Radial Distribution Functions for the Gaussian Model*

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Radial distribution functions g are computed for the "Gaussian model" using the Monte Carlo (MC) method and the convolution-hypernetted-chain (CHNC) and Percus-Yevick (PY) integral equations. These results are compared with the density-expansion results obtained by Helfand and Kornegay (HK). For low density, the MC, PY, and CHNC g's show excellent agreement with HK data, indicating that the errors introduced in the numerical solutions are small. At higher densities the HK data are no longer applicable, but the PY, CHNC, and MC results continue to show good agreement, with closest agreement between CHNC and MC results.

I. INTRODUCTION

IN recent years much effort has gone into the study of radial distribution functions g since a complete knowledge of g gives the complete thermodynamic behavior of a fluid (if the potential energy may be expressed as a sum of pair potentials).[1] In this paper we are concerned with the comparison of approximate methods for computing g for the "Gaussian model."

Two important integral equations have been put forward as methods for computing approximate g's. The Percus-Yevick (PY) equation[2] was originally derived using a method of collective coordinates. The convolution hypernetted chain (CHNC) equation[3] was derived by summing a certain set of terms from the density expansion for g. The PY equation is also equivalent to summing a (different) set of terms from the density expansion.[4] In the notation of Klein and Green,[5] the exact density expansion[6] for g can be written

$$g(\mathbf{r})-1=G(\mathbf{r})=f(\mathbf{r})+[1+f(\mathbf{r})]\times[S(\mathbf{r})+B(\mathbf{r})+P_1(\mathbf{r})], \quad (1)$$

$$f(\mathbf{r})=\exp[-V(\mathbf{r})/kT]-1, \quad (2)$$

where V is the pair potential function, and S, B, and P_1, are power series in density corresponding to the series, bridge, and parallel diagrams, respectively. A summation of the "CHNC diagrams" is equivalent to the integral equation

$$G(\mathbf{r})=\bar{n}\int c(\mathbf{r}-\mathbf{s})G(\mathbf{s})d\mathbf{s}+c(\mathbf{r}),$$
$$c(\mathbf{r})=g(\mathbf{r})-1-\ln g(\mathbf{r})-V(\mathbf{r})/kT, \quad (3)$$

where $\bar{n}$ is the number density.

A summation of the "PY diagrams" gives the integral equation

$$G(\mathbf{r})=\bar{n}\int c(\mathbf{r}-\mathbf{s})G(\mathbf{s})d\mathbf{s}+c(\mathbf{r}),$$
$$c(\mathbf{r})=g(\mathbf{r})\{1-\exp[V(\mathbf{r})/kT]\}. \quad (4)$$

Recently, Helfand and Kornegay[7] (HK) evaluated several of the terms in the density expansion for g for the "Gaussian model." They computed the exact coefficients, Eq. (1), through the fifth power in density and the CHNC and the PY coefficients through the fourth power in density.

A third method for obtaining approximate g's is the Monte Carlo (MC) method of Metropolis *et al.*[8] In previous work MC results have often been taken as standards for judging the accuracy of the integral equations. Because it is taken as a standard and yet contains certain approximations, it seems wise to test the MC method against exact or near exact results whenever possible.

Solving the PY and CHNC integral equation is equivalent to summing the appropriate terms in the density expansion for g to all orders of density. The equations are nonlinear and require high-speed digital computers for their solutions. Iteration methods are used which require certain approximations in the numerical procedures. The most important of these approximations are (1) the truncation of the range of integration, (2) the use of a finite number of points in numerical integration procedures, and (3) the use of a finite number of iterations.

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[1] Terrell L. Hill, *Introduction to Statistical Thermodynamics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1960); J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954).

[2] J. K. Percus and G. J. Yevick, Phys. Rev. **110**, 1 (1958); J. K. Percus, Phys. Rev. Letters **8**, 462 (1962); J. L. Lebowitz and J. K. Percus, J. Math. Phys. **4**, 116 (1963).

[3] E. Meeron, J. Math. Phys. **1**, 192 (1960); T. Morita, Progr. Theoret. Phys. (Kyoto) **23**, 385 (1960); J. M. J. Van Leeuwen, J. Groeneveld, and J. DeBoer, Physica **25**, 792 (1959); M. S. Green, Tech. Rept. Hughes Aircraft Corporation (unpublished).

[4] G. Stell, Physica **29**, 517 (1963); A. A. Khan, Phys. Rev. **134**, A367 (1964).

[5] Max Klein and M. S. Green, J. Chem. Phys. **39**, 1367 (1963).

[6] J. E. Mayer and E. W. Montroll, J. Chem. Phys. **9**, 626 (1941).

[7] E. Helfand and R. Kornegay, Bell Telephone Laboratories, Inc., Murray Hill, New Jersey (unpublished).

