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FOR CLASSICAL FLUIDS II.
APPLICATIONS FOR A HARD SPHERE
REFERENCE SYSTEM

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CLUSTER PERTURBATION THEORY FOR CLASSICAL FLUIDS II.
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ABSTRACT

The thermodynamic properties and the radial distribution functions for systems with inverse power potential and for a Lennard-Jones fluid at high temperature are calculated using a new perturbation method applied for a hard sphere reference system. The results are compared to those obtained from the Andersen-Weeks-Chandler theory and to the Monte Carlo results.

АННОТАЦИЯ

Термодинамические свойства и парные корреляционные функции для системы частиц, отталкивающихся по закону $1/r^n$, и для жидкости Ленард-Джонса были вычислены с помощью нового метода возмущения для системы референции твердых сфер. Результаты были сравнены с соответствующими величинами теории Андерсен-Викс-Чендлера и с Монте-Карло "машинными" экспериментами.

KIVONAT

Az $1/r^n$ taszító potenciállal kölcsönható rendszerek és a magas hőmérsékletű Lennard-Jones folyadék termodinamikai tulajdonságait és radiális eloszlásfüggvényét számítottuk ki egy új perturbációs módszer segítségével, kemény-gömb referencia rendszert használva. Az eredményeket összevetettük az Andersen-Weeks-Chandler módszerrel számoltakkal és Monte Carlo számítógépes kísérletek eredményeivel.

Introduction

In the first part of this work¹ (hereafter referred to as paper I) a perturbational method was developed for the description of the thermodynamic and structural properties of real fluids in terms of a reference system, the properties of which are assumed to be known. In this paper we apply this method for a hard sphere reference system, for which convenient analytic formulae are available both for the equation of state² and the pair correlation function^{3,4}.

During the last years the relationship between the properties of this idealized model system and those of real fluids with smoothly varying repulsive forces has been discussed in several papers. Rowlinson⁵ considered fluids with an inverse n th power potential and expanded the thermodynamic properties in powers of $1/n$. Barker and Henderson⁶ generalized the Rowlinson method by applying it to a wide class of repulsive potentials. One of the most successful method was proposed by Andersen, Weeks and Chandler /AWC/⁷. In this method a series expansion is obtained for the free energy in powers of a "softness parameter" ξ by writing down its functional Taylor expansion in powers of the Boltzmann factor differences. The hard sphere diameter is chosen in such a way which causes the first order term of the free energy to vanish, at the same time reducing the magnitude of the higher order terms as well. However, if the interaction potential is not steep enough, the accuracy of these methods is not satisfactory in many cases, especially for the radial distribution function of the system.

The inaccuracy of the treatment of softening the core reflects in the results of the perturbation calculations for realistic potentials, when an attractive tail is added to a smoothly varying short range repulsive potential. Although the different theoretical methods for treating slowly varying attractive perturbations can be tested by ruling out this inaccuracy⁸, the accurate treatment of soft cores has still remained an unsolved problem in the theory of classical fluids.

In this paper we calculate the thermodynamic properties and radial distribution functions for systems with inverse n th power potentials ($n= 6, 9, 12$) and for a Lennard-Jones fluid at high temperature using the method developed in I. This method enables us to take into account an important part of the higher order terms of the usual g -dependent form of the thermodynamic quantities using only the radial distribution function of the hard sphere reference system (those parts that can be expressed in terms of the derivatives of this function with respect to the density). This will be demonstrated on the system with an inverse twelfth power potential. We discuss the problems related to the optimal choice of the hard sphere reference system and the condition $g = g_0$ proposed in I is compared to that given by Andersen et al⁷. The thermodynamic consistency will also be investigated: the equation of state is calculated both from the virial equation and from the derivative of the free energy with respect to the density. The results are compared to those obtained from the AWC method. In the last

part of the paper the calculated radial distribution function for the system with inverse twelfth power potential is compared to the Monte Carlo results and to that obtained from the AWC theory.

Description of the method for a hard sphere reference system

In this section we reformulate the method described in paper I for a hard sphere reference system, assuming that we know only the hard sphere pair correlation function. In this case the basic equations of the method (equations (11a-b) in paper I) will have the form

$$\rho(\eta, d^*) = \frac{\beta P}{S} = [\rho_0(\eta_0) + I(\eta_0, d^*)] \left[1 + \frac{(\eta_0 I)'}{(\eta_0 \rho_0)'} \right]^{-1} \quad (1a)$$

and

$$\frac{\eta}{\eta_0} d^{*3} = 1 + \frac{(\eta_0 I)'}{(\eta_0 \rho_0)'} \quad (1b)$$

where, to simplify the formulas, we introduced the quantity $\eta = \frac{\pi}{6} \rho \sigma^3$ instead of the density (σ stands for the characteristic length of the potential $u(\frac{r}{\sigma})$) and the packing fraction $\eta_0 = \frac{\pi}{6} \rho_0 d^3$ for the hard sphere reference system (d is the hard sphere diameter).

