

## Coulomb Self-Energy of Axial Figures\*

ROBERT BERINGER

*Department of Physics, Yale University, New Haven, Connecticut*

(Received 5 April 1963)

A new method of computing the Coulomb self-energy of uniform axial figures is developed. The energy is expressed as a sum of slice-slice interactions plus the self-energy of each slice. Analytical formulas are derived for these energies and are presented in numerical tables. The method is tested numerically by comparing its results with the exact self-energies of certain simple figures.

THE problem of the self-energy of an extended body due to the gravitational attraction or electrostatic repulsion of its matter is very old. Beginning with Newton, Clairaut, and Maclaurin the subject<sup>1</sup> was developed in connection with the figure of the earth and the equilibrium shapes of rotating, gravitating liquid masses.<sup>2</sup> In this study the Maclaurin spheroids and Jacobi ellipsoids were found to be the stable shapes for low angular momentum, and for these figures the self-energy was integrated. Indeed, to this day, uniform ellipsoids are the only solid figures for which an exact self-energy formula is known. In this early period the Legendre expansion for distorted-sphere potentials was also developed. At the turn of this century Poincaré, Darwin, Liapounov, and Jeans studied the "pear-shaped" figure which terminates the stability of the Jacobi shapes for high angular momentum. In this they used Lamé expansions for the distorted-ellipsoid potential.

In recent times the same problem has been studied extensively in connection with the liquid-drop model of nuclear fission.<sup>3</sup> The same expansion techniques were used to find the Coulomb self-energies of Legendre-distorted spheres and spheroids.<sup>3,4</sup>

We are not concerned here with the successes or failures of liquid-drop calculations in explaining fission but only with the accuracy of those Coulomb self-energy calculations which use expansion techniques; yet even this is difficult to assess. The formulas themselves, which are power series in the distortion parameters, show very slow apparent convergence even for rather small distortions. In addition, there are unanswered questions on the convergence of the method because of difficulties in determining the perturbed

potential. In the fission literature this is not seriously investigated<sup>5</sup> although the distortions of interest are frequently large, whereas in the gravitational stability studies<sup>2</sup> small distortions sufficed and terms beyond the second order in the expansion coefficients were not required. Even so, the history of the pear-shaped figures records several mistakes arising from convergence difficulties. It should also be noted that the prediction of fission saddle points and trajectories requires very high accuracy in the self-energy calculations because of the partial cancellation of the Coulomb and surface-tension distortion energies.

These impressions, formed during attempts<sup>6</sup> to study liquid-drop equilibrium shapes for nuclei with high angular momentum, led me to examine a different method of calculating Coulomb self-energies. This method, named the *slice method*, is applicable to any uniform solid body which is a figure of revolution and is slicable into circles.

### THE SLICE METHOD

Consider a uniformly charged body which is a figure of revolution around the  $z$  axis. Suppose it to be cut by planes perpendicular to  $z$  into  $N$  circular slices each of thickness  $\Delta$ . With no approximation, the self-energy is given by the sum of the self-energies of the  $N$  slices plus the sum of the interaction energies of each pair of slices. Now replace each slice by a flat, circular cylinder of height  $\Delta$  and radius equal to some average radius of the slice. To some approximation its self-energy is equal to that of the slice. In the slice-slice interaction the same cylinders may be used or in a cruder approximation each slice can be replaced by a midplane disk onto which the total slice charge is uniformly spread. To some approximation the cylinder-cylinder (or disk-disk) interaction energy equals the true slice-slice interaction energy.

In order to compute the cylinder self-energies and the interaction energies only one basic formula is needed; a formula which gives the interaction energy of two uniform disks. All other energies are integrals of this interaction. When this formula is obtained the accuracy of the slice method can be tested with spheres, spheroids, and sets of nonintersecting spheres. Of

\* Supported in part by the U. S. Atomic Energy Commission.

<sup>1</sup> I. Todhunter, *A History of Mathematical Theories of Attraction* (MacMillan and Company Ltd., London, 1873; reprint, Dover Publications, Inc., New York, 1962).

