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1987 J. Phys. A: Math. Gen. 20 1193

(http://iopscience.iop.org/0305-4470/20/5/028)

J. Phys. A: Math. Gen. 20 (1987) 1193-1204. Printed in the UK

On the car parking problem

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Received 16 April 1986

Abstract. The radial distribution functions of randomly distributed one-dimensional spheres are studied. The differences between equilibrium fluids and sequentially constructed systems are discussed in terms of the corresponding configuration spaces and numerical simulations. It is shown that for the sequentially constructed systems, which correspond to the car parking problem, a 'memory effect' occurs, such that the sequential spheres are temporally distinguishable. Exact solutions for some simple cases and numerical simulations for large systems are shown, discussed and compared with the equilibrium fluid results.

1. Introduction

Models of rigid spheres in one, two and three dimensions, distributed more or less randomly in space, have been widely used as reference systems to represent a large variety of disordered physical situations: fluids, glasses, alloys, implanted systems, porous and granular materials, etc (e.g. Bernal 1964, Finney 1970, Ziman 1979). Of course the model has been employed with modifications appropriate to the systems under study, including spheres of different diameters, charged or with other interaction potentials beyond the hard core, etc (e.g. Abramo *et al* 1983, Singh and Holz 1983, Montroll and Lebowitz 1982). The properties studied include equations of state, thermodynamic functions and phase transitions, as well as two essentially geometrical aspects whose importance lies in their direct relationship with observable physical properties: the random close packing, in connection with the maximum density, and the radial distribution function, which is directly related to the structure factor and therefore to the microscopic description of the systems.

However, even in the simplest version of rigid identical spheres, exact analytical solutions for the random close packing and the radial distribution function are limited to some one-dimensional cases: for two and three dimensions there are some good approximate solutions (Montroll and Lebowitz 1982), experimental results (Scott and Kilgour 1969, Stillinger *et al* 1964) and a growing number of numerical simulations (Alder and Wainwright 1959, 1960, McNeil and Madden 1982), not always totally concident.

There are three main models of packing (Finney 1970).

(i) The ordered close packing of spheres of radius σ admits geometrical definitions, with packing fractions $\eta = 1$, $\pi/\sqrt{12}$ and $\pi/\sqrt{18}$ for one, two and three dimensions.

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0305-4470/87/051193+12$02.50

(ii) The random loose packing may be defined, rather vaguely, as the packing 'observed by dumping ball bearings into a container and measuring the resulting density without shaking' (Berryman 1983). In the absence of gravity, which obviously complicates a numerical simulation, one could define it as the packing resulting from a sequential introduction of spheres into the system, without relaxation, until it is geometrically impossible to introduce another sphere. With this definition the one-dimensional random loose packing corresponds to the densest car parking problem, and has an analytical solution with $\eta = 0.7476$ for infinite systems (Solomon 1964).

(iii) The random close packing corresponds to an intermediate situation and is observed experimentally by dumping spheres into a container which is 'conveniently shaken' (Scott and Kilgour 1969). This shaking is defined experimentally and gravity plays an important role. Berryman (1983) has recently proposed a variety of possible theoretical definitions which lead to values of η which are attractively coincident between them and with experimental three-dimensional results (Scott and Kilgour 1969).

Recently, Roman and Majlis (1983), in the context of ion implantation, have studied a three-dimensional system of N randomly distributed rigid spheres. They performed numerical experiments using the following procedure: they considered a cubic box of volume L^3, with a sphere of diameter σ in its centre, and generated sequentially random numbers to define the position of the centres of subsequent spheres; if such a sphere overlaps previously existing ones, the point is rejected, and if not the sphere is incorporated into the system; no relaxation is allowed. Considering an ensemble of such systems, Roman and Majlis calculated the density of bodies around the central sphere and the corresponding radial distribution function, $G(R)$, associated with this non-equilibrium situation. The numerical experiments performed with packing densities $\eta = \pi N\sigma^3/6L^3 = 0.105$, 0.209 and 0.314 show that $G(R)$ differs from those corresponding to fluids in thermodynamic equilibrium, $G^{\mathrm{F}}(R)$, obtained from molecular dynamics calculations (Barker and Henderson 1971): $G(\sigma) < G^{\mathrm{F}}(\sigma)$, and $G(R)$ does not exhibit the characteristic oscillations of $G^{\mathrm{F}}(R)$.