In these equations the prime denotes a derivative with respect to η_0 and $d^* = d/\sigma$. The integral $I(\eta_0, d^*)$ is defined as

$$I(\eta_0, d^*) = 12 \eta_0 \int_0^{\infty} y_2^0(\eta_0, x) [e(d^*x) - e_0(x)] x^2 dx \quad (2)$$

Here $e_0(x) y_2^0(\eta_0, x)$ stands for the hard sphere radial distribution function (which coincides with y_2^0 for $r > d$), $e(\frac{r}{\sigma})$ and $e_0(\frac{r}{\sigma})$ are the Boltzmann factors for the system under consideration and for the reference system, respectively. The excess chemical potential of the system can be obtained from the equation (19) of paper I:

$$\beta \mu_{ex}(\eta, d^*) = \beta \mu_{ex}^0(\eta_0) - \ln \left[1 + \frac{(\eta_0 I)'}{(\eta_0 \rho_0)'} \right] \quad (3)$$

The excess free energy per particle $a = \frac{\beta A_{ex}}{N}$ can be determined now from the thermodynamic relation

$$a(\eta, d^*) = \beta \mu_{ex} - p + 1 \quad (4)$$

The calculation can be carried out in two steps. First, one has to determine the packing fraction η_0 of the hard sphere system for a given value of η from the equation (1b). After this calculation the corresponding thermodynamic quantities can be obtained from the equations (1a), (3) or (4) using this value for η_0 . We can, however, proceed in an other way, starting from the usual density-dependent form for the thermodynamic quantities; expressions of this kind for the excess chemical potential and excess free energy can be obtained from the

equations (20) and (21) in paper I, respectively (first order in ξ):

$$\beta\mu_{ex}(\eta, d^*) = \beta\mu_{ex}^0(\bar{\eta}) - [\bar{\eta} I(\bar{\eta}, d^*)]' \quad (5a)$$

$$a(\eta, d^*) = a_0(\bar{\eta}) - I(\bar{\eta}, d^*) \quad (5b)$$

To simplify the formulae, here we introduced the notation $\bar{\eta} = \eta d^{*3}$. The two kinds of description, in general, are not equivalent with each other: the results of a calculation based on the equations (1b) and (3) or (4) differ from those obtained from the equations (5a-b) in the sum of an infinite subseries. They are equivalent only if the hard sphere reference system is determined from the condition $\mathcal{G} = \mathcal{G}_0$ proposed in paper I, when the sum of this subseries equals to zero. The equivalency of the two descriptions can be seen by comparing the equations (5a-b) to (3) and (4) and taking into account the condition $\mathcal{G} = \mathcal{G}_0$, which now has the form

$$[\bar{\eta} I(\bar{\eta}, d^*)]' = 0 \quad (6)$$

This equation specifies the reference system for a given value η through determining the function $d^*(\eta)$. To illustrate the difference between the two descriptions, we consider a system with an inverse twelfth power potential and calculate the excess free energy and the excess chemical potential as a function of

the hard sphere diameter d^* at different values for η using both kinds of description. As it is well known, the thermodynamic functions of a system with an inverse power potential of the form

$$u(r) = \epsilon \left(\frac{\sigma}{r} \right)^n \quad (7)$$

depends only on the quantity $\eta(\epsilon\beta)^{3/n}$. In the present method this scaling property is preserved as we can see from the definition (2) for the function I, which does not depend on β , ϵ , and σ separately, but only on a "temperature dependent characteristic length" $\sigma(\epsilon\beta)^{1/n}$. Replacing σ by this new characteristic length (i.e. taking $\eta = \frac{\pi}{6} \rho \sigma^3 (\epsilon\beta)^{3/n}$ and $d^* = \frac{d}{\sigma} (\epsilon\beta)^{-1/n}$), our formulae become appropriate for treating systems with a potential of the type (7).

To perform this calculation, one needs the knowledge of the hard sphere radial distribution function y_2^0 as a function of the packing fraction and the distance, and the equation of state for hard sphere fluids. For y_2^0 outside the core we used the analytic expressions obtained empirically by Verlet and Weis³ based on the solution of the Percus-Yevick equation⁴, while in the $r < d$ region we took the Thiele-Wertheim cubic polynomial form in r/d , with coefficients, which assure the continuity of the pair distribution function and its first and second derivatives at $r=d$ ⁹. Verlet and Weis state that the function y_2^0 obtained in this way differs from their Monte Carlo results by at most 3%. For the equation of state of hard sphere fluids we used the

expression suggested by Carnahan and Starling², which summarizes the available molecular-dynamics and Monte Carlo results within the statistical accuracy of these computer calculations. For the excess free energy and for the excess chemical potential this gives

$$\alpha_0(\bar{\eta}) = \frac{\bar{\eta}(4-3\bar{\eta})}{(1-\bar{\eta})^2} \quad (8a)$$

$$\beta\mu_{ex}^0(\bar{\eta}) = \frac{8\bar{\eta} - 9\bar{\eta}^2 + 3\bar{\eta}^3}{(1-\bar{\eta})^3} \quad (8b)$$

The calculated values for the excess free energy and for the excess chemical potential of the system with inverse twelfth power potential vs. d^* are shown in Fig. 1a and b at three different values for η ($\eta = 0.3, 0.4, 0.5$). The solid curves were obtained from the equations (1a), (1b), (4) or (3) by eliminating η_0 , while the results obtained from the equation (5b) or (5a) for α and $\beta\mu_{ex}$ respectively, are indicated by dashed lines. The Monte Carlo results¹⁰ are also shown in the figure by dotted lines for the corresponding values η . To interpret the results we call attention to the fact that if we knew all the higher order distribution functions of the hard sphere system, in principle we would obtain accurate results starting from any value of d^* . Thus the extension of the region in d^* , where these two kinds of first order calculation give reasonable results (the "flat" regions of the curves close to the dotted lines), characterizes, in some sense, the magnitude

of the neglected higher order terms. Therefore this figure clearly shows the advantages of a description which starts from the equations (1b) and (4) or (3). In the figure we also indicated the values d^* determined from the equation (6) and those obtained from the AWC condition $(I(\bar{\eta}, d^*) = 0)$. The two methods result in similar values for d^* , and therefore, for this system, they are nearly equivalent from the point of view of the thermodynamic quantities (but not from the point of view of the pair distribution functions, as we will see later). Furthermore, it is easy to show that at the value of d^* where $\rho = \rho_0$, not only the values of the free energies obtained from the two kinds of description equal to each other, but the slopes of the curves also coincide at this point¹¹:

$$\left(\frac{\partial a}{\partial \ln d^*}\right)_{\eta} = 3(p-1) - \left(\frac{\partial I}{\partial \ln d^*}\right)_{\bar{\eta}} \quad (9)$$

