and

$$
\begin{aligned}
h&=36\eta_1\eta_2(R_2-R_1)^2\,,\\
L_1(s)&=12\eta_2[(1+\tfrac{1}{2}\xi)+\tfrac{3}{2}\eta_1R_1^2(R_2-R_1)]R_2s^2\\
&\quad+[12\eta_2(1+2\xi)-hR_1]s+h\,,\\
S(s)&=h+[12(\eta_1+\eta_2)(1+2\xi)-h(R_1+R_2)]s\\
&\quad-18(\eta_1R_1^2+\eta_2R_2^2)^2s^2-6(\eta_1R_1^2+\eta_2R_2^2)\\
&\qquad\times(1-\xi)s^3-(1-\xi)^2s^4\,,
\end{aligned}
\tag{43}
$$

and $G_{22}(s)$, $L_2(s)$ can be found from $G_{11}(s)$ and $L_1(s)$ by interchanging η_1, R_1 with η_2, R_2. We may now verify explicitly our previous assumptions on $G_{ij}(s)$ as well as its correct behavior when η_1 or R_1 vanishes or $R_1=R_2$.

The pressure given in (39), which comes from the compressibility relation (13), yields correctly the first three virial coefficients,[15] i.e., coefficients of $\rho_1{}^l\rho_2{}^k$ for $l+k\leq 3$. It is also in very good agreement with the Monte-Carlo computations[16] of the pressure done for $R_1=\frac{3}{5}R_2$, $\rho_1=\rho_2$, $\xi<0.2$. The reduced volume of mixture is always negative which implies that there is no phase separation of the components.[17] The pressure may be obtained from $g_{ij}(r)$, in addition to the compressibility relation (13), also by use of the virial theorem. For a mixture of hard spheres this has the form,[18]

$$\beta p^v=\rho_1+\rho_2+\tfrac{2}{3}\pi\sum_{i,j}\rho_i\rho_jR_{ij}{}^3g_{ij}(R_{ij})\,. \tag{44}$$

For the correct g_{ij} the two relations, (13) and (44), will yield the same result. For our approximate g_{ij} we find from (40),

$$\beta p^v=\beta p-\frac{18}{\pi}\frac{\xi}{(1-\xi)^3}(\eta_1R_1^2+\eta_2R_2^2)^3\,, \tag{45}$$

where we continue to label the compressibility pressure (39) by p. The generalization of the above results to an m-component mixture of hard spheres is immediate. The generalization of Eqs. (39), (45), and (40) are

$$\beta p=\Big\{[\sum_{i=1}^m\rho_i][1+\xi+\xi^2]-\frac{18}{\pi}\sum_{i<j}\eta_i\eta_j(R_i-R_j)^2\times[2R_{ij}+R_iR_j(\sum\eta_lR_l^2)]\Big\}(1-\xi)^{-3}\,, \tag{46}$$

$$\beta p^v=\beta p-\frac{18\xi}{\pi}[\sum_{l=1}^m\eta_lR_l^2]^3(1-\xi)^{-3}\,,\quad \xi=\sum_{l=1}^m\eta_lR_l^3\,, \tag{47}$$

$$g_{ij}(R_{ij})=[R_jg_{ii}(R_i)+R_ig_{jj}(R_j)]/2R_{ij}\,, \tag{48}$$

$$g_{ii}(R_i)=\{(1-\xi)+\tfrac{3}{2}(\sum_{l=1}^m\eta_lR_l^2)R_i\}(1-\xi)^{-2}\,. \tag{49}$$

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I would like to thank M. Wertheim and J. K. Percus for many very valuable discussions, and Jim Steadman for help with some of the computations.

[15] A. G. McLellan and B. J. Alder, J. Chem. Phys. 24, 115 (1956).

[16] E. B. Smith and K. R. Lea, Nature 186, 714 (1960).

[17] I am indebted for the above results to Professor J. S. Rowlinson. Professor Rowlinson also obtained independently the pressure (39) for the case $R_1=0$.

[18] *Note added in proof.* B. J. Alder has kindly informed me that both p and p^v are in very good agreement (with p slightly above and p^v slightly below) with Monte-Carlo computations carried out by him and his co-workers for several values of R_2/R_1, ρ_2/ρ_1, and a large range of ξ.

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Simplified Approach to the Ground-State Energy of an Imperfect Bose Gas. II. Charged Bose Gas at High Density

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Foldy, and later Girardeau, calculated the ground-state energy of a charged Bose gas at high density. We rederive the common first term obtained by these authors by using a nonperturbation method developed previously. Our aims are: (i) to establish the validity of this common result, which has not been proved; (ii) to establish the validity and usefulness of our nonperturbation method. We also show that our method will give the correct functional dependence of the ground-state energy on the density at *low* density, although the exact coefficient must await a numerical computation.

I. INTRODUCTION

About two years ago Foldy[1] suggested investigating the charged Bose gas as a possible model for superconductivity and superfluidity. He derived formulas for the ground-state energy and elementary excitation spectrum of the system at high density (weak coupling constant) by applying Bogolyubov's well-known method.[2] Foldy derived the first two terms

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[1] L. L. Foldy, Phys. Rev. 124, 649 (1961) (hereafter referred to as F). See also Errata, *ibid.* 125, 2208 (1962).