Cohan and Weissmann (1983) also studied the radial distribution function of a system of randomly distributed rigid spheres, using a different, but apparently equivalent, method: the spheres are generated sequentially, without relaxation, as in the previous case, but no central sphere is included. Instead, periodic boundary conditions are imposed and the $N(N-1)/2$ relative distances between all pairs of spheres are considered to calculate $G(R)$. Both generating procedures correspond, in one dimension, to the car parking problem. It is also worthwhile to note that these procedures, continued until maximum density is attained would yield the packing fraction corresponding to the random loose packing without gravity.

In the present paper we will study a sequential system of randomly distributed rigid spheres without relaxation; we will try to clearly establish its differences with an equilibrium hard sphere fluid, and in particular focus our attention on a 'memory' or temporal distinguishability effect on the sequentially generated bodies, which is absent in equilibrium fluids. This situation occurs frequently in numerically simulated systems, and also in physical systems with restricted relaxation; we will be interested in the radial distribution functions. For the sake of simplicity we will limit ourselves to the simplest one-dimensional systems, which we believe to be, in this respect, qualitatively representative of general systems.

The paper is organised as follows: in the next section we introduce the definitions needed to avoid ambiguities, in § 3 we rededuce some results for one-dimensional

equilibrium fluids, § 4 is devoted to the car parking problem, in § 5 we discuss numerical simulation methods and their results and in § 6 we present and discuss the results and draw some conclusions.

2. Definitions

In general, we will discuss one-dimensional systems of N rigid rods of length σ located on a segment of length L; the rod centres may occupy sites in the interval $L_1 = L - \sigma$. The distributions are symmetrical with respect to the centre of the segment, since both ends are equivalent; therefore these boundaries may be looked at as another (the zeroth) body of the system, imposing periodic boundary conditions with period $L_p = L + \sigma$. Introducing a coordinate system with the centre of the zeroth body at $R_0' \pm nL_p$, n = integer, the coordinates of the body centres (coordinates of the body) R_i' may take values in the interval

$$R_0' + \sigma \leqslant R_i' \leqslant R_0' + L_p - \sigma = R_0' + L \qquad i = 1, 2, \ldots, N$$

and their translational equivalents. Due to the arbitrariness of the coordinate origin only N coordinates are independent and define the geometry of the problem: $R_i = R_i' - R_0'$, $\forall i$ ($R_0 = 0$, see figure 1). For finite systems (L and N finite) the average density ρ_0 and the packing fraction η_0 may have slightly different definitions, depending on if we use L_p and $N+1$ or L and N as the basic quantities; in this paper we will use

$$\rho_0 = N/L \qquad \eta_0 = N\sigma/L. \tag{1}$$

For a rigid rod problem, where the interaction energy between rods i, j, is zero if $|R_i - R_j| \geqslant \sigma$ and infinite otherwise, the calculation of the radial distribution function is essentially a geometrical problem. It is useful to introduce an N-dimensional configuration space C_N, in which every point $(R_1, R_2, \ldots, R_N)$ defines a possible geometry for the system; all the system's properties are periodic in all coordinates R_i with period L_p.

The volume of the configuration space corresponding to one period is

$$V(C_N) = L_p^N = (L + \sigma)^N. \tag{2a}$$

The accessible volume, due to the condition $|R_i - R_j| \geqslant \sigma$, is reduced to

$$V_N(L, \sigma) = (L - N\sigma)^N \tag{2b}$$

as can be seen by inspection or direct integration.