On the other hand - since in zeroth order $y_2(\eta, \frac{\tau}{\sigma}) = y_2^0(\bar{\eta}, \frac{\tau}{\sigma})$ as we can see from the equation 23 of paper I - the virial pressure p_V is related to the derivative $\left(\frac{\partial I}{\partial \ln d^*}\right)_{\bar{\eta}}$ by the equation

$$3(p_V - 1) = \left(\frac{\partial I}{\partial \ln d^*}\right)_{\bar{\eta}} \quad (10)$$

Thus we can see that $p = p_V$ when $\left(\frac{\partial a}{\partial \ln d^*}\right)_{\eta}$ equals to zero. From Fig. 1a we can see that this condition is approximately satisfied for all the three values of η at the point where $\rho = \rho_0$, which predicts a good zeroth order approximation for the radial distribution function by using the $\rho = \rho_0$ condition.

Results

A. Equation of state

In order to test the present method, in this section we calculate the equation of state for several systems from the condition $\rho = \rho_0$, and compare them to those obtained from the AWC method and to the results of computer simulations. The values for the free energy and the pressure for a system with inverse twelfth power potential are shown in Table 1. As was already indicated in Fig. 1, there are no reasonable differences between the results obtained from the condition $\rho = \rho_0$ (equation (6)) and those obtained from the AWC condition ($I=0$) when the equation of state is determined by numerical differentiation of the free energy with respect to the density. The virial equation of state, however, is more accurate in the case of the condition $\rho = \rho_0$, as we can expect on the basis of the discussion in connection with Fig. 1. The values for the pressure obtained from the equation (1a) using the condition $\rho = \rho_0$ are in good agreement with those obtained by numerical differentiation, demonstrating again how the thermodynamic consistency is fulfilled in the present method.

Other applications of the method are shown in Table 2 and in Fig. 2, where the equation of state is given for the systems with inverse ninth and sixth power potentials, respectively. In Fig. 2, the results obtained from the condition $\rho = \rho_0$ (solid line) are compared to those of the AWC method (dashed line).

The dotted lines show the virial equations of state and the full circles indicate the Monte Carlo results¹². We can conclude again that at low densities there are no essential differences between the results of the two methods, but for larger densities the condition $\rho = \rho_0$ reproduces more accurately the Monte Carlo values. The advantage of the condition $\rho = \rho_0$ is even more evident if one compares the virial pressure p_V to that obtained by numerical differentiation (p). Both the data in Table 2 and the curves plotted in Fig. 2 clearly show that $p \sim p_V$ for the condition $\rho = \rho_0$, while using the AWC method p_V is essentially larger than p at large densities.

Finally in Fig. 3 the calculated equation of state for a Lennard-Jones fluid is plotted at high temperature ($T^* = 5$), together with the Monte Carlo results¹³. The results show that in this temperature range the method can be applied directly for a Lennard-Jones system as well, but at low temperatures it fails to work for the reasons discussed in paper I (at low temperatures our zeroth order pair distribution function $n_2(r) = \frac{e(r)}{e_0(r)} n_2^0(r)$ is not a good approximation any more, and one should treat separately the short range repulsive and long range attractive parts of the potential).

B. Radial distribution function

The equation (23) in paper I gives an expression (first order in ξ) for the radial distribution function, and we suggested two different recipes for the choice of the reference system in the

zeroth and the first order calculation. In zeroth order (when $y_2(\eta, \frac{\tau}{\sigma}) = y_2^0(\bar{\eta}, \frac{\tau}{\alpha})$) the reference system can be determined from the condition $\rho = \rho_0$ (equation (6)). The results of such a zeroth order calculation are shown in the Fig. 4 and are compared to the results of a Monte Carlo computer calculation¹⁴ and to the pair distribution function obtained from the AWC method for the system with inverse twelfth power potential. In contrast to the case of the thermodynamic quantities, in this case there is an essential difference between the results obtained from the AWC method and from the condition $\rho = \rho_0$. While the first peak of the pair distribution function is too large in the AWC method, the condition $\rho = \rho_0$ almost exactly reproduces the results of the computer simulations in this region (here we used a moderately large value of η , indicated in the figure). In the region of the first minimum, however, both the AWC and the present method give too small values for the function $g_2(r)$.

These results can be improved by taking into account the next term in the expansion of the pair distribution function. In this case the reference system can be determined from the consistency criterion given by the equation (27) in paper I, which now has the form (for a hard sphere reference system)

$$(\bar{\eta} I)' = 2(\bar{\eta} \rho_0)' I(\bar{\eta}, d^*) \quad (11)$$

To perform the calculation, one should use some approximation for the three particle distribution function of the hard sphere system, which appears in the first order term in the equation (23)

in paper I. Using the Kirkwood superposition approximation for this function, we can obtain an approximate expression for y_2 from the equation (23) of paper I:

$$y_2(\eta, \frac{\tau}{\alpha}) = y_2^0(\eta, \frac{\tau}{\alpha}) \left[1 - 4I - 2I\eta \left[\ln y_2^0(\eta, \frac{\tau}{\alpha}) \right]' + 2\eta J(\eta, \frac{\tau}{\alpha}) \right] \quad (12)$$

where the integral J is defined by

$$J(\eta, x) = \frac{12}{x} \int_0^{\infty} dx' x' y_2^0(\eta, x') \left[e^{(d^*x')} - e_o(x') \right] \int_{\max(|x-x'|, 1)}^{x+x'} d\tau \tau y_2^0(\eta, \tau) \quad (13)$$

This expression for $J(x)$ was obtained by introducing a bipolar coordinate system.