[2] N. N. Bogolyubov, J. Phys. (U.S.S.R.) 11, 23 (1947). See also *The Many Body Problem*, edited by C. DeWitt (John Wiley & Sons, Inc., New York, 1959), p. 343.

in an asymptotic series for the ground-state energy, and conjectured that the first term at least was given correctly by Bogolyubov's formula—although no proof was offered to support this assertion. His result was

$$\text{Foldy:}\quad f\equiv E_0/(NR_H)=-0.803r_s^{-3/4}+0.213\,, \quad (1.1)$$

where E_0 is the ground-state energy, N is the number of particles, V is the volume, $\rho=N/V$ is the density, e is the particle charge, m is the particle mass, $R_H=me^4/2\hbar^2$ is a Rydberg, and $r_s=(3/4\pi\rho)^{1/3}e^2(m/\hbar^2)$ is the dimensionless coupling constant.

Girardeau[3] later recomputed the ground-state energy using the variational method of himself and Arnowitt.[4] He found

$$\text{Girardeau:}\quad f=-0.8037r_s^{-3/4}-\tfrac{1}{8}\ln r_s+O(1). \quad (1.2)$$

As far as the first term is concerned, Eqs. (1.1) and (1.2) agree, but this is not surprising since they are both derived from Bogolyubov's method. The reason the respective second terms disagree, and at the same time the reason Girardeau is probably more nearly correct, is the following: Foldy derived the second term by considering the difference between ρ and ρ_0 (the so-called ground-state depletion effect). He ignored, however, the expectation value of the quartic part of the many-body Hamiltonian. For the general short-range, finite potential, this quartic part will give a correction of the same order in the coupling constant as the ground-state depletion effect, and so in any event, ought to be included. But for the Coulomb potential it turns out that the expectation value of the quartic part in Bogolyubov's ground state contains a divergent integral. The dilemma is resolved by including the effect of the quartic part directly on the wave function (in the same manner that $\rho-\rho_0$ is usually incorporated into the wave function) with the result that the divergence gives place to a $\ln r_s$ term as found by Girardeau.

Thus, in order to calculate the second term consistently within the framework of the Bogolyubov method, one should include *all* so-called pair terms in the effective Hamiltonian. This program has already been carried out by Luban.[5] It is unfortunate that even the pair Hamiltonian cannot be diagonalized exactly because it is quartic, but Luban quotes a theorem of Wentzel[6] to the effect that the free energy (which at $T=0$ is the ground-state energy) can be calculated exactly in the limit of a large system by using the self-consistent procedure which is at the heart of the Bogolyubov method.

Although Luban did not actually calculate the ground-state energy for any specific system, it is clear that his integral equations are the same as in Girardeau's calculation. In short, Girardeau's result, Eq. (1.2), has a doubly validity. On the one hand, it is the correct solution of the pair Hamiltonian without omitting any terms. On the other hand, it arises from a variational calculation and hence is an upper bound for the ground-state energy.

It should be pointed out, by the way, that the second term of Eq. (1.1) or (1.2) is what would normally be called the third term. The reason is that for the Coulomb gas the usual first term is exactly cancelled out by the positive background. Now even for the short-range, hard-sphere Bose gas, Wu[7] found that the third term is logarithmic. Judging from Girardeau's calculation, the log term appears to be specifically connected with the long-range behavior of the Coulomb potential, but if we believe Wu's calculation, it may well be that the log term is somehow a general feature of the Bose gas.

In this paper we rederive the common first term of Eqs. (1.1) and (1.2) by a method introduced previously.[8] We do this by solving, to leading order, a nonlinear integrodifferential equation [I, Eq. (3.29)]. Our purpose is twofold: Firstly, since the result above has not been proved, the fact that we also obtain it by a method quite different from Bogolyubov's is support for its validity. Secondly, but closer to our real interest, we are attempting to establish the usefulness and validity of I, Eq. (3.29).

Judging from the results of the present paper and of I, it would seem that this same equation is valid (for weak-coupling constant at least) for both long-range and short-range potentials, with or without a hard core. This equation does not make use of pseudopotentials or other artifices which must be introduced in other methods if the potential is singular.

For weak-coupling constant, as in this present case and in the short-range case treated before, I Eq. (3.29) can be linearized to the extent that it can be solved analytically and the first two terms in a power series for the ground-state energy obtained. [For the Coulomb case this means that we obtain only the first term correctly, as explained before. Our next term is a constant, as in Eq. (1.1), but with a different coefficient. It is not clear whether we could obtain a log term by solving I Eq. (3.29) more accurately, or whether it is necessary to first construct an improved version of this equation by invoking higher correlation functions than the second.] Another case in which this equation acquits itself properly for *all* coupling is in the one-

[3] M. Girardeau, Phys. Rev. **127**, 1809 (1962).
[4] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).
[5] M. Luban, Phys. Rev. **128**, 965 (1962).
[6] G. Wentzel, Phys. Rev. **120**, 1572 (1960). Unfortunately, the theorem cannot be regarded as rigorously proved in all generality for the Bose gas, because it assumes that a certain unknown power series converges. For the particular case of the ground state (zero temperature), the case in which we are here interested, the theorem was proved previously by Girardeau and Arnowitt (cf. Ref. 4, Appendix B). However, their proof also suffers from having to make the same assumption as Wentzel.
[7] T. T. Wu, Phys. Rev. **115**, 1390 (1959).
[8] E. H. Lieb, Phys. Rev. **130**, 2518 (1963) (hereafter referred to as I).

dimensional model proposed by one of us[9] where the exact solution is known.