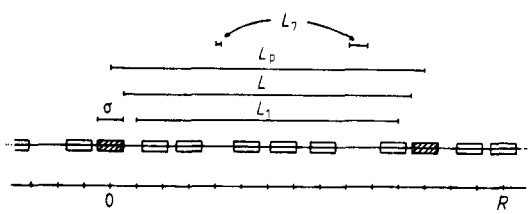

Figure 1. One-dimensional periodic rigid rod system with $N = 6$, $L_p = 12\sigma$. The accessible space for the seventh body, L_7, is also shown.

3. The one-dimensional equilibrium fluid

We define a finite equilibrium fluid as a system of N identical rods located on a segment of length L, with uniform probability density in the accessible configuration space. Given a configuration such that one body centre is located between R and $R+\Delta R$, with $(k-1)$ bodies on its left and the remaining $(N-k)$ on its right, the configuration space volume associated with it is

$$\Delta V(k, R) = \begin{cases} \Delta R N \binom{N-1}{k-1} V_{k-1}(R-\sigma, \sigma) V_{N-k}(L-R, \sigma) & k\sigma \leq R \leq L-(N-k)\sigma \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

where $V_{k-1}(R-\sigma, \sigma)$ and $V_{N-k}(L-R, \sigma)$ are given by $(2b)$ and the factor $N\binom{N-1}{k-1}$ comes from the different possibilities of choosing the right and left bodies. Since the equilibrium fluid configurations are uniformly distributed, the probability of finding the kth neighbour of the reference body at R is

$$p_k(R) = \Delta V(k, R)/\Delta R V_N(L, \sigma). \tag{4}$$

In terms of the packing fraction η_0, we may write

$$p_k(R) = \begin{cases} \dfrac{\eta_0}{\sigma(1-\eta_0)} \binom{N-1}{k-1} x_k^{k-1}(1-x_k)^{N-k} & 0 \leq x_k \leq 1 \\ 0 & \text{otherwise} \end{cases} \tag{5a}$$

where

$$x_k(R) = x_k = \frac{\eta_0}{N(1-\eta_0)}\left(\frac{R}{\sigma} - k\right) \tag{5b}$$

and $p_k(R)$ is normalised in the interval $(0, L_p)$.

The radial distribution function is then

$$G_N^F(R) = \frac{\rho(R)}{\rho_0} = (L/N) \sum_{k=1}^{N} p_k(R). \tag{6}$$

According to (5), the main peak of $G_N^F(R)$ at $R = \sigma$ takes the value

$$G_N^F(\sigma) = 1/(1-\eta_0) \qquad \forall N.$$

It can also be seen that the radial distribution function is symmetric, $G_N^F(R) = G_N^F(L_p - R)$. In the case of only one rod $(N=1)$, $G_1^F(R) = \text{constant}$; for $N=2$ it decreases linearly in the interval $\sigma \leq R \leq 2\sigma$ and is constant for $3\sigma \leq R \leq L_p/2$ (if $L_p > 6\sigma$). For $N=3$, $G_3^F(R)$ reaches a minimum for $R = 2\sigma$, already showing the typical oscillations of a liquid; for increasing values of N the number of oscillations increases, and in the limit for $N \to \infty$, $L \to \infty$ ($\eta_0 = \text{constant}$), equations (5) and (6) lead to the well known expression (Ziman 1979)

$$G(R) = \sum_{k=1}^{[R/\sigma]} z_k(R) \tag{7a}$$

$$z_k(R) = \begin{cases} \dfrac{1}{(k-1)!} \dfrac{\eta_0^{k-1}}{(1-\eta_0)^k} \left(\dfrac{R}{\sigma} - k\right)^{k-1} \exp\left[\dfrac{-\eta_0}{1-\eta_0}\left(\dfrac{R}{\sigma} - k\right)\right] & k\sigma \leq R \\ 0 & \text{otherwise.} \end{cases} \tag{7b}$$

4. The car parking problem

As stated in the introduction, the car parking problem (CPP) may be defined through a numerical experiment. The zeroth body is placed at an arbitrary origin; the coordinates of the centres of the N following rods are introduced sequentially by the generation of random numbers, R_i, in the interval $\sigma \leqslant R_i \leqslant L_p - \sigma$, where L_p is the period of the system. If the coordinate R_i fulfills the condition $|R_i - R_j| \geqslant \sigma$, $j = 0, 1, 2, \ldots, i-1$, the rod is incorporated into the system; otherwise, the coordinate is rejected and new random numbers are generated until the condition above is met. In practice, the numbers are generated in the interval $(0, 1)$, the origin is placed at $-\sigma$ and the period is $L_p = 1 + 2\sigma$.