<sup>2</sup> Reviews of this problem appear in: J. H. Jeans, *Problems of Cosmogony and Stellar Dynamics* (Cambridge University Press, New York, 1919); R. A. Lyttleton, *The Stability of Rotating Liquid Masses* (Cambridge University Press, New York, 1953); W. S. Jardetsky, *Theories of Figures of Celestial Bodies* (Interscience Publishers, Inc., New York, 1958).

<sup>3</sup> N. Bohr and J. A. Wheeler, *Phys. Rev.* **56**, 426 (1939).

<sup>4</sup> Many papers using Legendre distortions in Coulomb self-energy calculations have been published since N. Bohr and J. A. Wheeler. The most complete is that of W. J. Swiatecki, in *Proceedings of the Second United Nations International Conference on the Peaceful Uses of Atomic Energy, Geneva, 1958* (United Nations, Geneva, 1958), Vol. 15, p. 651.

<sup>5</sup> It is, however, noted by Swiatecki (Ref. 4).

<sup>6</sup> R. Beringer and W. J. Knox, *Phys. Rev.* **121**, 1195 (1961).

course, with very large  $N$  the method will be accurate, but since the number of interaction terms is  $\frac{1}{2}N(N-1)$  the calculation will become very laborious. The practical question is whether the errors are small for moderate values of  $N$ . We guessed that the total error would be small because of compensating errors in the geometry of the method, and this is the fact.

It is clear that the slice method amounts to nothing more than a particular arrangement of the double summation which defines the self-energy. It would not have appeared attractive or even reasonable before the era of high-speed computers. On the other hand, the method is completely general. Results are as easily obtained for one figure as for another and the accuracy should have little dependence on the shape of the figure.

THE DISK-DISK INTERACTION

The interaction energy of two coaxial and parallel disks of radii  $R_1$  and  $R_2$ , uniform surface charge densities  $\sigma_1$  and  $\sigma_2$ , and spacing  $L$  is obtained by integrating the potential due to one disk over the charge on the other. Considering the larger disk, No. 1, as the source, the well-known potential convergent inside the hemisphere  $r \leq R_1, \theta \leq \frac{1}{2}\pi$  is

$$V(r, \theta) = 2\pi\sigma_1 R_1 \left\{ 1 - \frac{r}{R_1} P_1(\cos\theta) + \sum_{n=1}^{\infty} C_{2n} \left(\frac{r}{R_1}\right)^{2n} P_{2n}(\cos\theta) \right\},$$

where  $r$  is measured from the center of disk,  $C_{2n}$  are the binomial coefficients of  $x^{2n}$  in the expansion of  $(1+x^2)^{1/2}$ , and  $P_{2n}(\cos\theta)$  are the Legendre polynomials. The interaction energy of the two disks is

$$E_c(\text{disk-disk}) = \int_0^{\tan^{-1}(R_2/L)} V(r, \theta) 2\pi\sigma_2 L^2 \sin\theta \cos^{-3}\theta d\theta,$$

which can be integrated term-by-term to give a power series in  $R_2/L$  with coefficients which are themselves power series in  $L/R_1$ . When this expression is rearranged as a series in ascending powers of  $R_2/R_1$ , the coefficients of these terms are recognized as products of binomial coefficients and hypergeometric series,

$$E_c(\text{disk-disk}) = 4\pi^2\sigma_1\sigma_2 R_1^3 \left\{ -\frac{k}{2}g^2 + \sum_{n=0}^{\infty} \frac{g^{2n+2}}{2(n+1)} \times C_{2n} P_{2n}(0) F\left(n+\frac{1}{2}, n-\frac{1}{2}, \frac{1}{2}, -k^2\right) \right\},$$

where  $k=L/R_1, g=R_2/R_1$ , and  $F(a, b, c, -k^2)$  are hypergeometric series.<sup>7</sup> The series can be transformed to hypergeometric polynomials and the resulting

expression written as,

$$E_c(\text{disk-disk}) = 4\pi^2\sigma_1\sigma_2 R_1^3 \left\{ -\frac{k}{2}g^2 + \sum_{n=0}^{\infty} \frac{g^{2n+2}(1+k^2)^{-2n-\frac{1}{2}}}{2(n+1)} \times C_{2n} P_{2n}(0) F\left(-n, -n+1, \frac{1}{2}, -k^2\right) \right\}.$$

This formula has several virtues: (a) By its arrangement in powers of  $g$ , the coefficients of the series are polynomials in  $k^2$  and thus exact. (b) The formula converges to the correct value not only within the hemisphere but for all  $R_2 < R_1$  and, thus, a separate far-field solution is not needed. (c) The formula is convenient for high-speed computers.