[8] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953); W. W. Wood and F. R. Parker, *ibid.* **27**, 720 (1957).

For low densities, the contribution of the terms of power greater than five in density is negligible, and the HK results provide nearly exact answers. We use these solutions for low density to test the Monte Carlo method and to study errors in the numerical methods of solving the integral equations.

When the major contribution to G comes from the first few terms in the density expansion, much can be learned about the approximations by looking at the neglected diagrams. However, the number of diagrams increases rapidly with density and even for diagrams of only three field points the number of diagrams makes such analysis difficult. Also, it is quite possible that at moderate densities there is cancellation of errors from the higher order terms. To study these cancellation effects, we obtain solutions to the integral equations and compare these results with the HK data at moderate densities. We also obtain a MC g for high density to estimate the correctness of the PY and CHNC g's.

II. THE GAUSSIAN MODEL

The Gaussian model takes the Mayer f function to be a negative Gaussian.

$$f(r)=-\exp[-(r/a)^2]. \tag{5}$$

Figure 1 compares the Mayer f function for the Gaussian model with the Lennard-Jones and hard-sphere models. The Gaussian model has received considerable attention recently because the integrals appearing in various density expansions can be evaluated.[7,9] It is hoped that the study of this model will bring out certain characteristics common to the more realistic but more difficult models. Since the pair potential is temperature-dependent, it does not correspond to a physical potential. However, this is not important in the applications made here as we may consider the comparisons to be made at fixed temperatures.

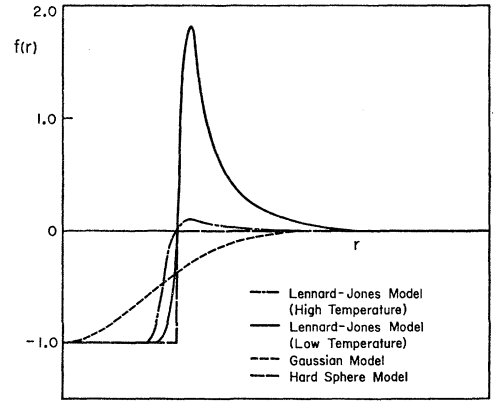

FIG. 1. Schematic drawing of the Mayer f function for the Gaussian, Lennard-Jones, and hard-sphere models.

We use the same units as in the HK paper taking (1.100 a) as our unit of length. We let

$$x=r/(1.100\,a). \tag{6}$$

For this model, the density expansion for g may be rewritten

$$g(x)=[1-\exp(-1.210x^2)][1+\sum_{n=1}^{\infty}\rho^n g_n(x)]. \tag{7}$$

In Eq. (7), ρ is the number density and the g_n are, of course, different for the exact expansion and the PY and CHNC approximations. Helfand and Kornegay determined g_n for n through 5 for the exact expansion and through 4 for the PY and CHNC approximations.

III. METHODS OF SOLUTION

The numerical solution of the integral equation is an iterative process and has been previously discussed.[10] In these computations we use one-hundred points with intervals of 0.05 giving a range of integration of 5. All solutions show good convergence (small changes in g in successive iterations) after 10 iterations.

The Monte Carlo method we use is that of Metropolis *et al.*, and a discussion of the method can also be found in the Wood and Parker paper.[8] The discussion here is very brief and the reader is referred to the papers above for a more complete account. The method consists of putting a number N of particles in a cubic cell of length L. Periodic cubic cells are assumed so that a particle in the basic cell has periodic images in the surrounding cells. One of the particles is chosen and given a new position at random within a cubic cell surrounding the original position. If the energy of configuration is lower for the new position, the move is allowed. If the energy is higher, the move is allowed with a probability of $\exp(-\Delta E/kT)$, where ΔE is the change in the configurational energy. Continuing in this manner a large number of configurational states can be generated on a high-speed digital computer. The process described above generates configurational states with a probability proportional to the Boltzmann factor. Thus, to obtain average values of quantities depending upon the configuration, it is necessary only to average these quantities over the configurations generated. Although the Monte Carlo method has often been taken as a standard for checking other methods, there are approximations involved. Some of these approximations are: (1) the necessity of using a small number of particles in the basic cell (usually of the order of 10^2), (2) the truncation of the pair potential, (3) the elimination of

[9] G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics* (American Mathematical Society, Providence, Rhode Island, 1963); J. DeBoer and G. E. Uhlenbeck, *Studies in Statistical Mechanics* (North-Holland Publishing Company, Amsterdam, 1962); H. N. V. Temperly, Atomic Weapons Research Establishment, Aldermaston, Berks, 1963 (unpublished); H. N. V. Temperly, Proc. Phys. Soc. (London) **83**, 3 (1964).

