{\rho \mathbf{h}(p)^2}{1 + \rho \mathbf{h}(p)} \end{aligned} \quad (10)$$

and we denote by  $\mathbf{h}(p)$  the Fourier transform of  $h(x)$ .

This equation can be derived by minimizing with respect to  $h(x)$  the following free energy per unit volume, in the space of functions of  $|x|$ :

$$2\beta F = \int d^d x \rho^2 g(x) [\ln(g(x)) - 1 + \beta U(x)] + \int \frac{d^d q}{(2\pi)^d} L(\rho \mathbf{h}(q)) \quad (11)$$

where  $L(x) \equiv -\ln(1+x) + x - x^2/2$ .

We now implement the programme outlined in section 2, using this HNC approximation. We start from  $n$  replicas of our system of  $N$  particles, described by the Hamiltonian  $H_n$  of (3), which includes, besides the usual pair interaction  $U(x_i^a - x_k^a)$  between particles of the same type, an arbitrary but small pair attraction  $\epsilon \phi_{ab}(x_i^a - x_k^b)$  between particles of different types. It is straightforward to go through one of the usual textbook derivations of the HNC equation in the present case, for any  $n$  (positive integer). Specifically we have followed the physical approach of Percus [26], but a purely diagrammatical derivation is also certainly possible. The HNC equation reads in this case:

$$g_{ab}(x) = \exp(-\beta(U(x)\delta_{a,b} + \epsilon \phi_{ab}(x)) + W_{ab}(x)) \quad (12)$$

where:

$$g_{ab}(x) = 1 + h_{ab}(x)$$

$$W_{ab}(x) \equiv \int \frac{d^d p}{(2\pi)^d} e^{-ipx} (\rho \mathbf{h}(p))^2 (1 + \rho \mathbf{h}(p))^{-1}{}_{ab}. \quad (13)$$

This equation derives from the following replicated free energy:

$$2\beta F = \rho^2 \int d^d x \sum_{a,b} g_{ab}(x) [\ln(g_{ab}(x)) - 1 - \beta(U(x)\delta_{a,b} + \epsilon\phi_{ab}(x))] + \text{Tr} L(\rho \mathbf{h}) \quad (14)$$

where  $\mathbf{h}$  is now an operator both in  $x$  space and in replica space.

If in the limit  $\epsilon \rightarrow 0$  one finds that at large enough densities  $g_{ab}$  is non zero off the diagonal, replica symmetry is broken. In the case where  $g_{ab}$  is of the form shown in (8), this equation can be used to compute the properties of the correlation function in the glassy phase, as discussed in section 2.

Within the one step breaking scheme (8), the free energy is:

$$\lim_{n \rightarrow 0} \frac{2\beta F}{n\rho^2} = \int d^d x \{ \tilde{g}(x) [\ln(\tilde{g}(x)) - 1 + \beta U(x)] - (1-m)g_1(x) [\ln(g_1(x)) - 1] \}$$

$$- \int \frac{d^d q}{(2\pi)^d} \left( \frac{\tilde{\mathbf{h}}(q)^2}{2} - (1-m) \frac{\mathbf{h}_1(q)^2}{2} - \frac{\tilde{\mathbf{h}}(q)}{\rho} \right.$$

$$+ \frac{1}{m\rho^2} \ln[1 + \rho\tilde{\mathbf{h}}(q) - (1-m)\rho\mathbf{h}_1(q)]$$

$$\left. - \frac{1-m}{m\rho^2} \ln[1 + \rho\tilde{\mathbf{h}}(q) - \rho\mathbf{h}_1(q)] \right). \quad (15)$$