The convergence is very rapid for  $k > 0$  if  $g < 1$ . Only in the region  $k \sim 0, g \sim 1$  is the convergence slow. However, the value of  $E_c$  at  $k=0, g=1$  is known from the analytic solution of the self-energy of a single disk<sup>8</sup> which may be thought of as the self-energies of two coincident disks plus their interaction energy. This gives

$$E_c(\text{disk-disk}) = (16\pi/3)\sigma_1\sigma_2 R_1^3$$

for  $k=0, g=1$ .

The disk-disk interaction energy has been calculated for various  $g$  and  $k$  by hand and with electronic computers. A short table of the interaction function  $E(k, g) = E_c/4\pi^2\sigma_1\sigma_2 R_1^3$  is given in Table I.

THE FLAT-CYLINDER SELF-ENERGY

For extremely flat cylinders the self-energy is that of a single disk,  $(8\pi/3)\sigma^2 R^3$ , but for cylinders of finite height it is smaller. An accurate value can be calculated with the disk-disk interaction formula. This is conveniently carried out by fitting an integrable function to  $E(k, 1)$  and performing the double integration

$$E_c(\text{cyl}) = 4\pi^2\rho^2 R^5 \int_0^{\Delta/R} \int_0^p E(k, 1) dk d\rho,$$

where  $\rho$  is the volume charge density,  $R$  the cylinder radius, and  $\Delta$  its height. It was found that a fit with a maximum residual of 0.01% in the range  $0 \leq k \leq 0.5$  could be arranged with the semiempirical formula

$$E(k, 1) = \frac{4}{3\pi} - \frac{1}{2}k + Bk^2 - Ak^2 \ln k,$$

where  $B=0.257729, A=0.155241$  were determined by

<sup>7</sup> E. T. Whittaker and G. N. Watson, *Modern Analysis* (Cambridge University Press, New York, 1958), Chap. XIV.

<sup>8</sup> A. S. Ramsey, *Theory of Newtonian Attraction* (Cambridge University Press, New York, 1940).

TABLE I. The (disk-disk) interaction function  $E(k, g)$ . The larger disk is of radius  $R_1$  and the smaller of radius  $R_2$ .  
 $k = \text{disk separation}/R_1$ ,  $g = R_2/R_1$ .