[10] A. A. Broyles, S. U. Chung, and H. L. Sahlin, J. Chem. Phys. **37**, 2462 (1962); D. D. Carley, dissertation, University of Florida, 1963 (unpublished).

fluctuations in the number of particles in the basic cell, (4) the introduction of spurious correlations due to the periodicity conditions, and (5) the necessity of generating only a finite number of configurations (usually of the order of 10^4 or 10^5).

Two MC calculations are made for the Gaussian model. The first, for a density of $\rho=0.35$, we use as a check of the MC method (and our computer code) and the second, for a density of $\rho=1.00$, we use as a check on the PY and CHNC integral equations where the HK data are no longer applicable.

For the $\rho=0.35$ calculation we take N equal to 64, thus determining L to be 5.676. For $\rho=1.00$, we again take N to be 64 thus making L equal to 4.00. In both cases we truncate the pair potential at $\frac{1}{2}L$ and determine $g(x)$ at intervals of 0.05 (conforming to the HK data)

TABLE I. Radial distribution functions for $\rho=0.10$.

	Radial distribution function					
x	E5[a]	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0138	0.0138	0.0138	0.0139	0.0138	0.0139
0.20	0.0542	0.0542	0.0540	0.0544	0.0539	0.0544
0.30	0.1179	0.1179	0.1173	0.1182	0.1173	0.1182
0.40	0.1999	0.1999	0.1990	0.2003	0.1990	0.2003
0.50	0.2943	0.2943	0.2931	0.2948	0.2930	0.2948
0.60	0.3948	0.3948	0.3934	0.3954	0.3933	0.3953
0.70	0.4954	0.4954	0.4940	0.4961	0.4939	0.4960
0.80	0.5913	0.5913	0.5899	0.5918	0.5898	0.5918
0.90	0.6785	0.6785	0.6773	0.6790	0.6772	0.6789
1.00	0.7547	0.7547	0.7537	0.7551	0.7536	0.7550
1.10	0.8187	0.8187	0.8179	0.8191	0.8178	0.8189
1.20	0.8706	0.8706	0.8700	0.8709	0.8700	0.8707
1.30	0.9111	0.9111	0.9107	0.9113	0.9107	0.9112
1.40	0.9416	0.9416	0.9414	0.9417	0.9413	0.9416
1.50	0.9637	0.9637	0.9636	0.9638	0.9635	0.9636
1.60	0.9790	0.9790	0.9789	0.9791	0.9789	0.9789
1.70	0.9891	0.9892	0.9891	0.9892	0.9891	0.9891
1.80	0.9955	0.9955	0.9955	0.9955	0.9955	0.9954
1.90	0.9992	0.9992	0.9992	0.9992	0.9992	0.9991
2.00	1.0011	1.0010	1.0011	1.0011	1.0011	1.0010
2.40	1.0015	1.0015	1.0015	1.0015	1.0015	1.0015
2.80	1.0003	1.0003	1.0003	1.0003	1.0003	1.0003
3.20	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

[a] This notation is presented in Sec. IV.

from zero to $\frac{1}{2}L$. In each case we generate a total of 16 000 configurations.

IV. DISCUSSION OF RESULTS

In Tables I–VIII and in the discussion we use the following notation:

E5: g as determined from the HK data for the exact expansion using the g_n [Eq. (7)] through $n=5$.

E4: g as determined from the HK data for the exact expansion using the g_n through $n=4$.

PY4: g as determined from the HK data for the PY approximation using the g_n through $n=4$.

CHNC4: g as determined from the HK data for the CHNC approximation using the g_n through $n=4$.

PY: g as determined from a numerical solution of the PY integral equation.

TABLE II. Radial distribution functions for $\rho=0.20$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0157	0.0157	0.0154	0.0158	0.0154	0.0158
0.20	0.0614	0.0614	0.0603	0.0618	0.0603	0.0618
0.30	0.1328	0.1328	0.1307	0.1337	0.1306	0.1336
0.40	0.2238	0.2238	0.2206	0.2251	0.2204	0.2250
0.50	0.3270	0.3270	0.3229	0.3285	0.3227	0.3284
0.60	0.4348	0.4348	0.4302	0.4365	0.4300	0.4363
0.70	0.5406	0.5406	0.5360	0.5423	0.5357	0.5420
0.80	0.6388	0.6388	0.6347	0.6405	0.6343	0.6400
0.90	0.7258	0.7259	0.7224	0.7274	0.7220	0.7267
1.00	0.7995	0.7997	0.7970	0.8010	0.7966	0.8001
1.10	0.8594	0.8597	0.8577	0.8609	0.8573	0.8597
1.20	0.9061	0.9065	0.9052	0.9076	0.9048	0.9062
1.30	0.9410	0.9415	0.9406	0.9425	0.9403	0.9409
1.40	0.9659	0.9664	0.9660	0.9675	0.9657	0.9658
1.50	0.9828	0.9834	0.9831	0.9844	0.9829	0.9827
1.60	0.9935	0.9942	0.9939	0.9952	0.9938	0.9934
1.70	0.9998	1.0005	1.0002	1.0015	1.0002	0.9998
1.80	1.0030	1.0037	1.0033	1.0047	1.0034	1.0030
1.90	1.0042	1.0050	1.0045	1.0058	1.0046	1.0043
2.00	1.0043	1.0048	1.0044	1.0057	1.0046	1.0044
2.40	1.0014	1.0015	1.0010	1.0020	1.0016	1.0016
2.80	1.0000	0.9997	0.9994	0.9999	1.0000	1.0000
3.20	1.0000	0.9994	0.9993	0.9995	0.9999	0.9999