This sequential incorporation of bodies causes the system to be essentially different from an equilibrium fluid: in the CPP the rods are temporally distinguishable, i.e. they 'remember' the order in which they were generated, giving rise to a non-equilibrium distribution in the configuration space. In order to illustrate this, let us take the simplest case: $N = 2$; R_1, R_2 are the coordinates of the respective rod centres and the reference zeroth rod is at the origin. Figure 2 shows the corresponding configuration space; it is clear that, by definition, R_1 may take any value in the accessible space L_1, with probability density

$$p_1(R_1) = \theta(R_1)/L_1 \tag{8}$$

where $\theta(R_1, R_2, \ldots, R_k)$ is defined in general as

$$\theta(R_1, R_2, \ldots, R_k) = \begin{cases} 1 & \text{if } |R_i - R_j| \geqslant \sigma, \quad i, j = 0, 1, 2, \ldots, k \\ 0 & \text{otherwise.} \end{cases} \tag{9}$$

The accessible space for locating the second rod at R_2 depends on R_1 (see figure 2) and the corresponding probability density is

$$p_2(R_2/R_1) = \theta(R_1, R_2)/L_2(R_1) \tag{10a}$$

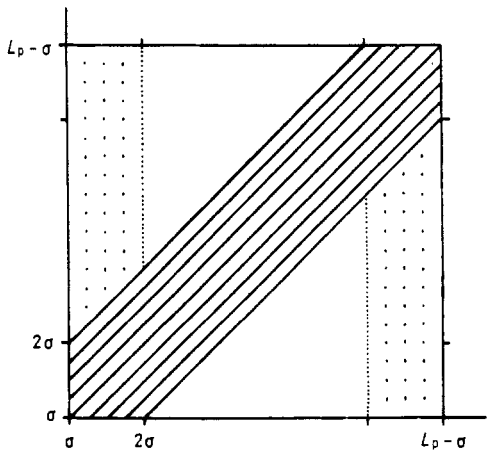

Figure 2. Asymmetry and non-uniform distribution of points in configuration space of the two-body CPP.

with

$$L_2(R_1)=\begin{cases} L_p-2\sigma-R_1 & \sigma\leq R_1\leq 2\sigma \\ L_p-4\sigma & 2\sigma\leq R_1\leq L_p-2\sigma \\ R_1-2\sigma & L_p-2\sigma\leq R_1\leq L_p-\sigma. \end{cases} \tag{10b}$$

The probability of a particular configuration (R_1, R_2) is $p_1(R_1)p_2(R_2/R_1)$, which is in general different from $p_1(R_2)p_2(R_1/R_2)$, as shown in figure 2. This asymmetry indicates the non-equivalence of the bodies; therefore it is necessary to introduce different radial distribution functions for the different bodies. In general, the radial distribution function $G_{ij}(R)$, $R=|R_i-R_j|$, $G_{ij}(R)=G_{ji}(R)$, indicates the spatial distribution of the jth body around the ith body, $i,j=0,1,2,\ldots,N$, indicating the order in which each body is introduced into the sample. The radial distribution function of rods about the ith one is

$$G_i(R)=(1/N)\sum_{j\neq i} G_{ij}(R) \tag{11}$$

and the average radial distribution function

$$\bar{G}(R)=\frac{1}{N+1}\sum_{i=0}^{N} G_i(R). \tag{12}$$

For the case $N=2$ it is easy to see that $G_{01}=L\theta(R_1)/L_1=$ constant and $G_{02}(R)=G_{12}(R)$ and therefore $G_0(R)=G_1(R)$. The expressions for $G_{02}(R)$ may be obtained by direct integration of the corresponding probability density over configuration space. The results depend on the relative magnitude of L_p and σ and are