$\frac{g}{k}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0	0.004994	0.019899	0.044488	0.078366	0.120961	0.171486	0.228893	0.291764	0.358092	0.424413
0.1	0.004519	0.018001	0.040220	0.070792	0.109153	0.154540	0.205942	0.262025	0.321016	0.380594
0.2	0.004093	0.016301	0.036410	0.064052	0.098699	0.139643	0.185971	0.236538	0.289965	0.344746
0.3	0.003715	0.014792	0.033033	0.058101	0.089514	0.126639	0.168686	0.214710	0.263649	0.314425
0.4	0.003380	0.013460	0.030060	0.052876	0.081480	0.115322	0.153730	0.195931	0.241090	0.288378
0.5	0.003086	0.012289	0.027449	0.048299	0.074464	0.105471	0.140755	0.179681	0.221574	0.265771
0.6	0.002827	0.011261	0.025160	0.044292	0.068333	0.096880	0.129457	0.165536	0.204564	0.245994
0.7	0.002600	0.010358	0.023153	0.040781	0.062966	0.089365	0.119575	0.153155	0.189643	0.228579
0.8	0.002400	0.009565	0.021389	0.037697	0.058254	0.082765	0.110891	0.142259	0.176478	0.213159
0.9	0.002224	0.008866	0.019835	0.034981	0.054102	0.076946	0.103226	0.132623	0.164804	0.199436
1.0	0.002069	0.008249	0.018462	0.032580	0.050429	0.071794	0.096428	0.124059	0.154403	0.187168
1.1	0.001931	0.007702	0.017245	0.030449	0.047166	0.067212	0.090373	0.116416	0.145094	0.176154
1.2	0.001809	0.007215	0.016161	0.028551	0.044257	0.063120	0.084956	0.109564	0.136728	0.166228
1.3	0.001699	0.006780	0.015192	0.026853	0.041652	0.059451	0.080092	0.103397	0.129181	0.157248
1.4	0.001601	0.006390	0.014322	0.025328	0.039310	0.056148	0.075705	0.097826	0.122347	0.149096
1.5	0.001513	0.006038	0.013539	0.023953	0.037196	0.053163	0.071734	0.092774	0.116137	0.141671
1.6	0.001433	0.005721	0.012831	0.022709	0.035281	0.050456	0.068128	0.088177	0.110475	0.134888
1.7	0.001361	0.005433	0.012188	0.021579	0.033540	0.047992	0.064841	0.083980	0.105298	0.128672
1.8	0.001295	0.005171	0.011603	0.020549	0.031952	0.045742	0.061835	0.080137	0.100549	0.122960
1.9	0.001235	0.004932	0.011068	0.019608	0.030499	0.043681	0.059078	0.076608	0.096180	0.117697
2.0	0.001180	0.004712	0.010578	0.018744	0.029165	0.041787	0.056542	0.073357	0.092151	0.112836
2.5	0.000963	0.003846	0.008640	0.015325	0.023875	0.034258	0.046435	0.060361	0.075988	0.093262
3.0	0.000811	0.003242	0.007286	0.012932	0.020162	0.028958	0.039293	0.051141	0.064470	0.079245
3.5	0.000700	0.002799	0.006292	0.011171	0.017427	0.025044	0.034007	0.044298	0.055895	0.068774
4.0	0.000615	0.002461	0.005532	0.009826	0.015333	0.022045	0.029950	0.039035	0.049285	0.060685
4.5	0.000549	0.002194	0.004935	0.008765	0.013682	0.019677	0.026743	0.034869	0.044046	0.054262
5.0	0.000495	0.001980	0.004452	0.007909	0.012348	0.017763	0.024148	0.031495	0.039798	0.049047
6.0	0.000414	0.001655	0.003722	0.006614	0.010328	0.014861	0.020210	0.026371	0.033338	0.041107
7.0	0.000355	0.001421	0.003197	0.005681	0.008872	0.012769	0.017369	0.022670	0.028667	0.035359
8.0	0.000311	0.001245	0.002801	0.004978	0.007775	0.011191	0.015225	0.019874	0.025137	0.031010
9.0	0.000277	0.001108	0.002492	0.004429	0.006918	0.009958	0.013549	0.017689	0.022376	0.027609
10.0	0.000249	0.000997	0.002244	0.003988	0.006231	0.008970	0.012205	0.015935	0.020160	0.024876
15.0	0.000166	0.000666	0.001498	0.002663	0.004161	0.005991	0.008153	0.010647	0.013473	0.016630
20.0	0.000125	0.000500	0.001124	0.001998	0.003122	0.004496	0.006119	0.007992	0.010113	0.012484

least squares. The integration gives

$$E_c(\text{cyl}) = \frac{8\pi}{3} \rho^2 \Delta^2 R^3 \left\{ 1 - \frac{\pi}{8} \left( \frac{\Delta}{R} \right) + \frac{\pi}{8} \left( \frac{\Delta}{R} \right)^2 \left[ B + \frac{7}{12} A - A \ln \frac{\Delta}{R} \right] \right\}.$$

The terms following unity are corrections to the disk value. This  $E_c(\text{cyl})$  formula is believed to be accurate to 0.005% in the range  $0 \leq \Delta/R \leq 0.5$ .