Having thus established the validity of I, Eq. (3.29) for weak coupling, but for a wide variety of potentials, it is our ultimate aim to solve it numerically for intermediate and strong coupling and hopefully to obtain a decent estimate of the ground-state energy of liquid helium. We shall not discuss this question further here except to note that for the Coulomb case, as we shall show, the equation will give the correct functional dependence of the ground-state energy on the coupling constant in the limit of *large* coupling constant. Whether or not the coefficient will turn out to be nearly correct when the equation is solved numerically remains to be seen.

II. THE INTEGRO-DIFFERENTIAL EQUATION METHOD

The Hamiltonian of the problem is[10]

$$H=-\tfrac{1}{2}\sum_{1}^{N}\nabla_i^2+\sum_{\langle i,j\rangle}v(\mathbf{x}_i-\mathbf{x}_j)\,, \tag{2.1}$$

where[11]

$$v(r)=e^2r^{-1}e^{-\epsilon r}\,, \tag{2.2}$$

and e is the electric charge of each particle. We have N particles in a volume V with a density $\rho=N/V$.

In I we introduced certain correlation functions, namely,

$$g(\mathbf{x}_1,\cdots,\mathbf{x}_s)\equiv V^S\int_V\psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)\prod_{S+1}^{N}d^3x_j \times\left(\int_V\psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)\prod_{1}^{N}d^3x_j\right)^{-1},$$

where ψ is the N particle ground-state wave function. We then found a recursion relation between the two-, three-, and four-particle functions, viz.,

$$[-\tfrac{1}{2}(\nabla_1^2+\nabla_2^2)+v_{12}]g(1,2)=M(1,2)\,, \tag{2.3}$$

where

$$M(1,2)=E_0g(1,2)-2V^{-1}(N-2)\int_V g(123)v_{23}d_3 -\tfrac{1}{2}V^{-2}(N-2)(N-3)\int\int_V g(1234)v_{34}d_3d_4\,, \tag{2.4}$$

and E_0 is the ground-state energy (before subtracting the background). We further argued that for weak interaction, at least, we needed to know the function M only for large values of $r=|\mathbf{x}_1-\mathbf{x}_2|$, and that this could be obtained from the superposition *ansatz*. The approximation to M thus obtained (for a large system) is

$$M(1,2)=\rho g(1,2)\{2K(1,2)-\rho L(1,2)\}\,, \tag{2.5}$$

where

$$K(1,2)=\int u(1,3)g(2,3)v_{23}d_3\,, \tag{2.6}$$

and

$$L(1,2)=\int\int u(1,3)u(2,4)\{g(1,4)g(2,3) -\tfrac{1}{2}u(1,4)u(2,3)\}g(3,4)v_{34}d_3d_4\,. \tag{2.7}$$

The function u is the finite part of the two-particle correlation function, $g(1,2)=g(|\mathbf{x}_1-\mathbf{x}_2|)$ defined by

$$g(r)=1-u(r)\,. \tag{2.8}$$

The energy before subtracting the background is defined in terms of $g(r)$ by

$$E_0=\frac{1}{2}\frac{N(N-1)}{V}\int_V g(r)v(r)d^3r\,, \tag{2.9}$$

and we notice that the term 1 in Eq. (2.8) will just cancel the background term.[11] If we define f to be the energy per particle in Rydbergs,[12] then

$$f=-\frac{1}{2}\frac{(N-1)}{VR_H}\int_V u(r)v(r)d^3r \to -2(6\pi^2)^{1/3}r_s^{-1}\rho^{2/3}\int_0^\infty ru(r)dr\,, \tag{2.10}$$

where in Eq. (2.10) we have passed to the limit of an infinite system and then to the limit of a Coulomb potential.

Equations (2.3) and (2.5) are Eq. (3.29) of I. In arriving at this approximate form for M we argued that M was needed only for large distances and in I we justified this need for short-range forces by taking the hard-sphere case as a typical example. Even for the long-range Coulomb case it is still true that M is needed only for large distances and in Appendix A we justify this assertion.

Granted that we need M only for large distances (for weak-coupling constant), we can further simplify M by replacing the factor in braces in Eq. (2.7) by unity so that

$$L(\mathbf{x}_1-\mathbf{x}_2)=\int\int u(\mathbf{x}_1-\mathbf{x}_3)S(\mathbf{x}_3-\mathbf{x}_4) \times u(\mathbf{x}_4-\mathbf{x}_2)d_3d_4\,, \tag{2.11}$$

where

$$S(r)=g(r)v(r)\,. \tag{2.12}$$

[9] E. Lieb and W. Liniger, Phys. Rev. **130**, 1605 and 1616 (1963). E. Lieb and W. Liniger (to be published).