$$\begin{aligned}
&3\sigma\leq L_p\leq 4\sigma\text{: } G_{02}(R)=B(R) && \sigma\leq R\leq L_p-2\sigma \\
&\qquad\qquad\qquad\quad =0\text{ (impossible)} && L_p-2\sigma\leq R\leq 2\sigma \\
&4\sigma\leq L_p\leq 5\sigma\text{: } G_{02}(R)=A(R) && \sigma\leq R\leq L_p-3\sigma \\
&\qquad\qquad\qquad\quad =B(R) && L_p-3\sigma\leq R\leq 2\sigma \\
&\qquad\qquad\qquad\quad =B(R)+B(L_p-R) && 2\sigma\leq R\leq L_p-2\sigma \\
&5\sigma\leq L_p\leq 6\sigma\text{: } G_{02}(R)=A(R) && \sigma\leq R\leq 2\sigma \\
&\qquad\qquad\qquad\quad =A(R)+B(L_p-R) && 2\sigma\leq R\leq L_p-3\sigma \\
&\qquad\qquad\qquad\quad =B(R)+B(L_p-R) && L_p-3\sigma\leq R\leq 3\sigma \\
&6\sigma\leq L_p\text{: } \quad G_{02}(R)=A(R) && \sigma\leq R\leq 2\sigma \\
&\qquad\qquad\qquad\quad =A(R)+B(L_p-R) && 2\sigma\leq R\leq 3\sigma \\
&\qquad\qquad\qquad\quad =A(R)+A(L_p-R) && 3\sigma\leq R\leq L_p-3\sigma
\end{aligned} \tag{13a}$$

where

$$\begin{aligned}
A(R)&=(L_p-3\sigma-R)/(L_p-4\sigma)+\ln[(L_p-3\sigma)/(L_p-4\sigma)] \\
B(R)&=\ln[(L_p-3\sigma)/(R-\sigma)].
\end{aligned} \tag{13b}$$

The average number of random numbers to be generated is

$$\mathcal{N}(N=2)=2+2\ln[(L_p-3\sigma)/(L_p-4\sigma)] \tag{14}$$

except for the case $L_p\leq 4\sigma$, where impossible situations may occur.

Similarly, for arbitrary N, the probability density of locating the ith rod at R_i is $\theta(R_1, \ldots, R_i)/L_i(R_1, \ldots, R_{i-1})$. However, for increasing i, the expressions rapidly become extremely cumbersome and complicated; we have worked out in full the case of $N=3$; the formulae are already very lengthy and will not be given here, although some results are discussed in § 6. It is probably not worthwhile to pursue the procedure further, and unfortunately we have not been able to find general expressions for arbitrary values of N, nor for $N \to \infty$.

5. Numerical simulations

Since general analytical solutions for the radial distribution functions of the car parking problem are not available, we must rely on numerical simulations to study general systems. It is clear that the rejection rate for the body coordinates will increase rapidly with the packing densities, and there will be 'impossible' or 'nearly impossible' configurations for densities well below the maximum $\eta_0 = 0.7476$, i.e. $N' < N$ bodies will occupy all, or almost all, the available space; this will produce the necessity of generating and checking very many random numbers.

We have found that an alternative simulation method is completely equivalent to that described in the previous section. In order to build up a system, only N random numbers are generated; the first body is located as usual. For successive bodies, the accessible space is calculated and the corresponding random number is renormalised accordingly; the body is then located at this position in the accessible space. In this way, impossible samples are easily detected—and rejected—through the condition that the available space must be larger than zero. The numerical examples given in the next section were calculated using this procedure, since we verified that, in that particular case, it was about 20% faster than the usual simulation method; the preferability of either will depend, of course, on the density of the system. It is worthwhile to note that, although from the numerical simulation point of view both methods yield identical results, they would seem to represent quite different physical situations. Let us think, stressing somewhat the imagination, of a one-dimensional ion implantation. In the usual picture, if an ion finds the site it is directed to occupied, it simply evaporates; in the 'accessible space' picture, it just goes on until it finds some free space, a much more reasonable behaviour. Although the translation of our alternative simulation method to two or three dimensions poses serious practical problems, it seems to us that the above interpretation lends some additional credibility to the random sphere model of ion implantation.