CHNC: g as determined from a numerical solution of the CHNC integral equation.

MC: g as determined from the Monte Carlo procedure.

The low-density comparisons (see Tables I–III) provide a means for checking the errors introduced in the numerical solutions of the integral equations. When E4 and E5 are nearly the same, it is reasonable to believe that the contribution from the terms of ρ^5 and higher are small. Thus PY4 and CHNC4 should agree with PY and CHNC, respectively, if the errors in the numerical solutions to the integral equations are small;

TABLE III. Radial distribution functions for $\rho=0.30$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0176	0.0176	0.0170	0.0178	0.0170	0.0178
0.20	0.0686	0.0685	0.0665	0.0693	0.0663	0.0693
0.30	0.1478	0.1476	0.1435	0.1491	0.1432	0.1491
0.40	0.2474	0.2472	0.2411	0.2494	0.2405	0.2493
0.50	0.3587	0.3584	0.3509	0.3613	0.3500	0.3608
0.60	0.4728	0.4725	0.4645	0.4759	0.4634	0.4749
0.70	0.5823	0.5821	0.5745	0.5858	0.5730	0.5840
0.80	0.6815	0.6816	0.6749	0.6856	0.6733	0.6826
0.90	0.7669	0.7674	0.7621	0.7718	0.7603	0.7675
1.00	0.8370	0.8381	0.8342	0.8430	0.8323	0.8371
1.10	0.8919	0.8937	0.8908	0.8993	0.8891	0.8917
1.20	0.9330	0.9356	0.9334	0.9417	0.9318	0.9327
1.30	0.9621	0.9656	0.9636	0.9723	0.9622	0.9620
1.40	0.9816	0.9859	0.9838	0.9929	0.9827	0.9819
1.50	0.9938	0.9986	0.9961	1.0059	0.9955	0.9944
1.60	1.0006	1.0058	1.0029	1.0130	1.0027	1.0016
1.70	1.0037	1.0091	1.0057	1.0161	1.0061	1.0052
1.80	1.0045	1.0098	1.0061	1.0164	1.0071	1.0063
1.90	1.0040	1.0089	1.0050	1.0150	1.0066	1.0061
2.00	1.0029	1.0073	1.0033	1.0128	1.0055	1.0051
2.40	0.9993	1.0002	0.9971	1.0033	1.0010	1.0010
2.80	0.9994	0.9971	0.9953	0.9984	0.9998	0.9998
3.20	1.0006	0.9966	0.9959	0.9972	0.9999	0.9999

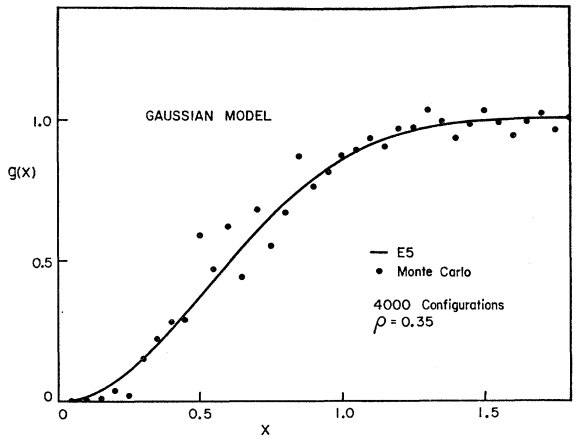

FIG. 2. The Monte Carlo radial distribution function compared with the density expansion through the fifth power in density. The number density is 0.35 and 4000 configurations have been generated.