The static transition is identified as the temperature (or density) at which there exists a non trivial solution to the replicated HNC equations  $\partial F/\partial \tilde{g}(x) = 0$ ,  $\partial F/\partial g_1(x) = 0$  and  $\partial F/\partial m = 0$ , for  $m \in [0, 1]$  (in fact we must minimize the free energy with respect to  $\tilde{g}$ , but maximize with respect to  $g_1$  and  $m$ ). The equations to be solved for the statics are thus:

$$\tilde{g}(x) = \exp(-\beta U(x) + \tilde{W}(x)) \quad g_1(x) = \exp(W_1(x)) \quad (16)$$

$$\int d^d x g_1(x) [\ln(g_1(x)) - 1] = \int \frac{d^d q}{(2\pi)^d} \left( \frac{\mathbf{h}_1(q)^2}{2} + \frac{1}{m\rho} \frac{\mathbf{h}_1(q)}{1 + \rho\tilde{\mathbf{h}}(q) - (1-m)\rho\mathbf{h}_1(q)} \right.$$

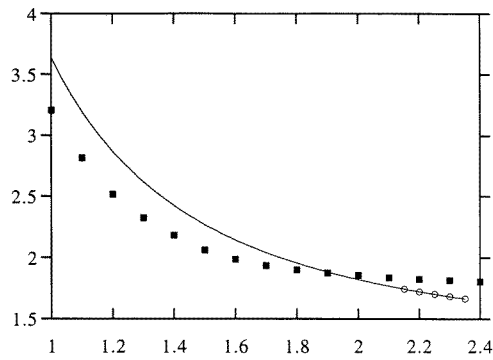
$$\left. - \frac{1}{m^2\rho^2} \ln \frac{1 + \rho\tilde{\mathbf{h}}(q) - (1-m)\rho\mathbf{h}_1(q)}{1 + \rho\tilde{\mathbf{h}}(q) - \rho\mathbf{h}_1(q)} \right) \quad (17)$$

where the Fourier transforms  $\tilde{\mathbf{W}}(q)$  and  $\mathbf{W}_1(q)$  of  $\tilde{W}(x)$  and  $W_1(x)$  verify:

$$\tilde{\mathbf{W}}(q) - (1-m)\mathbf{W}_1(q) = \rho \frac{(\tilde{\mathbf{h}}(q) - (1-m)\mathbf{h}_1(q))^2}{1 + \rho(\tilde{\mathbf{h}}(q) - (1-m)\mathbf{h}_1(q))} \quad (18)$$

$$m\mathbf{W}_1(q) = \frac{\rho(\tilde{\mathbf{h}}(q) - (1-m)\mathbf{h}_1(q))^2}{1 + \rho(\tilde{\mathbf{h}}(q) - (1-m)\mathbf{h}_1(q))} - \frac{\rho(\tilde{\mathbf{h}}(q) - \mathbf{h}_1(q))^2}{1 + \rho(\tilde{\mathbf{h}}(q) - \mathbf{h}_1(q))}.$$

The dynamical transition may be characterized as the highest temperature at which there is a non-trivial solution of the stationarity equations  $\partial F/\partial \tilde{g}(x) = 0$  and  $\partial F/\partial g_1(x) = 0$  at  $m = 1^-$ . The corresponding equations are obtained by substituting  $m \rightarrow 1$  in the first two equations of (17). The equation for  $\tilde{g}$  is identical to the usual HNC equation (10), while  $g_1$  is a solution of  $g_1(x) = \exp(W_1(x))$ , with  $W_1$  given by the second equation of (18) at  $m = 1$ . The computation of the dynamical energy follows the strategy defined in the previous section.



**Figure 1.** The static energy of a system of soft spheres as a function of the dimensionless inverse density  $\gamma$  from numerical simulation (full squares), from the replica symmetric HNC equation (full curve) and from one-step replica symmetry-broken HNC equation (open circles).