Equilibrium fluids may also be obtained through a random number simulation. In this case, N random numbers are generated and the sample is checked for overlapping; if any occurs, the sample is rejected as a whole, and another set of N numbers is generated. It is clear that the 'memory effect' of the CPP does not exist any more, since all bodies are perfectly equivalent; we have verified in some simple cases that this simulation method fully coincides with the analytical results of (6).

6. Results and discussion

Figure 3 shows the radial distribution functions $G_i(R)$ for two simple cases of the car parking problem, $N=2$, $L_p = 6\sigma$ and $N=3$, $L_p = 6.5\sigma$, obtained from the analytical

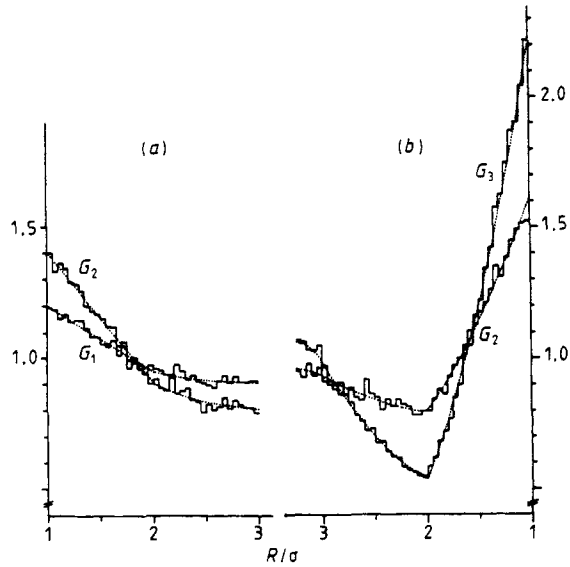

Figure 3. CPP radial distribution functions for (*a*) $N=2$, $L_p=6\sigma$; (*b*) $N=3$, $L_p=6.5\sigma$. Broken line: calculated from the exact solutions; full line: numerical simulations.

solution and from numerical simulations; all functions are normalised as

$$\int_0^{L_p} G(R)\,\mathrm{d}R = L_1 .$$

It can be seen that the agreement is excellent, as it should be. In figure 3(*a*), $G_1(R)$ and $G_2(R)$ decrease in the interval $2\sigma \leqslant R \leqslant 3\sigma$, while for the equilibrium fluid with $N=2$, $G^F(R)=$ constant (see (6)). In figure 3(*b*) we have omitted, for the sake of clarity, $G_0(R)=G_1(R)$ which is almost indistinguishable from $G_2(R)$ (see figure 4); the characteristic minima of the radial distribution functions at $R=2\sigma$ clearly appear already for $N=3$. Figure 4 shows the analytical results for $N=3$, $L_p=6.5\sigma$ in detail. It should be noted that each $G_{ij}(R)$ depends only on the ratio L_p/σ, and not on the total number of bodies in the system. In general, by construction, $G_{0j}(R)=G_{1j}(R)$, $\forall j>1$, and therefore $G_0(R)=G_1(R)$. It is seen that $G_i(\sigma)$ grows with i and so do the amplitudes of the corresponding oscillations.

In figure 5, we compare the results of the CPP and the finite equilibrium fluid. $G^F(R)$ is intermediate between the average radial distribution $\bar{G}(R)$ and $G_3(R)$. In this case, $G^F(R)$ is constant for $R>3\sigma$, while $\bar{G}(R)$ oscillates until $R=5\sigma$; this long range of the radial distribution function oscillations seems to be a general feature of the CPP.