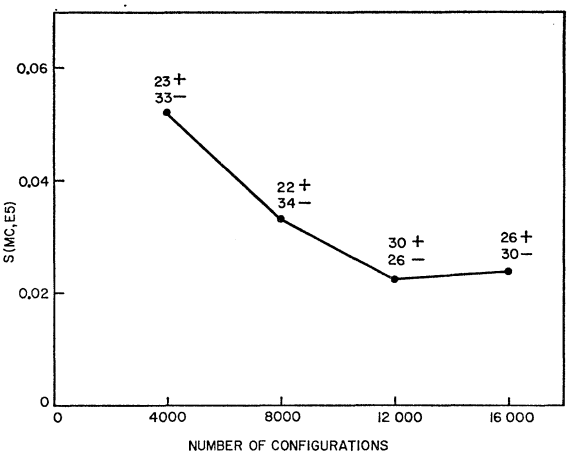

FIG. 4. The standard deviation between the Monte Carlo radial distribution function and E5 plotted as a function of the number of generated configurations for the $\rho=0.35$ case. The number preceding the plus (minus) sign indicates the number of times the MC point is above (below) the E5 point in the radial distribution curves.

examination of Tables I–III show this to be the case. The increasing differences between the density expansion and integral equation solutions at the higher densities is probably largely due to the neglect of higher terms in the density expansion, since E4 and E5 also begin to show differences. It should not be concluded, however, that all numerical solutions of the integral equations are as good as this comparison seems to indicate, since longer range forces, attractive forces, higher densities, and lower temperatures usually tend to destroy their accuracy.

Figures 2 and 3 show the results of the MC calculation at $\rho=0.35$. Since E4 and E5 are nearly the same at this density, it is again reasonable to believe that E5 is very close to the exact g. Taking E5 as the standard, we see the MC points to be scattered quite closely about the curve with nearly an equal number of points above and below. As a means for comparison, we use the standard deviation S between two functions, defined by

$$S(f,f')=\left[\frac{1}{n}\sum_{i=1}^{n}(f_i-f_i')^2\right]^{1/2}. \tag{8}$$

Since the MC method is statistical in nature, S(MC,E5) will vary with the number of configurations generated m and should approach zero as $m\rightarrow\infty$, if the MC approximations are valid. In Fig. 4, S(MC,E5) is plotted as a function of m. The increase in S(MC,E5) as m goes from 12 000 to 16 000 is largely due to certain points near $x=0$ where the small number of particles at these separations cause major fluctuations in $g(x)$. The nearly equal number of MC points above and below E5 and their tendency to bracket the curve indicates that the finite value of S(MC,E5) arises from a natural

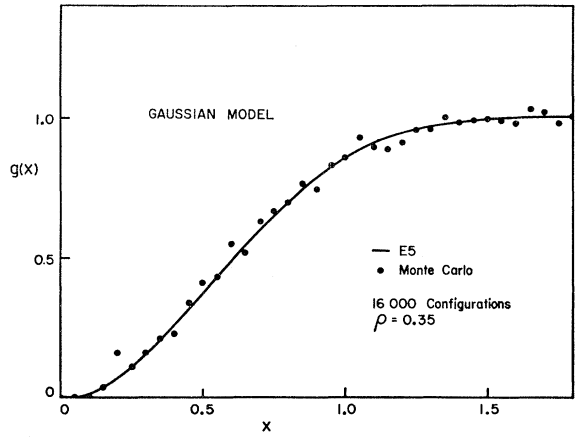

FIG. 3. The Monte Carlo radial distribution function compared with the density expansion through the fifth power in density. The number density is 0.35 and 16 000 configurations have been generated.

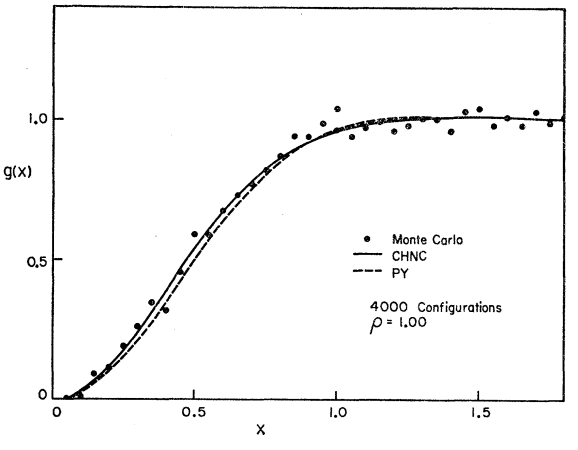

Fig. 5. The Monte Carlo radial distribution function compared with the PY and CHNC integral equation solutions. The number density is 1.00 and 4000 configurations have been generated.

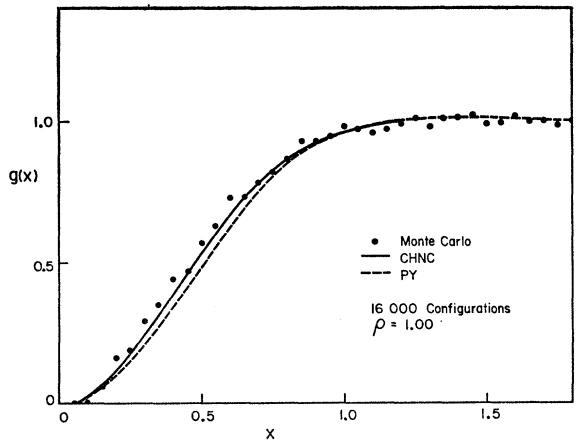

FIG. 6. The Monte Carlo radial distribution function compared with the PY and CHNC integral equation solutions. The number density is 1.00 and 16 000 configurations have been generated.

scatter of MC points rather than a systematic deviation from E5.