[10] We use units in which $\hbar^2/m=1$.

[11] To avoid confusion about subtracting the uniform background contribution, we first replace $v(r)$ by a shielded Coulomb potential with a fictitious, large cutoff length ϵ^{-1}, which is independent of and much smaller than the length of the system. The shielding allows us to continue the potential periodically, so that for a finite V and ϵ the wave function is homogeneous and periodic. Moreover, the additional energy due to the Boson-continuum and the continuum-continuum interactions, $-N\rho\int v_{12}d_2+\frac{1}{2}\rho^2\int v_{12}d_1d_2$, becomes a constant equal to $-2\pi e^2N\rho\epsilon^{-2}$ which is to be added to the total energy. At the end of the calculations we put $V\to\infty$ and then $\epsilon\to 0$.

[12] We use f instead of e (as in I) in order to avoid confusion with the electric charge.

In I we made a further simplification, namely, that since $v(r)$, and hence $S(r)$, was short range compared to $u(r)$ we could replace $S(r)$ (in the integrals for K and L) by $\delta^3(\mathbf{r})\frac{1}{2}e\rho^{-1}$, where e was the energy per particle. In the present case we obviously cannot make such a replacement. Thus, for the Coulomb case, while we are still using the same basic equation, I, (3.29), we must treat it a little more carefully.

To this end we combine Eqs. (2.3), (2.5), (2.6), (2.11), and (2.12), and take Fourier transforms of both sides with the result that

$$-k^2u(k)+S(k)=\rho S(k)\{2u(k)-\rho u(k)^2\} \quad (2.13)$$

and

$$S(k)=\frac{4\pi e^2}{k^2}-\frac{4\pi e^2}{(2\pi)^3}\int\frac{1}{(\mathbf{k}-\mathbf{q})^2}u(q)d^3q. \quad (2.14)$$

We have defined

$$u(k)=\int u(r)e^{i\mathbf{k}\cdot\mathbf{r}}d^3r, \quad (2.15)$$

with a similar definition for $S(k)$.

If we change to the dimensionless variable

$$p^4=k^4(8\pi e^2\rho)^{-1},$$

and perform the angular integration in Eq. (2.14) we obtain (cf. latter part of Appendix B)

$$\rho u(p)=1+p^4/H-(p^2/H)(p^4+2H)^{1/2} \quad (2.16)$$

and

$$H(p)=1-\frac{2}{\pi}6^{-1/4}r_s{}^{3/4}\rho\int_0^\infty pq\ln\left|\frac{p+q}{p-q}\right|u(q)dq$$
$$\equiv 1-H'(p). \quad (2.17)$$

The energy is given by

$$f=-\frac{2}{\pi}6^{1/4}r_s{}^{-3/4}\rho\int_0^\infty u(p)dp, \quad (2.18a)$$

$$=-\tfrac{1}{2}6^{1/2}r_s{}^{-3/2}\lim_{p\to 0}p^{-2}H'(p). \quad (2.18b)$$

We propose to solve the coupled equations (2.16) and (2.17) by iteration in the following manner: Let u_n and H_n denote the nth approximations to u and H, respectively, and take $H_1=1$. This gives

$$\rho u_1(p)=1+p^4-p^2(p^4+2)^{1/2}. \quad (2.19)$$

We then insert u_1 into Eq. (2.17) and derive H_2; the process is then repeated indefinitely.

In Appendix B we prove that for $r_s<R_s$ (where R_s is some constant) this iteration procedure converges to a $u(p)$, which is a unique solution of Eqs. (2.13) and (2.14). We prove, moreover, that if f_n is obtained from u_n via Eq. (2.18a) then f_{odd} forms a decreasing sequence of upper bounds and f_{even} forms an increasing sequence of lower bounds for the true f. Both sequences have a common limit, of course.

Having thus bounded f we can proceed to find an asymptotic expansion for f in powers of $r_s{}^{3/4}$ by expanding u in a power series in H about $H=1$ and retaining the first n terms in u_n. To find the first two terms we we must go to u_2, whereupon

$$f=Ar_s{}^{-3/4}+B \quad (2.20)$$

and

$$A=\frac{2}{\pi}6^{1/4}\int_0^\infty\{p^2(p^4+2)^{1/2}-p^4-1\}dp=-0.803, \quad (2.21)$$

$$B=\frac{4}{\pi^2}\int_0^\infty\int_0^\infty p^3\{p^4+1-p^2(p^4+2)^{1/2}\}(p^4+2)^{-1/2}$$
$$\times q\{q^4+1-q^2(q^4+2)^{1/2}\}\ln\left|\frac{p+q}{p-q}\right|dpdq$$
$$=0.0597. \quad (2.22)$$

The integral in Eq. (2.22) can be done by Mellin transforms and details of its evaluation, as well as of the integral in Eq. (2.21), are given in Appendix C. The A coefficient is the same as in Eqs. (1.1) and (1.2).