Figure 6 shows the results of a numerical simulation performed on 20 000 samples with $N=24$, $L_p=42\sigma$ and a channel width of $\sigma/20$; a simulation performed with $N=12$ and the same density yields statistically identical results.

It may be observed that the general results are qualitatively similar to those obtained for $N=3$. Although $\bar{G}(R)$ is not too different from $G_1(R)$, it can be better approximated by a $G_i(R)$ with $i\simeq\frac{2}{3}N$. The 'memory effect' gets more pronounced for values of $i>\frac{2}{3}N$; this can be observed in figure 7, which shows $G_i(\sigma)$ as a function of i. It is to be noted that, for low densities, this effect is minimal and actually the equilibrium fluid and the car parking systems tend to be identical, whereas for maximum densities

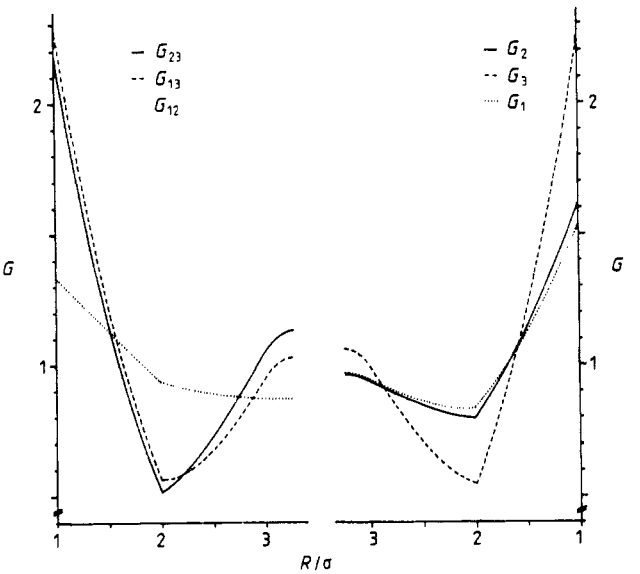

Figure 4. Calculated CPP radial distribution functions for $N = 3$, $L_p = 6.5\sigma$.

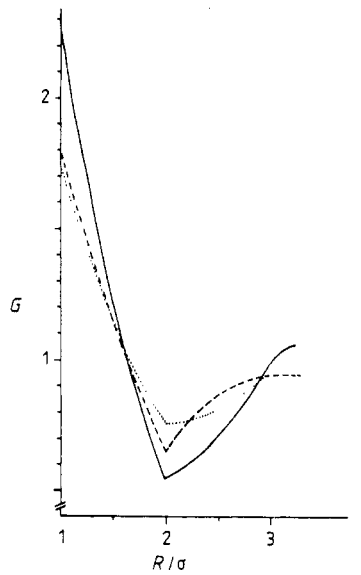

Figure 5. Calculated radial distribution functions for the finite equilibrium fluid and CPP. $N = 3$, $L_p = 6.5\sigma$. (——, G_3; ---, G_{liq}; . . . , G.)

corresponding to the loose packing problem the $G_i(R)$ are most sensitive to the order in which the bodies have been introduced in the system.

So far, we have been concerned with one-dimensional systems; however, the qualitative results probably hold also for two and three dimensions. It is clear now that the apparently similar numerical experiments of Roman and Majlis (1983) and Cohan and Weissmann (1983), mentioned in § 1, are essentially different. Whereas the computation of all distances to a central sphere yields $G_0(R)$, the calculation which