The result of the first order calculation (solid line) is plotted in Fig. 5 for a system with inverse twelfth power potential, together with the Monte Carlo results (full circles)^{1,4}.

The zeroth order curve (dashed line) is also shown. One can see from the figure that the result of the first order calculation agrees remarkably well with the Monte Carlo data not only in the neighbourhood of the first peak, but the agreement is essentially improved in the region of the first minimum as well compared to the zeroth order case.

Conclusion

To summarize we can say that the application of the method developed in I for the systems with inverse power potential using a hard sphere reference system, verifies our expectations that using this method a more accurate and more consistent description can be achieved compared to the calculations which start from the usual density-dependent form for the thermodynamic quantities. This result can be ascribed to the fact that the present method makes a more complete use of the information content of the radial distribution function. The advantage of the method can be seen clearly from the remarkable agreement between the values for the pressure calculated from the virial equation and those obtained from the derivative of the free energy with respect to the density, and from the reasonable agreement between the calculated radial distribution functions and the Monte Carlo results.

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The reason for changing the original procedure by Verlet and Weis³ was the fact that at large densities it gives large negative values for y_2^0 inside the core already at a distance as large as (0.8-0.9)d.

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Figure Captions

Figure 1.

The excess free energy (a) and the excess chemical potential (b) of the system with inverse twelfth power potential vs. d^* at different values for η . The solid curves were obtained from the equations (1b), (1a), (3) or (4) by eliminating η_0 , while the results obtained from the equation (5b) or (5a) for α and $\beta\mu_{ex}$, respectively, are indicated by dashed lines. The Monte Carlo results¹⁰ are shown by dotted lines. The arrows show the values of d^* determined from the condition $\mathcal{G} = \mathcal{G}_0$ (equation (6)) (\downarrow) and obtained from the AWC - condition (\downarrow).

Figure 2.

The equation of state of the system with inverse sixth power potential. The dashed curve was obtained from the AWC - condition by numerical differentiation of the free energy with respect to the density, while the dotted curves show the virial equation of state coming from both the AWC - method, and the condition $\mathcal{G} = \mathcal{G}_0$. The pressure obtained from the condition $\mathcal{G} = \mathcal{G}_0$ by numerical differentiation is indicated by solid line. The Monte Carlo results are denoted by full circles.

Figure 3.

The equation of state for a Lennard-Jones fluid at high temperature ($T^* = 5$). The solid line shows the result obtained from the condition $\mathcal{G} = \mathcal{G}_0$, the MC - results¹³ are indicated by black circles.

Figure 4.

The pair distribution function of the system with inverse twelfth power potential at $\eta = 0.4215$. The zeroth order result obtained from the condition $\rho = \rho_0$ (solid line) is compared to that calculated from the AWC theory (dashed line) and to the MC results (black circles).

Figure 5.

The pair distribution function of the system with inverse twelfth power potential at $\eta = 0.3746$. The full line shows the result of a first order calculation, where the three particle distribution function is given by the Kirkwood superposition approximation. The results of the zeroth order calculation and the MC - results are indicated by dashed line and black circles, respectively.