Returning to the full nonlinear version of $L(1,2)$, Eq. (2.7), we see at once, by changing to the dimensionless variable $\mathbf{x}=\rho^{1/3}\mathbf{r}$, that for large r_s (low-density limit) the second derivative term in Eq. (2.3) may be dropped and we obtain a pure integral equation for $u(r)$. Assuming the solution is properly integrable, we see from Eq. (2.10) that in this limit $f\sim$constant $\times r_s{}^{-1}$—the correct result found by Wigner.[13] If this constant turns out to be close to the value -1.792 found by Fuchs[14] then it may be supposed that for all values of r_s our nonlinear equation yields an accurate value for the ground-state energy.

We conclude this section by displaying the two-particle correlation function $g(r)=1-u(r)$. To leading order in r_s we may use the function u_1 found before. The inverse Fourier transformation is facilitated by performing a contour integration around the branch cuts of the square root. We also change variables to

$$z=a_0{}^{-1}r_s{}^{-3/4}r, \quad (2.23)$$

where $a_0=\hbar^2/me^2$ is the Bohr radius. The result is

$$u(z)=\frac{16}{\pi\sqrt{3}}r_s{}^{3/4}\frac{1}{z}\int_0^1 p^3(1-p^4)^{1/2}$$
$$\times\exp(-3^{1/4}pz)\sin(3^{1/4}pz)dp. \quad (2.24)$$

The asymptotic behavior of $u(z)$ is not $\sim z^{-5}$ as one might have guessed from the usual argument that small p is important in the integral when z is large.

[13] E. Wigner, Phys. Rev. **46**, 1002 (1934); Trans. Faraday Soc. (London) 34, 678 (1938).
[14] K. Fuchs, Proc. Roy. Soc. (London) **A151**, 585 (1935).

Rather, one can prove that

$$u(z)=\frac{8}{3\sqrt{\pi}}(12)^{1/8}r_s^{3/4}e^{-8^{1/4}z}\times\left\{z^{-5/2}\cos\left(3^{1/4}z+\frac{3\pi}{8}\right)+\Delta\right\}, \quad (2.25)$$

where $\Delta=0(z^{-7/2})$. An outline of this proof is given in Appendix C. Note that for large r, $g(r)$ has an oscillating component.

It is to be noted also that the range of u decreases with r_s like $r_s^{3/4}$, but more important u itself is proportional to $r^{3/4}$. This means that if r_s is not too large, $u(r)$ is everywhere less than 1, so that $g(r)$ is positive as it is known to be on general grounds [cf. I, Eq. (3.6d)]. In fact for all z,

$$u(z)\leqslant(16/\pi)3^{-1/4}r_s^{3/4}\int_0^1 p^4(1-p^4)^{1/2}dp =3^{-1/4}4r_s^{3/4}\Gamma\left(\frac{5}{4}\right)\Gamma\left(\frac{3}{2}\right)\Big/\pi\Gamma\left(\frac{11}{4}\right).$$

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APPENDIX A: JUSTIFICATION OF THE INTEGRODIFFERENTIAL EQUATION

We want to solve Eq. (2.3), which may be written (suppressing all irrelevant factors):

$$\nabla^2u(r)-(1/r)u(r)=-1/r+M(r). \quad (A1)$$

From the solution to this equation we must compute the ground-state energy per particle,

$$f=-\int r^{-1}u(r)d^3r=-4\pi\int_0^\infty ru(r)dr. \quad (A2)$$

What we wish to show here is that the quantity f is determined primarily by the asymptotic behavior of $M(r)$.

We first observe that since $u(r)$ must be integrable (in three dimensions), the right-hand side of Eq. (A1) must go to zero faster than r^{-1}. This means that $M(r)=r^{-1}+M'(r)$, where $M'(r)$ is what we might call the finite part of $M(r)$. For a short-range potential, M would have only a finite part. Any approximation to M must give the r^{-1} term correctly or the answer will be nonsensical. Indeed, the superposition *ansatz* gives the r^{-1} term providing $\int u(r)d^3r=\rho^{-1}$. In any event, the r^{-1} part of M is still a part of the asymptotic behavior of M, so that to obtain it we do not require knowledge of M for small r.

If we now write $u(r)=r^{-1}\phi(r)$, with $\phi(0)=0$, multiply Eq. (A1) by r^2, and integrate by parts, we obtain [using the fact that

$$\int_0^\infty r\ddot{\phi}(r)dr=r\dot{\phi}(r)\Big|_0^\infty-\int_0^\infty\dot{\phi}(r)dr=\phi(0)=0],$$

$$f=4\pi\int_0^\infty r^2M'(r)dr. \quad (A3)$$

We thus conclude that the situation here is quite analogous to that expressed by I Eq. (3.22). Assuming that $M(r)$ is reasonably smooth, we see that we need to know it for distances of the order of its cutoff length, whatever that may be. The superposition *ansatz* then tells us that the cutoff length is $\sim r_s^{3/4}a_0$.

APPENDIX B: THE ITERATIVE SOLUTION OF EQS. (2.16) AND (2.17)

We observe that since the kernel appearing in Eq. (2.17) is a positive function, if $u_1(p)$ and $u_2(p)$ are any two functions satisfying the relation $u_1(p)>u_2(p)$ for all p, then $H(u_1,p)<H(u_2,p)$ for all p. On the other hand, since $\rho\partial u(H,p)/\partial H(p)=(p^2/H)^{-1/2}u(p)>0$ for $H(p)>0$, then if $H_1(p)<H_2(p)$ for all p, $u(H_1,p)<u(H_2,p)$ for all p.