#### CALCULATIONS WITH THE DISK-DISK INTERACTION

In the simplest slice-method calculation the disk-disk interaction replaces the true interaction. As indicated earlier, the calculation consists in (a) slicing the figure into  $N$  slices of equal height  $\Delta$ , (b) evaluating the self-energy of each slice by replacing it with a cylinder whose volume is that of the slice, (c) adding to this the interaction energy of each pair of midplane disks having charge density  $\sigma = \rho\Delta$  and the radii of (b). In step (c) it is convenient to evaluate the interaction terms in order  $i$  starting at one end of the figure and

to include an interaction with disk  $j$  if  $R_i > R_j$ . This automatically counts each interaction only once.

It should be mentioned that with the method as described no volume or charge renormalization is required. In some early calculations midplane radii were used for the disks and cylinders, but no simple and accurate volume renormalization of the final answer was possible.

In our earliest calculations we used tabular values of  $E(k, g)$ , but it was not possible to find simple formulas for the two-dimensional interpolation. In the calculations reported here each interaction term was computed for the  $k$  and  $g$  values which occurred. A complete calculation of  $E_c$  for forty slices takes about thirty seconds on an IBM-7090 computer.

Table II lists results for the sphere and other figures for which exact analytical answers are known. It is seen that the accuracy improves fairly rapidly with the number of slices [the errors vary quite accurately as  $1/(N-1)$ ] but for a given number of slices the errors are higher for figures which are long in the axial direction. Also, all of the computed answers are low.

There are several inherent sources of error in the slice method and particularly in the approximation which uses disk-disk interactions. These errors were

studied for the figures of Table II and for other figures, in particular, cylinders within the range of validity of our  $E_c(\text{cyl})$  formula. It was concluded that for  $N \geq 20$  the predominant source of error is the disk-disk approximation to the slice-interaction energy. Errors arising from the replacement of the slice by a cylinder are much smaller. To improve the calculation an interaction-energy formula for flat cylinders was developed.

### THE CYLINDER-CYLINDER INTERACTION

The interaction energy of two parallel and coaxial cylinders of radii  $R_1$  and  $R_2$ , thickness  $\Delta$ , uniform volume-charge density  $\rho$ , and midplane spacing  $m\Delta = k_0 R_1$  can be found by a double integration of the disk-interaction function  $E(k, g)$

$$E_c(\text{cyl-cyl}) = 4\pi^2 \rho^2 R_1^5 \int_0^{\Delta/R_1} \int_{k_0+p-\Delta/R_1}^{k_0+p} E(k, g) dk dp.$$

The integration can be performed formally and results in a correction to  $E_c(\text{disk-disk})$  which can be arranged as a power series in  $\Delta/R_1 = k_0/m$ . The same formula is obtained more easily by the double integration of  $E(k, g)$  written as a Taylor expansion around  $(k_0, g)$ . The resulting formula is

$$E_c(\text{cyl-cyl}) = 4\pi^2 \sigma^2 R_1^3 \left\{ E(k_0, g) + \frac{1}{2 \times 3 \times 2!} \left( \frac{k_0}{m} \right)^2 \left( \frac{\partial^2 E}{\partial k^2} \right)_{k_0} + \frac{1}{3 \times 5 \times 4!} \left( \frac{k_0}{m} \right)^4 \left( \frac{\partial^4 E}{\partial k^4} \right)_{k_0} + \dots \right\},$$

where  $\sigma$  is the disk charge density,  $\sigma = \rho\Delta$ . The deriva-

TABLE II. Self-energy calculations with the (disk-disk) interaction. All figures have unit charge and the volume of the unit sphere.  $N$  is the number of slices. Flat-cylinder energies were computed with the volume-average radius. The (disk-disk) interactions used these same radii. In the (disk-disk) interactions the series terms in  $E(k, g)$  were computed until two successive terms were less than  $10^{-7}$  or until  $n=50$  was reached.