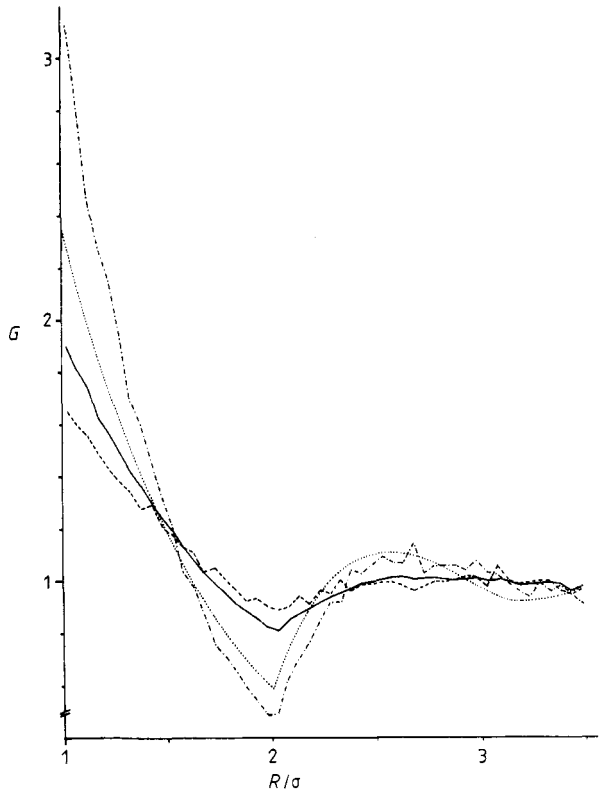

Figure 6. Calculated radial distribution for the finite equilibrium fluid and numerical simulation of some radial distribution functions for the CPP. $N = 24$, $L_p = 42\sigma$; 20 000 samples, channel width: $\sigma/20$. (. . . . , G_{liq}; ---, G_1; —·—, G_{24}; ——, $\bar{G}$.)

takes into account all possible distances among spheres in the sample gives $\bar{G}(R)$. Although it is probably more appropriate in general to use $\bar{G}(R)$, it must be kept in mind that if the properties of interest are fast varying functions of R, both approaches may give rise to erroneous results and the contribution of each $G_i(R)$ should be considered separately.

Another important result, regarding binary mixtures of random spheres (frequently used to represent alloys) is implicit in the existence of the 'memory effect': even if the radii of the two types of spheres are similar, the arrangement will be highly dependent on the way in which the binary system was constructed.

In conclusion, the difference between equilibrium fluids and random sphere systems is clearly established and may be equated to the absence or presence of 'memory effect', or temporal indistinguishability or distinguishability of the bodies.

Of course relaxation or interaction between the bodies will take the non-equilibrium random system to the equilibrium fluid. However one could pose the question: to what extent will 'appropriate shaking' whether mechanical or numerically simulated, of very dense systems like the loosely packed system, completely erase the memory effect? In that sense, it is probable that the best approximation to the random close packing problem would come from the compression of equilibrium fluids (Visscher and Bolsteri 1972, Anonymous 1972).

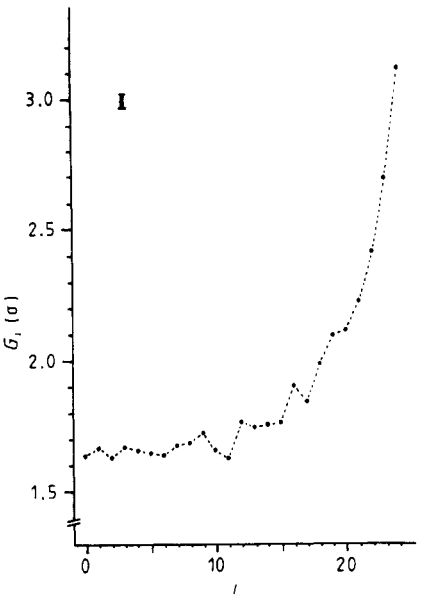

Figure 7. Maxima of the radial distribution functions, $G_i(\sigma)$, as a function of the sequential order i.

Very recently, two papers regarding stable two-dimensional random packing have appeared (Williams 1985, Uhler and Shilling 1985). The systems under study are clusters of identical discs, where the central one is in contact with three, four or five discs. It is clear that this problem is trivially mapped onto a one-dimensional periodic system with $L_p = 6\sigma$, to which all the formalism and conclusions of this paper may be applied. Work on the influence of 'memory effects' on this problem has been completed (Burgos and Bonadeo 1986).

Acknowledgment

We wish to thank Héctor Martin for helpful discussions.

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