Now, starting with $H_1=1$ and $u_1=u(H_1,p)$ [cf. Eq. (2.19)], we insert u_1 into Eq. (2.17) and obtain $H_2=H(u_1,p)<H_1$. In general, $u_n=u(H_n,p)$ and $H_n=H(u_{n-1},p)$. One easily concludes from the above inequalities [assuming for the moment that $H_n(p)>0$ for all n and p] that if n is any odd integer, then for all p

$$u_1>u_3>\cdots>u_n>u_{n+1}>u_{n-1}>\cdots>u_4>u_2>0, \quad (B1)$$

and

$$H_1>H_3>\cdots>H_n>H_{n+1}>H_{n-1}>\cdots>H_4>H_2>0. \quad (B2)$$

Thus, the odd u's and the odd H's form a decreasing sequence for all p, while the even u's and the even H's form an increasing sequence. Since the odd sequences are bounded below, and the even sequences are bounded above, it follows that each of these sequences must converge to limit functions. We denote these by u_e, H_e, u_0, and H_0, respectively. We have, however, glossed over one point: The above inequalities, (B1) and (B2), are true only if $H_n(p)>0$ for all n and p. Since $H_2(p)$ is always the smallest H, it is sufficient to show that it is positive. But $H_2=H(u_1,p)$, and when we insert Eq. (2.19) into Eq. (2.17) we see that $H_2'(p)$ is given by an integral which is not only convergent but which is bounded for all p. In other words, we can write

$$H_{\rm odd}(p)\geqslant H_{\rm even}(p)\geqslant H_2(p)\geqslant 1-\tfrac{1}{2}(r_s/R_s)^{3/4}, \quad (B3)$$

where R_s is some constant. Therefore, if $r_s<2^{4/3}R_s$, then Eqs. (B1) and (B2) are true.

We next must show that the limit functions satisfy $u_e=u_0$ and $H_e=H_0$ (at least for sufficiently small r_s). Unless these limit functions agree, the iterative solution to Eqs. (2.16) and (2.17) will not exist.

The limit functions satisfy

$$u_0=u(H_0);\quad u_e=u(H_e),$$

$$H_0(p)=1-\int K(p,q)u_e(q)dq, \tag{B4}$$

$$H_e(p)=1-\int K(p,q)u_0(q)dq,$$

where we have used an obvious notation for the kernel appearing in Eq. (2.17). Assuming $r_s<2^{4/3}R_s$, and observing that $\partial^2u/\partial H^2<0$ we have (from the remainder theorem on Taylor series)

$$u_0-u_e\leqslant (H_0-H_e)\partial u_e/\partial H<(H_0-H_e)(u_e/H_e)\leqslant (H_0-H_e)u_eA\,, \tag{B5}$$

where $A=[1-\frac{1}{2}(r_s/R_s)^{3/4}]^{-1}$. Let $h(p)=H_0(p)-H_e(p)\geqslant 0$, which satisfies

$$\begin{aligned} h(p)&\leqslant A\int K(p,q)h(q)u_e(q)dq\\ &\leqslant AM\int K(p,q)u_e(q)dq\\ &=AM[1-H_0(p)]\leqslant M(A-1)\,, \end{aligned} \tag{B6}$$

where $M=\max_p h(p)$. If $A-1<1$, Eq. (B6) is a contradiction unless $M=0$, and hence if $r_s<R_s$, $H_e(p)=H_0(p)$. Q.E.D.

We conclude by showing that the iterative solution is the unique solution. To do this we must first show that the only meaningful solution is one for which $H(p)>0$ (all p). The argument is as follows: (1) f exists [cf. Eq. (2.10)] because it is bounded from above by zero (from a variational calculation with $\psi=1$) and from below by[13] $-1.8r_s^{-1}$, the minimum value of the potential energy. For any admissible u, therefore, $\int_0^\infty ru(r)dr$ exists. (2) $u(r)$ is bounded since g is. In particular, $u(r=0)$ is finite. (3) Since $H'(p)=\text{const}\times p^2\int_0^\infty ru(r)\times(\sin pr/pr)dr$, $H'(p)$ is continuous and differentiable in p. Also $|H'(p)|<\text{const}\times p\int_0^\infty u(r)dr=\text{const}\times p$. (4) We now come to the question of the choice of the plus or minus sign before the square root in Eq. (2.16). Whichever choice we make, by the bound on $|H'(p)|$, $u(p=0)=\rho^{-1}$. This means $\int ud^3r$ exists, and hence $u(p)$ is continuous and differentiable and bounded for $p>0$. (5) Since $u(p)$ is supposed to be the three-dimensional Fourier transform of a real, symmetric function, $u(p)$ is real, which means that $H(p)\geqslant -\frac{1}{2}p^4$. (6) On the face of it, there is no need to retain one sign of the square root in Eq. (2.16) for all p but, by continuity of $u(p)$, we can change the sign only when the square root vanishes, i.e., either when $H=\pm\infty$ (which never happens) or when $H(p)=-\frac{1}{2}p^4$. (7) Let u_- be given by Eq. (2.16) and u_+ be the u with a plus sign in front of the square root. If $H(p)<0$ someplace it must be negative for all p, because when $H=0-$, $u_-=-\infty$ and when $H=0+$, $u_+=+\infty$. Since $u(p)$ is bounded, and since we cannot switch from u_+ to u_- when $H=0$, we conclude that $H(p)\neq 0$. By continuity of H, it is either always negative or always positive. In the latter case we must use u_-, as we have done, in order that $u(p=\infty)=0$. (8) If $-\frac{1}{2}p^4<H<0$ both u_+ and u_- are negative, but by Eq. (2.17) H would be positive—a contradiction.