Figure	$N$	$E_c$	Error
Sphere	10	0.596335	-0.611%
	20	0.598948	-0.175
	30	0.599508	-0.082
	40	0.599715	-0.047
Two equal, touching spheres	20	0.533921	-0.288%
	40	0.534999	-0.087
Prolate spheroid of 2:1 axis ratio	10	0.566265	-1.482%
	20	0.572193	-0.451
	30	0.573545	-0.216
	40	0.574059	-0.126
Oblate spheroid of 2:1 axis ratio	10	0.575077	-0.133%
	20	0.575612	-0.041
	30	0.575734	-0.019
	40	0.575779	-0.011

TABLE III. Self-energy calculations with the (cyl-cyl) interaction. The figures and procedures are the same as for Table II. The columns list calculated self-energies and errors with two different degrees of approximation to the true (cyl-cyl) interaction.

Figure	$N$	Including $\partial^2 E / \partial k^2$ terms		Including $\partial^2 E / \partial k^2$ and $\partial^4 E / \partial k^4$ terms	
		$E_c$	Error (%)	$E_c$	Error (%)
Sphere	10	0.598501	-0.250	0.598512	-0.248
	20	0.599602	-0.066	0.599606	-0.066
	30	0.599819	-0.030	0.599821	-0.030
	40	0.599897	-0.017	0.599897	-0.017
Two equal, touching spheres	20	0.535289	-0.0332	0.535294	-0.0323
	40	0.535411	-0.0103	0.535414	-0.0098
Prolate spheroid of 2:1 axis ratio	10	0.571838	-0.513	0.571800	-0.519
	20	0.574028	-0.132	0.574040	-0.130
	30	0.574446	-0.059	0.574448	-0.059
	40	0.574593	-0.033	0.574597	-0.033
Oblate spheroid of 2:1 axis ratio	10	0.575751	-0.0163	0.575756	-0.0155
	20	0.575807	-0.0067	0.575807	-0.0067
	30	0.575825	-0.0035	0.575825	-0.0035
	40	0.575832	-0.0022	0.575832	-0.0022

tives yield hypergeometric polynomials which can be transformed into those already appearing in the disk-disk interaction, and the resulting formula is no more difficult for calculation than the disk-disk interaction formula. Including terms in  $\partial^2 E / \partial k^2$ ,

$$E_c(\text{cyl-cyl}) = 4\pi^2 \sigma^2 R_1^3 \left\{ -\frac{1}{2} k g^2 + \frac{1}{2} (1+k^2)^{1/2} g^2 + \sum_{n=1}^{\infty} C_{2n} P_{2n}(0) \left[ \frac{g^{2n+2}}{2(n+1)} - \frac{n g^{2n} k^2}{6 m^2} \right] \times (1+k^2)^{-2n+1/2} F(-n, -n+1, \frac{1}{2}, -k^2) \right\},$$

or including terms in  $\partial^2 E / \partial k^2$  and  $\partial^4 E / \partial k^4$ ,

$$E_c(\text{cyl-cyl}) = 4\pi^2 \sigma^2 R_1^3 \left\{ -\frac{1}{2} k g^2 + \frac{1}{2} (1+k^2)^{1/2} g^2 - (1+k^2)^{-3/2} g^4 \left[ \frac{1}{16} - \frac{1}{24} \frac{k^2}{g^2 m^2} \right] + \sum_{n=2}^{\infty} C_{2n} P_{2n}(0) \times \left[ \frac{g^{2n+2}}{2(n+1)} - \frac{n g^{2n} k^2}{6 m^2} + \frac{n^2(n-1)}{45} \frac{k^4}{g^{2n-2} m^4} \right] \times (1+k^2)^{-2n+1/2} F(-n, -n+1, \frac{1}{2}, -k^2) \right\}.$$

The procedure can be extended to higher order derivatives but we have not found it useful to do so.

Slice-method calculations with the (cyl-cyl) interaction are considerably more accurate than those with the (disk-disk) interaction. Table III lists results for the figures used in Table II. As in Table II the errors vary inversely as the number of interactions but the shape-dependent errors of Table II have been reduced.