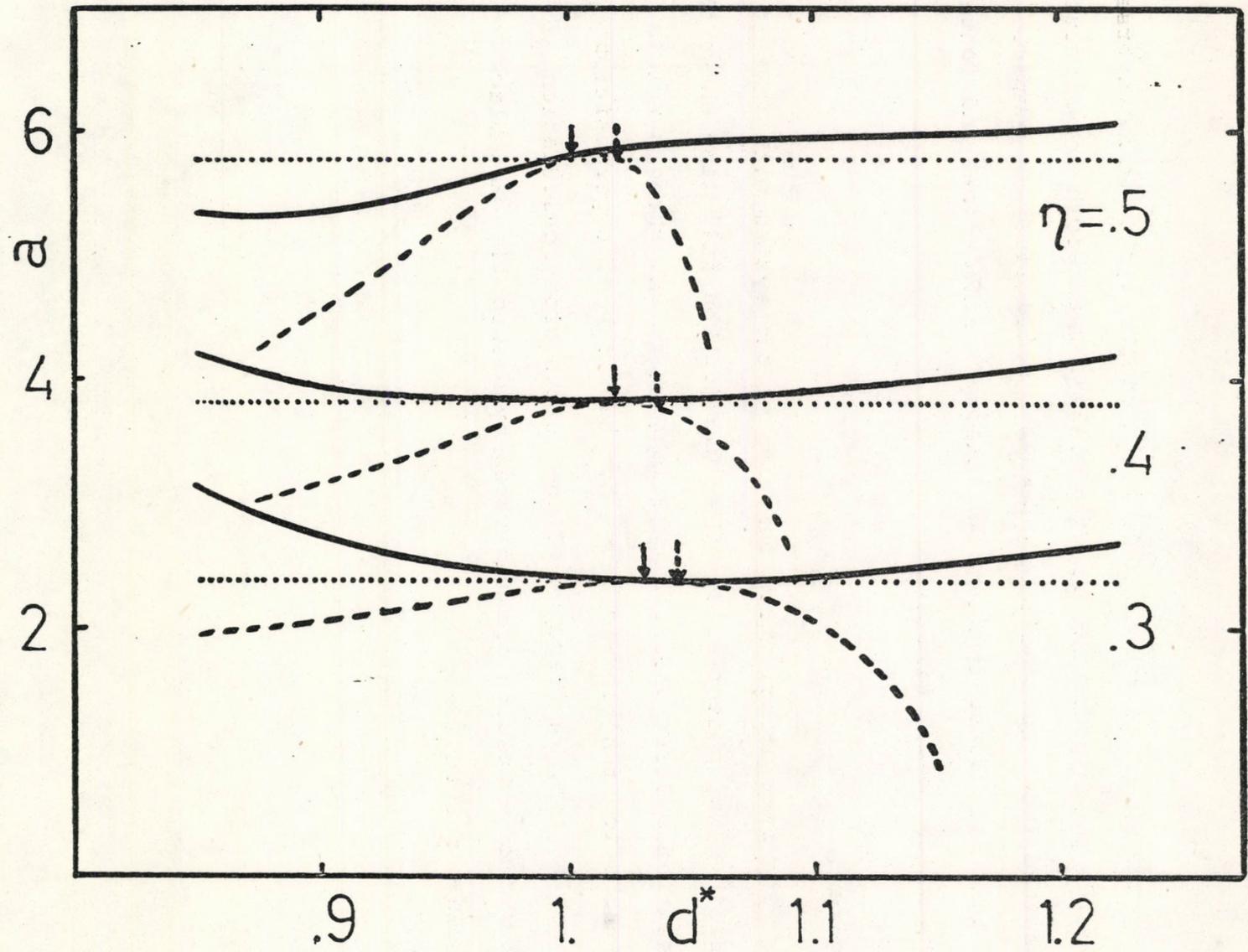


Fig. 1/a

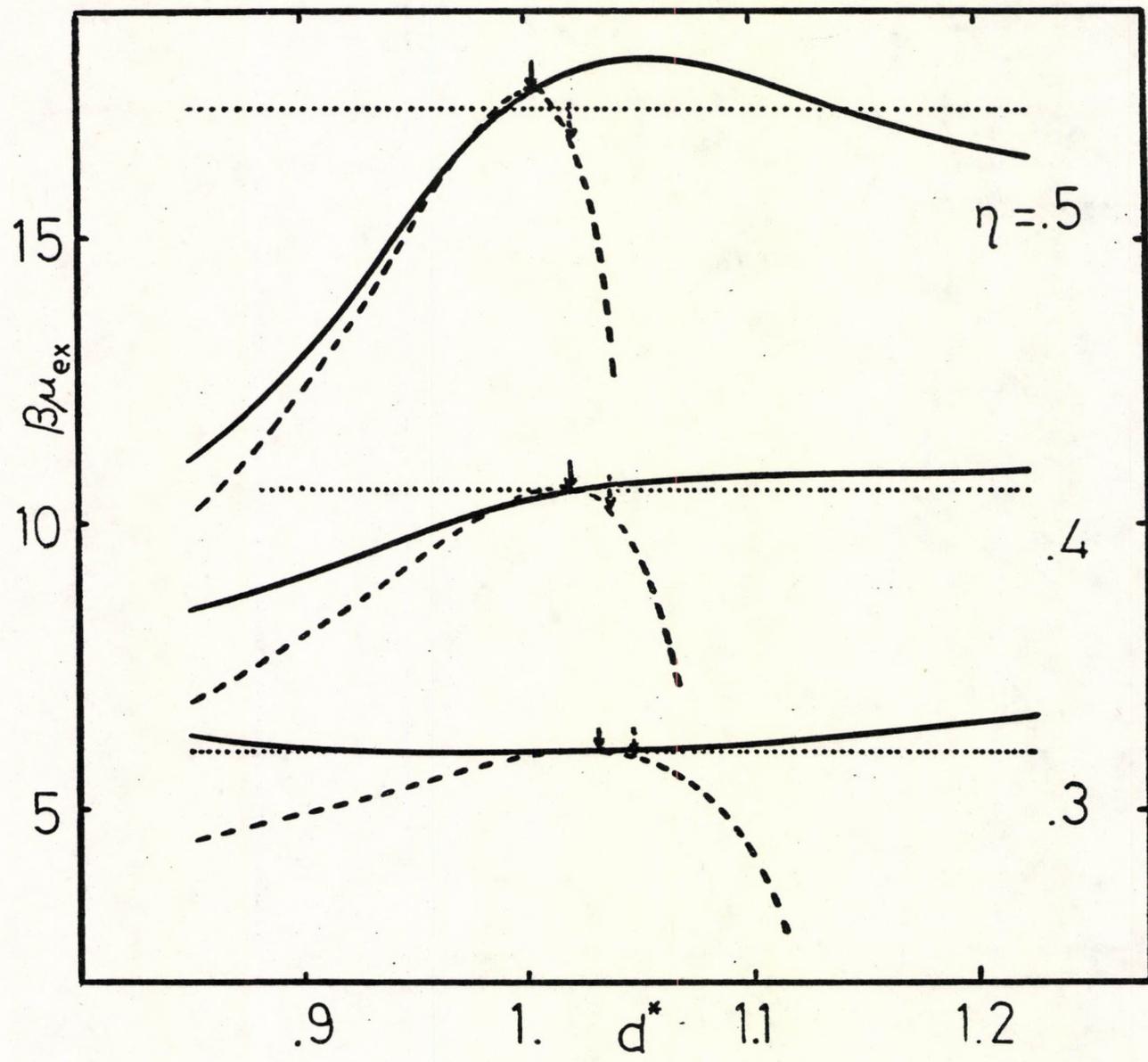


Fig. 1/b

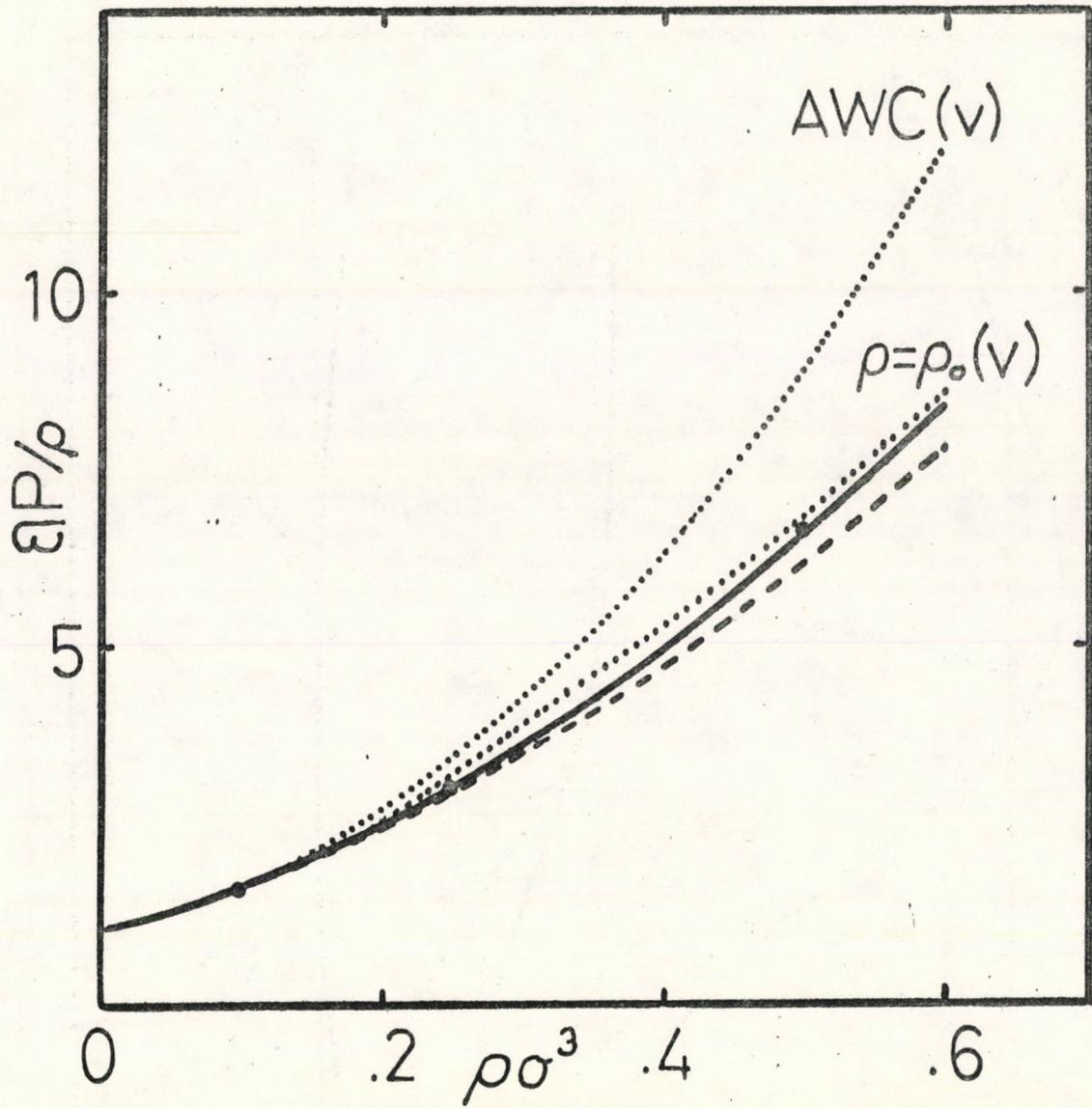


Fig. 2

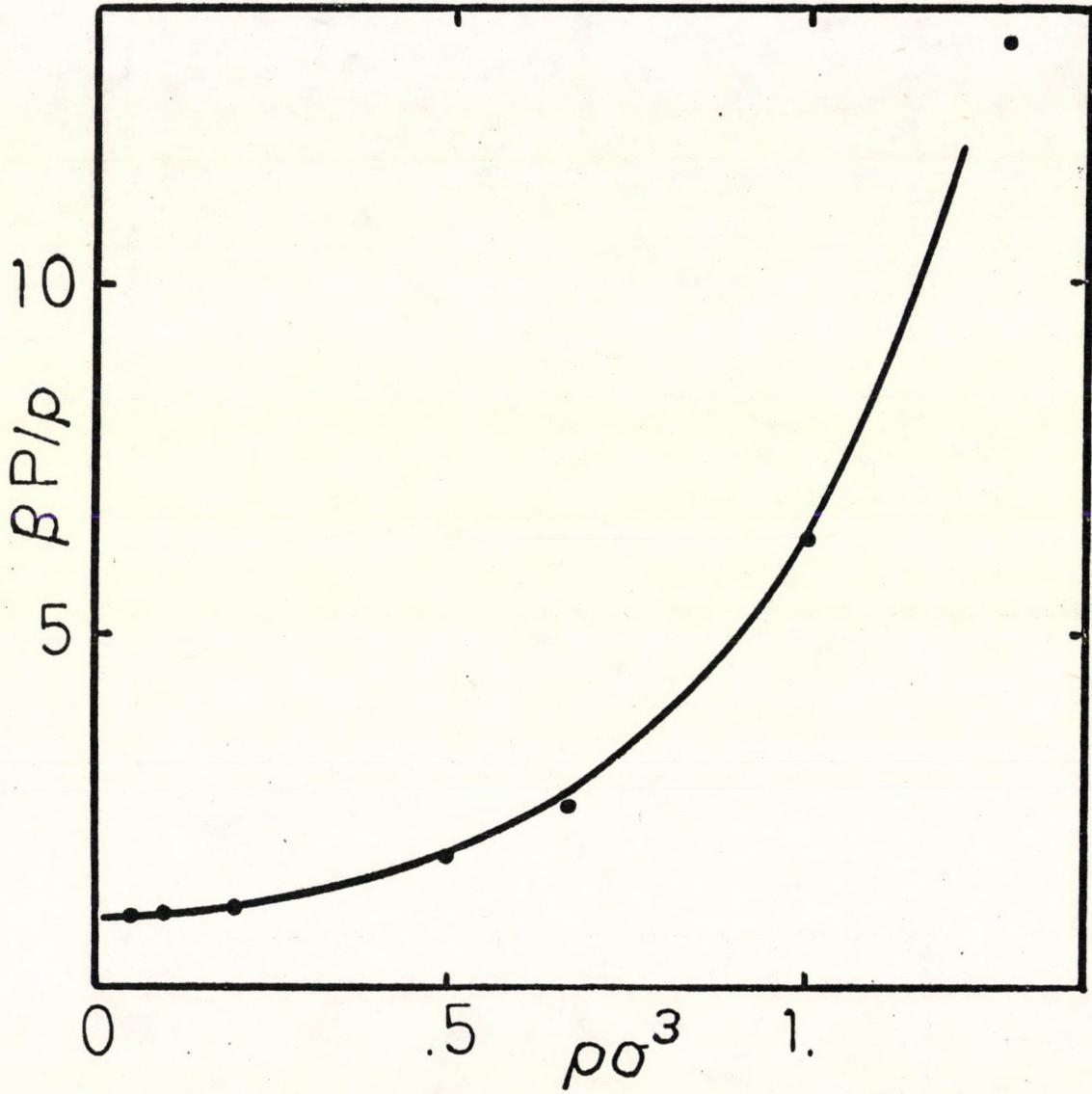


Fig. 3

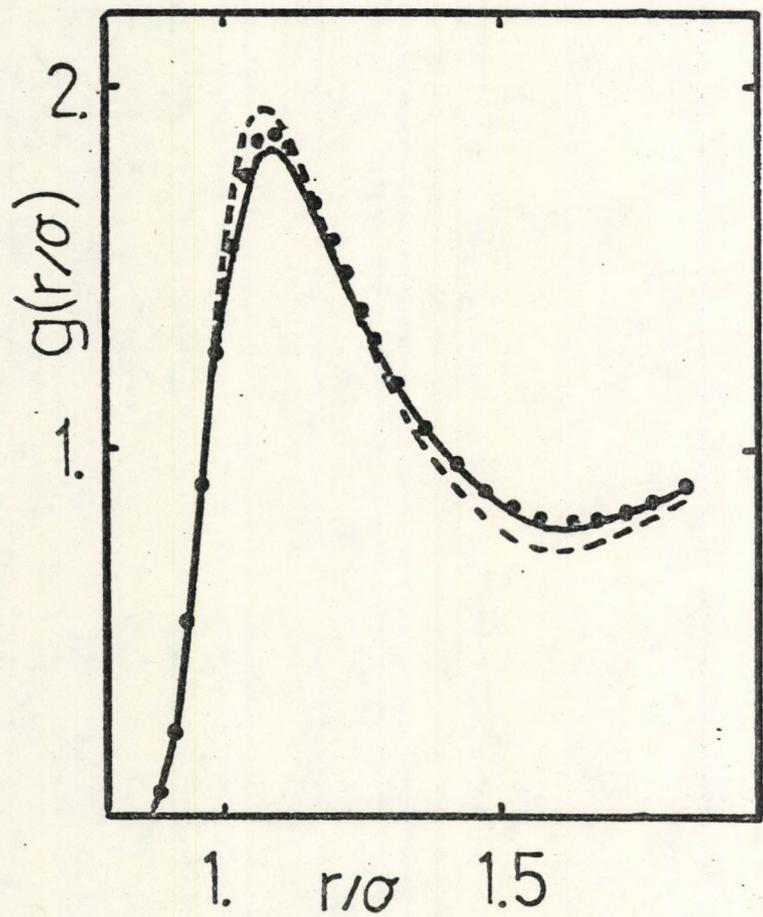


Fig. 5

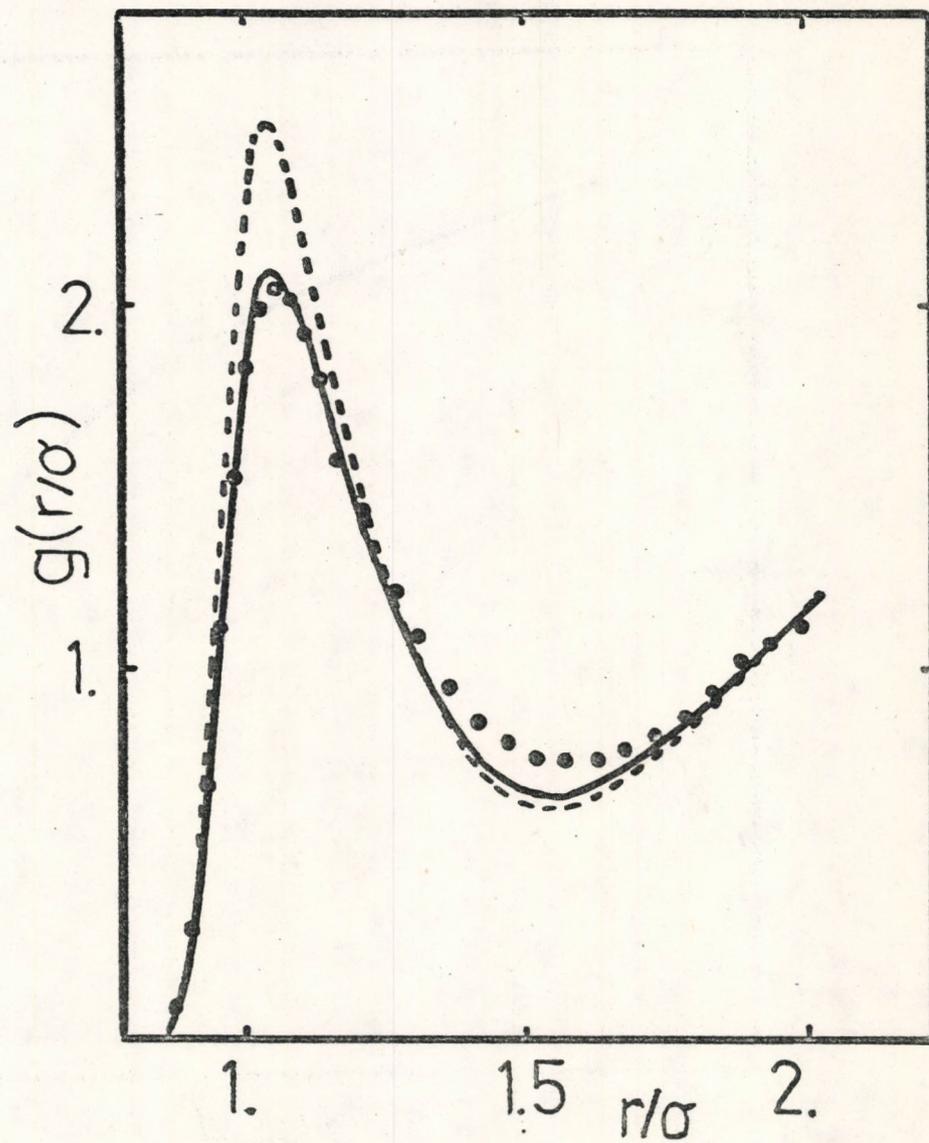


Fig. 4

Table Captions

Table 1.

The thermodynamic properties of a system with inverse twelfth power potential. MC = results of Monte-Carlo experiments¹⁰; AWC = prediction of the AWC - theory, $\beta = \beta_0$ = results obtained from the equation (6). The equation of state is obtained by numerical differentiation of the free energy; AWC(v) and $\beta = \beta_0(v)$ are the predictions of the AWC - theory and the condition $\beta = \beta_0$, respectively, based on the virial theorem. The values for the pressure obtained from the equation (1a) using the condition $\beta = \beta_0$ are also shown ($\beta = \beta_0$ (1a)). The AWC values shown in the table differ slightly from those of Ref. 7 as a consequence of the different extrapolation procedure for $y_2^0(r)$ inside the core.

Table 2.

The equation of state of a system with inverse ninth power potential. The notations are the same as in Table 1. The MC values were taken from Ref. 12.

| $\eta \frac{6}{\pi \sqrt{2}}$ | a | | | p | | | | | |
|-------------------------------|------|-------|-----------------|------|-------|-------------|-----------------|----------------------|--------------------|
| | MC | AWC | $\rho = \rho_0$ | MC | AWC | AWC (v) | $\rho = \rho_0$ | $\rho = \rho_0(1/a)$ | $\rho = \rho_0(v)$ |
| 0.1 | 0.40 | 0.404 | 0.404 | 1.45 | 1.450 | 1.455 | 1.450 | 1.449 | 1.454 |
| 0.2 | 0.91 | 0.907 | 0.908 | 2.12 | 2.123 | 2.155 | 2.124 | 2.123 | 2.143 |
| 0.3 | 1.53 | 1.537 | 1.540 | 3.12 | 3.116 | 3.232 | 3.123 | 3.119 | 3.166 |
| 0.4 | 2.33 | 2.331 | 2.337 | 4.58 | 4.556 | 4.873 | 4.580 | 4.571 | 4.631 |
| 0.5 | 3.34 | 3.332 | 3.347 | 6.66 | 6.616 | 7.334 | 6.665 | 6.669 | 6.640 |
| 0.6 | 4.61 | 4.599 | 4.623 | 9.56 | 9.539 | 10.945 | 9.591 | 9.688 | 9.256 |

Table 1.

| $\eta \frac{6}{\pi \sqrt{2}}$ | p | | | | |
|-------------------------------|------|------|--------|-----------------|--------------------|
| | MC | AWC | AWC(v) | $\rho = \rho_0$ | $\rho = \rho_0(v)$ |
| 0.1 | 1.50 | 1.50 | 1.51 | 1.50 | 1.51 |
| 0.25 | 2.70 | 2.69 | 2.84 | 2.70 | 2.77 |
| 0.5 | 6.60 | 6.48 | 7.74 | 6.61 | 6.65 |

Table 2.

63.105



Kiadja a Központi Fizikai Kutató Intézet
Felelős kiadó: Krén Emil
Szakmai lektor: Bergou János
Nyelvi lektor: Tüttő István
Példányszám: 500 Törzsszám: 80-738
Készült a KFKI sokszorosító üzemében
Felelős vezető: Nagy Károly
Budapest, 1980. december hó