Thus, Eq. (2.16) is correct and $H>0$ and $u>0$. (for physically meaningful solutions). Consequently, since $0<H(p)<1$, $u(p)<u_1(p)$. But this in turn implies that $H(p)>H_2(p)$. Proceeding in this way we conclude that for any odd integer n

$$u_1>u_3>\cdots u_n\geqslant u\geqslant u_{n+1}>u_{n-1}>\cdots>u_2. \tag{B7}$$

Since the even and odd sequences converge to a common limit function, $u(p)$ must be that limit function, and hence is identical to the iterative solution.

APPENDIX C: THE EVALUATION OF INTEGRALS

The integrals appearing in this paper are readily evaluated by utilizing the Mellin-representation.

$$\log\left|\frac{x+y}{x-y}\right|=\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}\frac{\pi}{s}\tan\frac{\pi s}{2}\left(\frac{x}{y}\right)^{-s}ds\,, \tag{C1}$$

and the integral

$$a^{-y}\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}=\int_0^\infty t^{x-1}(a+t)^{-x-y}dt\,, \tag{C2}$$

with Rex and Re$y>0$.

(α). The coefficient A [Eq. (2.21)], is a particular case of (C2).

$$\begin{aligned} A&=-\frac{2}{\pi}6^{1/4}\int_0^\infty \{p^4+1-[(p^4+1)^2-1]^{1/2}\}dp\\ &=-\frac{8}{5\pi}\left(\frac{3}{4}\right)^{1/4}\frac{\Gamma(3/4)^2}{\Gamma(3/2)}=-0.803\,, \end{aligned} \tag{C3}$$

where we have changed variables to p^4 and integrated twice by parts to reduce the integral to the form (C2).

(β). The constant B is obtained by noting that

$$\int_0^\infty dq q^{s+1}\{q^4+1-[(q^4+1)^2-1]^{1/2}\}=\frac{2^{s/4-1/2}}{4(\frac{1}{4}s+\frac{1}{2})(\frac{1}{4}s+\frac{3}{2})}\frac{\Gamma(1+\frac{1}{4}s)\Gamma(\frac{1}{2}-\frac{1}{4}s)}{\Gamma(\frac{3}{2})},\quad 2>\mathrm{Re}s>-2 \tag{C4}$$

and

$$\int_0^\infty dp p^{5-s}\left\{-1+\frac{p^4+1}{[(p^4+1)^2-1]^{1/2}}\right\}=\frac{1}{4}\frac{2^{-s/4-1/2}}{(\frac{3}{2}-\frac{1}{4}s)}\frac{\Gamma(1-\frac{1}{4}s)\Gamma(\frac{1}{2}+\frac{1}{4}s)}{\Gamma(\frac{3}{2})},\quad 4>\mathrm{Re}s>-2, \tag{C5}$$

where we have changed variables to q^4 and p^4 and integrated by parts once and twice, respectively.

Thus,

$$\begin{aligned}B&=\frac{4}{\pi^2}\int_0^\infty p^5\left\{-1+\frac{p^4+1}{[(p^4+1)^2-1]^{1/2}}\right\}dp\int_0^\infty q\{q^4+1-[(q^4+1)^2-1]^{1/2}\}\log\left|\frac{p+q}{p-q}\right|dq\\
&=\frac{1}{2\pi^3}\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}\frac{\pi}{s}\tan\frac{\pi s}{2}\frac{\Gamma(1+\frac{1}{4}s)\Gamma(\frac{1}{2}-\frac{1}{4}s)}{(\frac{3}{2}-\frac{1}{4}s)}\frac{\Gamma(1-\frac{1}{4}s)\Gamma(\frac{1}{2}+\frac{1}{4}s)}{(\frac{1}{2}+\frac{1}{4}s)(\frac{3}{2}+\frac{1}{4}s)}\\
&=\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}\frac{1}{4\cos\frac{1}{2}\pi s}\frac{ds}{(\frac{3}{2}-\frac{1}{4}s)(\frac{1}{2}+\frac{1}{4}s)(\frac{3}{2}+\frac{1}{4}s)}\\
&=-\frac{1}{6}+\frac{1}{2\pi}\sum_{n=0}^\infty\frac{(-1)^n}{[\frac{1}{2}(3-n)-\frac{1}{4}][\frac{1}{2}(1+n)+\frac{1}{4}][\frac{1}{2}(3+n)+\frac{1}{4}]}\\
&=-1/6+32/45\pi=0.05969,\end{aligned} \tag{C6}$$

where we have closed the contour to the right and summed the series by decomposing the summand into partial fractions.