#### 4. Solution of the replicated HNC equations

We have solved these HNC equations numerically. Let us first discuss some technical points which are common to the soft- and hard-sphere cases. In both cases the first task is to solve the replica symmetric HNC equation. For spherically symmetric functions in dimension three we use the Fourier transform for the radial dependence, in the following form:

$$qh(q) = 2\pi \int_0^\infty dr \sin(qr)rh(r). \quad (19)$$

We discretize this formula introducing in  $r$  space a cut-off  $R$  and a mesh size  $a$ . In this way we have a simple formula for the inverse Fourier transform and we can also use the fast Fourier transform algorithm. In most of the computations we have taken  $a = 1/32.5$  and  $L = 128 * a \approx 4$ . We have tried smaller values of  $a$  and larger values of  $L$  without serious effects. The solution of the equations can be found either by using a library minimization program<sup>†</sup>, or a program which solves nonlinear equations. We have found first the solution at low enough density and then followed it by continuity while gradually increasing the density.

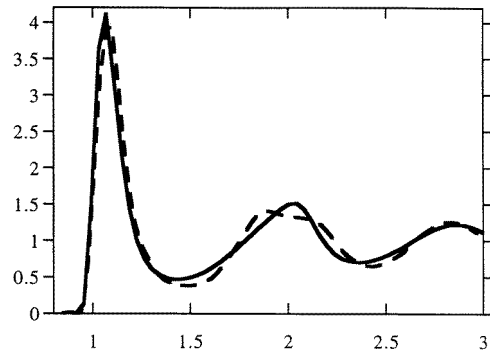
##### 4.1. The soft-sphere case

The HNC equation gives a description of the liquid phase which is not perfect, but precise enough for our purpose. The energy (or equivalently the pressure), does not depart more than 15% from the correct value (see figure 1), and the correlation function is also well reproduced (see figure 2).

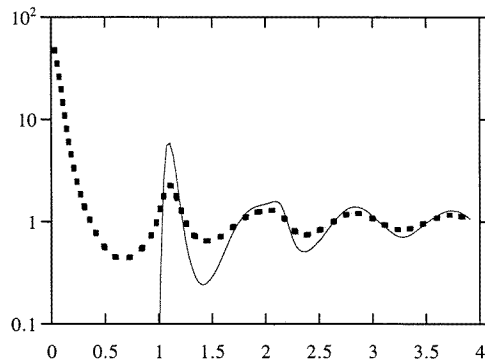
The numerical solution of the replicated HNC equations finds a dynamical transition at  $\gamma \simeq 2.05$ , and a static replica symmetry-breaking solution at  $\gamma \simeq 2.15$ . In numerical simulations the glass transition is found at a smaller value of  $\gamma$ , namely  $\gamma = 1.6$ . In the glass phase, the correlation function  $g_1(r)$  is essentially a smoothed form of the function  $\tilde{g}(r)$  plus an extra contribution at short distance which has integral near to 1 (see figure 3). This form seems very reasonable: considering the definition (4) of  $g_1$ , we see that it basically

<sup>†</sup> When one has to minimize the free energy with respect to one variable and maximize it with respect to another one, we first minimize with respect to the first variable, later maximize with respect to the second, and iterate the procedure until convergence.





**Figure 2.** The correlation function  $\tilde{g}(r)$  of a system of soft spheres as a function of the distance at the dimensionless density  $\gamma = 1.6$  corresponding to the numerical glassy transition: numerical simulations (broken curve) and replica symmetric HNC equation (full curve).

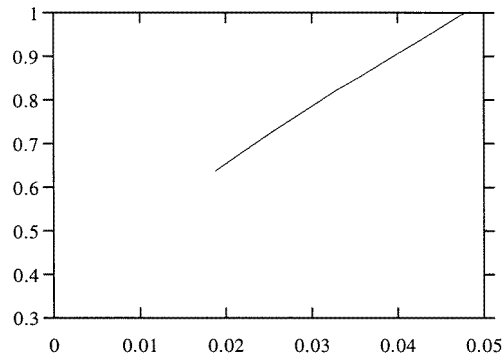


**Figure 3.** The correlations  $\tilde{g}(r)$  (full curve) and  $g_1(r)$  (broken curve) obtained from the replicated HNC equations, as functions of the distance, for soft spheres at the density where replica symmetry is broken ( $\gamma = 2.15$ ).

characterizes the average over  $\alpha$  of the product  $\rho_\alpha(x)\rho_\alpha(y)$ , which is precisely expected to have this kind of peak structure.