Figures 5 and 6 show the results of the MC calculation for $\rho=1.00$. Because the HK data are not applicable at this high density, we compare the MC result only with PY and CHNC. Figure 6 shows that both PY and CHNC are quite good even at this high density. The MC results are higher than PY and perhaps even slightly above CHNC in the range $0.2<x<1.0$. Figure 7, where S(MC,PY) and S(MC,CHNC) are plotted as functions of m, also confirms the conclusion that the MC points lie closer to CHNC than PY. Because of the small differences between PY and CHNC and the uncertainty in the MC points, we conclude that both PY and CHNC give reasonably good answers at this density, and that the CHNC equation is probably somewhat better. This study, and other similar comparisons,[4,10] indicate that it is meaningless to ask whether the PY or CHNC equation is superior, without also specifying the pair potential, temperature, and density.

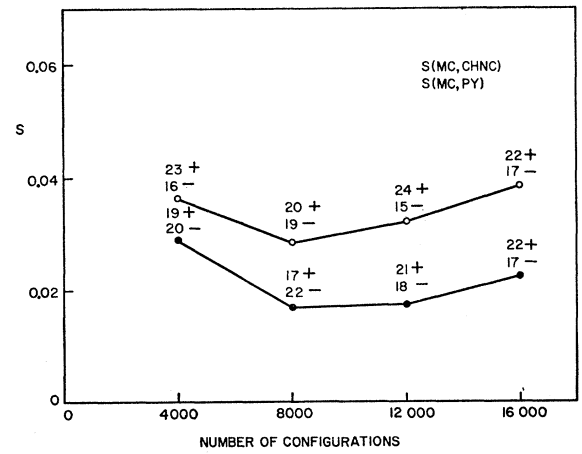

FIG. 7. The standard deviation between the Monte Carlo radial distribution function and PY and CHNC results, respectively, plotted as a function of the number of generated configurations for the $\rho=1.00$ case. The number preceding the plus (minus) sign indicates the number of times the MC point is above (below) the PY or CHNC point in the radial distribution curves. The upper curve is S(MC,PY).

TABLE IV. Radial distribution functions for $\rho=0.40$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0196	0.0195	0.0186	0.0198	0.0185	0.0198
0.20	0.0760	0.0756	0.0726	0.0768	0.0720	0.0768
0.30	0.1628	0.1620	0.1562	0.1645	0.1550	0.1643
0.40	0.2709	0.2696	0.2613	0.2735	0.2593	0.2727
0.50	0.3897	0.3881	0.3784	0.3934	0.3753	0.3914
0.60	0.5093	0.5078	0.4978	0.5146	0.4938	0.5105
0.70	0.6215	0.6204	0.6115	0.6292	0.6066	0.6218
0.80	0.7205	0.7206	0.7133	0.7317	0.7076	0.7198
0.90	0.8032	0.8052	0.7995	0.8190	0.7933	0.8018
1.00	0.8687	0.8733	0.8685	0.8902	0.8622	0.8671
1.10	0.9178	0.9256	0.9207	0.9457	0.9147	0.9166
1.20	0.9525	0.9638	0.9581	0.9868	0.9527	0.9524
1.30	0.9754	0.9901	0.9828	1.0154	0.9784	0.9768
1.40	0.9891	1.0069	0.9976	1.0337	0.9945	0.9925
1.50	0.9961	1.0165	1.0050	1.0437	1.0036	1.0015
1.60	0.9987	1.0207	1.0073	1.0475	1.0078	1.0060
1.70	0.9985	1.0211	1.0064	1.0468	1.0089	1.0076
1.80	0.9970	1.0191	1.0036	1.0430	1.0083	1.0074
1.90	0.9950	1.0158	1.0000	1.0375	1.0067	1.0062
2.00	0.9932	1.0117	0.9962	1.0311	1.0050	1.0048
2.40	0.9922	0.9963	0.9853	1.0067	1.0003	1.0005
2.80	0.9983	0.9886	0.9828	0.9932	0.9996	0.9997
3.20	1.0044	0.9876	0.9851	0.9893	0.9999	0.9999

The results discussed above indicate that the PY and CHNC integral equations provide reasonable answers for g for densities at least to $\rho=1.00$. In the light of this conclusion, it is interesting to compare E4, PY4, CHNC4, PY, and CHNC at intermediate densities (see Tables IV–VII). The differences between E4, PY4, and CHNC4, respectively, are in many instances