## DISCUSSION

As now developed, the slice method is accurate enough for studies in liquid-drop nuclear fission. This is being done and preliminary results will be published shortly. With its extension to elliptical disks the method should also be useful for further calculations of the equilibrium shapes of liquid-drop nuclei with high angular momentum<sup>6,9</sup> and for the dynamics of close binary stars.

<sup>9</sup>B. C. Carlson and Pao Lu, in *Proceedings of the Rutherford Jubilee International Conference, Manchester, 1961*, edited by J. B. Berks (Academic Press Inc., New York, 1961).

## ACKNOWLEDGMENTS

It is a pleasure to acknowledge the invaluable assistance of Joseph N. Vitale who programmed and computed, at the Yale Computer Center, all of the results of Tables II and III and numerous other studies of the slice method mentioned in the text. I also thank Lois Frampton for programming the early work which appears in Table I. I also thank Professor R. L. Gluckstern who assisted in the analysis which led to the disk-disk interaction formula.

## Computations of Radial Distribution Functions for a Classical Electron Gas\*

DAVID D. CARLEY

*University of Florida, Gainesville, Florida*

(Received 5 April 1963)

The radial distribution functions  $g$  for a classical electron gas computed using the Percus-Yevick (PY) equation, convolution hypernetted chain (CHNC) equation, and the Broyles-Sahlin (BS) method, have been compared with the Debye-Hückel (DH) theory. The quantities  $E \equiv \bar{U}/NkT$  and  $P \equiv p/\bar{n}kT$  have been computed from these  $g$ 's. Computations have been made for values of  $\theta$  of 20, 10, 5, 3, and 1;  $\theta = ka/q^2$ , where  $a$  is the ion sphere radius. The PY and BS results show the best agreement, particularly at  $\theta < 3$ . The BS method has been of particular value in this study of a long-range potential. In the range of  $\theta$  studied,  $g$  never exceeds one, that is, there is no oscillatory behavior of  $g$ .

## I. INTRODUCTION

IN a classical one-component fluid having an average number density  $\bar{n} = N/V$ , where  $N$  is the number of particles and  $V$  the volume, the average number density  $n(r)$  about a given particle is, in general, not constant. The radial distribution function  $g(r)$  is the factor by which  $n(r)$  differs from  $\bar{n}$  and is defined by  $n(r) = \bar{n}g(r)$ . As a result of the Maxwell-Boltzmann classical distribution law,  $g(r)$  may be written, in the limit as  $N$  approaches infinity, as<sup>1</sup>

$$g(r) = V^2 Z^{-1} \int \dots \int_V e^{-U/kT} dr_3 \dots dr_N, \quad (1)$$

$$Z = \int \dots \int_V e^{-U/kT} dr_1 \dots dr_N,$$

where  $U$  is the potential energy. In the following,  $U$  will be assumed to be the sum of pair potentials  $\phi(r)$ .

The radial distribution function is important because thermodynamic quantities can be calculated once  $g(r)$

and  $\phi(r)$  are known. Of particular interest here are the relations for the pressure and mean potential energy,<sup>1</sup>

$$E \equiv \bar{U}/NkT = 2\pi\bar{n}(kT)^{-1} \int_0^\infty \phi(r)g(r)r^2 dr, \quad (2)$$

$$P \equiv p/\bar{n}kT = 1 - 2\pi\bar{n}(3kT)^{-1} \int_0^\infty r^3 g(r) \frac{d\phi(r)}{dr} dr. \quad (3)$$

$\bar{U}/N$ , the mean potential energy per particle, is often referred to as the correlation energy.

A direct evaluation of Eq. (1) to determine  $g$  is not practical and, consequently, several approximate methods have been developed; there are four methods which are of interest here. Using a collective coordinate technique Percus and Yevick<sup>2</sup> formed an integral equation (PY) for  $g$ . A second integral equation was obtained by a summation procedure of Mayer-type diagrams and has been given the name convolution hypernetted chain equation (CHNC).<sup>3</sup> A third method,

<sup>2</sup>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).

<sup>3</sup>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).

\* This research was supported in part by funds from the U. S. National Science Foundation.

<sup>1</sup>Terrell L. Hill, *Introduction to Statistical Thermodynamics* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1960).