In spite of this nice form for  $g_1$ , this solution has some problems. A first one is found on the value of the energy. The static energy as a function of  $\gamma$  (or equivalently of  $T$  at density 1) is plotted in figure 1. Although there is a discontinuity in the specific heat, it is extremely small and the final effects on the internal energy are more or less invisible. The specific heat remains extremely large. Moreover, the value of  $m$  has a very unusual dependence on the temperature (see figure 4). In all the known models with one step replica symmetry breaking, the breakpoint  $m$  varies linearly with  $T$  at low temperatures. Here the behaviour is very different. We have also computed the dynamical internal energy and found out that it differs from the equilibrium one by an extremely small amount.

We conclude that if we consider the qualitative behaviour of the correlation functions, we find a reasonable form, on the other hand the energy in the glassy phase turns out to be quite wrong.



**Figure 4.** The value of the breakpoint  $m$  in the replica symmetry breaking solution for soft spheres as a function of the dimensionless density  $\gamma$ .

#### 4.2. The hard-sphere case

The situation is quite similar in the case of the hard sphere. The HNC approximation works reasonably in the liquid phase. The pressure, which can be extracted either from the free energy or from its relation with  $g(1^+)$ , does not depart from the correct one by more than 15% in the liquid phase. The main defect is the absence of the peak around  $r = \sqrt{3}$  and a too large value of the peak at  $r = 2$ . The pressure seems to diverge proportionally to  $(\rho_c - \rho)^{-2}$ , where  $\rho_c$  is around 1.6, while the maximum possible density, corresponding to the fcc lattice, is  $\sqrt{2}$ .

Here replica symmetry is broken around  $\rho \simeq 1.19$  and the dynamical transition is located at  $\rho \simeq 1.17$ . These values are very close to the result of the numerical simulations which find a freezing transition around  $\rho \simeq 1.15$ . Unfortunately also in this case the computed value for the pressure differs by a very small amount from the replica symmetric one and it is therefore unacceptable. Similar conclusions have also been reached for the Lennard–Jones potential.

## 5. Conclusions

The simple implementation of the replica approach to glasses which we have proposed here provides some interesting results, like the existence of a glass transition at a reasonable value of the density. However, it is not satisfactory, in the sense that the effects of the transition on the thermodynamic of the systems are much too small.

At the moment we do not have a clear understanding of the reasons for this failure to grasp the thermodynamic properties of the glassy phase. Two possible explanations came to mind. The first one would be that an approximation like that of HNC may miss some of the main physical characteristics of the problem in the glassy phase. A first look at the corrections to the free energy indicates that they are quite large, lending some support to this hypothesis. More work is needed to decide what class of diagrams should be added to cure this problem. On the other hand we must also admit that it is not obvious that this type of coupled equations for the two-point density is the best starting point for the discussion of the glass phase. This approach amounts to a study of the density modulations in the glass phase at the level of the two-point function. In the glass phase  $\rho_\alpha(x)$  becomes space dependent. It is the necessity of averaging over the states  $\alpha$  which forces us to study this  $x$  dependence at the level of the two point correlations; our correlation  $\tilde{g}$  reflects the structure

of  $\rho_\alpha(x)$  as a sum of peaks of unit weights, smoothed by the average over states. A more proper approach could be to work with a free energy expressed as a functional of the density  $\rho(x)$ , seeking all the (non-translational invariant) solutions corresponding to glass phases. Then the correlations and thermodynamics could be studied by giving to each solution a weight proportional to  $\exp(-\beta F_\alpha)$ ,  $F_\alpha$  being the free energy of the solution labelled by  $\alpha$ .

We think that finding an analytic approximation scheme which produces reasonable results in the glass phase is within reach. The method we propose seems to be promising in this respect and shows how the replica method could be used to study the glass phase.

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