TABLE V. Radial distribution functions for $\rho=0.50$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0216	0.0213	0.0203	0.0218	0.0199	0.0217
0.20	0.0836	0.0824	0.0790	0.0843	0.0774	0.0841
0.30	0.1784	0.1759	0.1695	0.1800	0.1661	0.1790
0.40	0.2949	0.2912	0.2825	0.2980	0.2768	0.2951
0.50	0.4212	0.4165	0.4071	0.4268	0.3988	0.4202
0.60	0.5460	0.5412	0.5326	0.5562	0.5216	0.5431
0.70	0.6603	0.6571	0.6502	0.6780	0.6368	0.6555
0.80	0.7583	0.7586	0.7533	0.7871	0.7379	0.7521
0.90	0.8372	0.8433	0.8382	0.8806	0.8217	0.8307
1.00	0.8967	0.9107	0.9040	0.9575	0.8873	0.8914
1.10	0.9382	0.9620	0.9513	1.0180	0.9356	0.9360
1.20	0.9646	0.9990	0.9829	1.0629	0.9689	0.9670
1.30	0.9789	1.0239	1.0013	1.0937	0.9903	0.9872
1.40	0.9843	1.0388	1.0096	1.1120	1.0026	0.9993
1.50	0.9839	1.0460	1.0109	1.1198	1.0086	1.0057
1.60	0.9801	1.0472	1.0074	1.1192	1.0104	1.0082
1.70	0.9750	1.0439	1.0011	1.1122	1.0098	1.0084
1.80	0.9701	1.0376	0.9935	1.1007	1.0081	1.0073
1.90	0.9662	1.0295	0.9856	1.0865	1.0060	1.0057
2.00	0.9641	1.0203	0.9781	1.0708	1.0040	1.0041
2.40	0.9732	0.9860	0.9573	1.0124	0.9998	1.0000
2.80	0.9973	0.9676	0.9529	0.9791	0.9996	0.9996
3.20	1.0172	0.9659	0.9597	0.9701	1.0000	0.9999

quite large (see Fig. 8) thus indicating relatively large errors in the PY and CHNC approximations to g_2, g_3, and g_4. However, the PY and CHNC results are nearly the same at these densities and, in light of the MC calculation, are probably very close to the true g. Thus, there must be a cancellation of errors among the contributions from the various density terms. It is, therefore, not always possible to judge the merit of the approximation by looking at the diagrams omitted by the first few terms of the density expansion. For the "Gaussian model" the CHNC and PY approximations seem to be much better than superficial inspection of the first few g_n would indicate.

TABLE VI. Radial distribution functions for $\rho=0.60$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0238	0.0230	0.0222	0.0238	0.0213	0.0237
0.20	0.0920	0.0890	0.0861	0.0921	0.0826	0.0913
0.30	0.1954	0.1892	0.1844	0.1963	0.1767	0.1933
0.40	0.3213	0.3118	0.3063	0.3244	0.2933	0.3165
0.50	0.4557	0.4439	0.4394	0.4644	0.4206	0.4470
0.60	0.5859	0.5741	0.5721	0.6057	0.5472	0.5730
0.70	0.7023	0.6943	0.6943	0.7405	0.6641	0.6856
0.80	0.7986	0.7994	0.7992	0.8639	0.7648	0.7801
0.90	0.8721	0.8872	0.8832	0.9727	0.8464	0.8550
1.00	0.9229	0.9578	0.9454	1.0652	0.9084	0.9112
1.10	0.9531	1.0121	0.9871	1.1402	0.9525	0.9511
1.20	0.9662	1.0517	1.0116	1.1970	0.9816	0.9778
1.30	0.9662	1.0781	1.0219	1.2356	0.9990	0.9944
1.40	0.9573	1.0930	1.0215	1.2568	1.0080	1.0037
1.50	0.9435	1.0981	1.0139	1.2623	1.0114	1.0080
1.60	0.9283	1.0951	1.0016	1.2543	1.0114	1.0091
1.70	0.9142	1.0856	0.9867	1.2356	1.0097	1.0084
1.80	0.9033	1.0714	0.9709	1.2092	1.0073	1.0068
1.90	0.8967	1.0540	0.9554	1.1778	1.0049	1.0050
2.00	0.8950	1.0349	0.9409	1.1440	1.0029	1.0033
2.40	0.9312	0.9630	0.9010	1.0193	0.9994	0.9997
2.80	0.9984	0.9247	0.8933	0.9488	0.9996	0.9997
3.20	1.0503	0.9226	0.9096	0.9316	1.0000	1.0000

TABLE VII. Radial distribution functions for $\rho=0.70$.

x	E5	E4	PY4	CHNC4	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0264	0.0247	0.0244	0.0260	0.0226	0.0256
0.20	0.1018	0.0953	0.0946	0.1006	0.0875	0.0982
0.30	0.2154	0.2022	0.2021	0.2144	0.1867	0.2070
0.40	0.3524	0.3320	0.3347	0.3552	0.3088	0.3367
0.50	0.4968	0.4712	0.4785	0.5106	0.4409	0.4721
0.60	0.6339	0.6084	0.6201	0.6706	0.5708	0.6002
0.70	0.7528	0.7355	0.7487	0.8280	0.6889	0.7124
0.80	0.8464	0.8481	0.8566	0.9780	0.7888	0.8044
0.90	0.9116	0.9444	0.9400	1.1165	0.8679	0.8754
1.00	0.9485	1.0241	0.9983	1.2395	0.9263	0.9273
1.10	0.9598	1.0875	1.0331	1.3429	0.9663	0.9629
1.20	0.9500	1.1349	1.0483	1.4228	0.9914	0.9859
1.30	0.9246	1.1666	1.0473	1.4767	1.0053	0.9995
1.40	0.8898	1.1832	1.0343	1.5038	1.0114	1.0064
1.50	0.8516	1.1858	1.0131	1.5053	1.0127	1.0091
1.60	0.8153	1.1758	0.9868	1.4842	1.0114	1.0092
1.70	0.7850	1.1555	0.9580	1.4446	1.0088	1.0079
1.80	0.7638	1.1271	0.9286	1.3917	1.0061	1.0060
1.90	0.7533	1.0933	0.9001	1.3300	1.0037	1.0042
2.00	0.7540	1.0565	0.8736	1.2643	1.0018	1.0025
2.40	0.8501	0.9188	0.8007	1.0250	0.9992	0.9996
2.80	1.0067	0.8473	0.7883	0.8926	0.9997	0.9997
3.20	1.1227	0.8467	0.8224	0.8634	1.0000	1.0000

TABLE VIII. Radial distribution functions for $\rho=0.80$, $\rho=0.90$, and $\rho=1.00$.

	$\rho=0.80$		$\rho=0.90$		$\rho=1.00$	
x	PY	CHNC	PY	CHNC	PY	CHNC
0.00	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0238	0.0274	0.0250	0.0292	0.0262	0.0310
0.20	0.0922	0.1050	0.0966	0.1117	0.1009	0.1181
0.30	0.1962	0.2202	0.2053	0.2329	0.2139	0.2452
0.40	0.3235	0.3560	0.3373	0.3743	0.3505	0.3917
0.50	0.4599	0.4955	0.4777	0.5174	0.4945	0.5378
0.60	0.5926	0.6252	0.6128	0.6481	0.6316	0.6691
0.70	0.7115	0.7364	0.7321	0.7580	0.7511	0.7773
0.80	0.8103	0.8256	0.8296	0.8441	0.8470	0.8604
0.90	0.8867	0.8927	0.9033	0.9075	0.9178	0.9201
1.00	0.9415	0.9404	0.9545	0.9513	0.9656	0.9602
1.10	0.9776	0.9722	0.9869	0.9796	0.9944	0.9854
1.20	0.9990	0.9919	1.0048	0.9965	1.0093	0.9998
1.30	1.0097	1.0029	1.0128	1.0053	1.0147	1.0069
1.40	1.0134	1.0081	1.0144	1.0090	1.0147	1.0094
1.50	1.0131	1.0095	1.0128	1.0095	1.0121	1.0093
1.60	1.0107	1.0089	1.0097	1.0084	1.0085	1.0078
1.70	1.0077	1.0072	1.0065	1.0065	1.0052	1.0058
1.80	1.0049	1.0053	1.0037	1.0045	1.0026	1.0038
1.90	1.0026	1.0034	1.0016	1.0028	1.0008	1.0022
2.00	1.0010	1.0019	1.0003	1.0014	0.9997	1.0010
2.40	0.9992	0.9994	0.9992	0.9994	0.9993	0.9994
2.80	0.9998	0.9997	0.9999	0.9999	1.0000	0.9998
3.20	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000

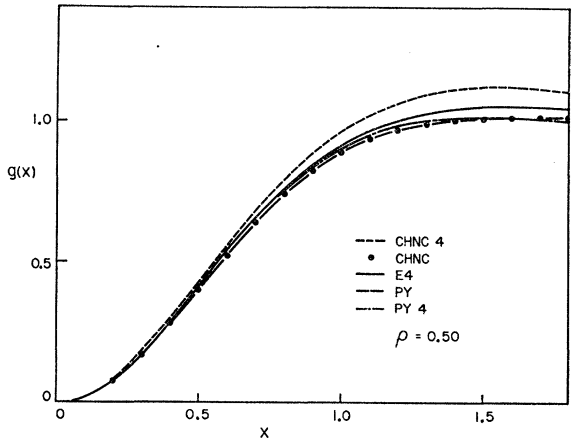

FIG. 8. The radial distribution functions for $\rho=0.50$.

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