(γ). The correlation function can be similarly obtained. We have

$$\begin{aligned}u(z)&=\frac{2}{3}\frac{\sqrt{6}}{\pi}\frac{r_s^{3/4}}{z}\int_0^\infty\{p^4+1-[(p^4+1)^2-1]^{1/2}\}\sin(6^{1/4}pz)p\,dp\\
&\equiv\frac{2}{3}\frac{\sqrt{6}}{\pi}\frac{r_s^{3/4}}{z}J(6^{1/4}z).\end{aligned} \tag{C7}$$

By using the Mellin representation,

$$\sin xy=\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}(xy)^{-s}\Gamma(s)\sin\frac{\pi s}{2}ds, \tag{C8}$$

we obtain, upon performing the p integration,

$$\begin{aligned}J(y)&=\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}y^{-s}\Gamma(s)\sin\left(\frac{\pi s}{2}\right)\frac{2^{-(s/4)-(1/2)}}{4}\frac{\Gamma(1-\frac{1}{4}s)\Gamma(\frac{1}{2}+\frac{1}{4}s)}{(\frac{1}{2}-\frac{1}{4}s)(\frac{3}{2}-\frac{1}{4}s)\Gamma(\frac{3}{2})}ds\\
&=\sqrt{\frac{\pi}{2}}\frac{1}{2\pi i}\int_{1>\mathrm{Re}s>-1}(\sqrt[4]{2}y)^{-s}\Gamma(s)\sin\left(\frac{\pi s}{4}\right)\frac{\Gamma(1-\frac{1}{4}s)}{\Gamma(\frac{5}{2}-\frac{1}{4}s)}ds.\end{aligned} \tag{C9}$$

If we now insert

$$\frac{\Gamma(1-\frac{1}{4}s)}{\Gamma(\frac{5}{2}-\frac{1}{4}s)}=\frac{1}{\Gamma(\frac{3}{2})}\int_0^1 t^{-(s/4)}(1-t)^{1/2}dt, \tag{C10}$$

and perform the Mellin inversion,

$$\begin{aligned}J(y)&=\frac{\sqrt{2}}{2i}\int_0^1(1-t)^{1/2}\{\exp[-(2t)^{1/4}ye^{-i\pi/4}]-\exp[-(2t)^{1/4}ye^{i\pi/4}]\}dt\\
&=\sqrt{2}\int_0^1(1-t)^{t/2}e^{-(t/2)^{1/4}y}\sin((t/2)^{1/4}y)dt,\end{aligned} \tag{C11}$$

so that

$$u(z)=\frac{4}{\pi\sqrt{3}}\frac{r_s^{3/4}}{z}\int_0^1(1-t)^{1/2}e^{-(3t)^{1/4}z}\sin((3t)^{1/4}z)dt. \tag{C12}$$

Note that

$$|u(r)|\leqslant u(0)=\frac{4}{\pi 3^{1/4}}\frac{\Gamma(3/2)\Gamma(5/4)}{\Gamma(11/4)}r_s^{3/4}. \tag{C13}$$

In order to obtain u for large z, consider

$$\int_C (1-s)^{1/2}\exp[-(-2s)^{1/4}y]ds=0,\quad y>0, \tag{C14}$$

where the contour C starts from $+\infty$, runs under the real axis to $x=0-$, and then to $+\infty$ above the real axis. Hence,

$$\int_\infty^1 \exp\left[-\left(\frac{x}{2}\right)^{1/4}(1+i)y\right]i(x-1)^{1/2}dx+\int_1^0 \exp\left[-\left(\frac{x}{2}\right)^{1/4}(1+i)y\right](1-x)^{1/2}dx$$
$$+\int_0^1 \exp\left[-\left(\frac{x}{2}\right)^{1/4}(1-i)y\right](1-x)^{1/2}dx+\int_1^\infty \exp\left[-\left(\frac{x}{2}\right)^{1/4}(1-i)y\right](-i)(x-1)^{1/2}dx=0. \tag{C15}$$

Thus,

$$J(y)=\sqrt{2}\int_1^\infty e^{-(x/2)^{1/4}y}\cos\left(\left(\frac{x}{2}\right)^{1/4}y\right)(x-1)^{1/2}dx$$
$$\equiv\frac{1}{\sqrt{2}}[F_+(2^{1/4}y)+F_-(2^{1/4}y)], \tag{C16}$$

where

$$F_\pm(y)=\int_1^\infty \exp[-yx^{1/4}e^{\mp i\pi/4}](x-1)^{1/2}dx$$
$$=8\exp[-ye^{\mp i\pi/4}]\int_0^\infty \exp[-yse^{\mp i\pi/4}]s^{1/2}(1+s)^3\left(1+\frac{6s+4s^2+s^3}{4}\right)^{1/2}ds, \tag{C17}$$

where we have changed variables to $s+1=x^{1/4}$. Thus,

$$F_\pm(y)=8\exp[-ye^{\mp i\pi/4}]\{\Gamma(3/2)\Psi(3/2,11/2;ye^{\mp i\pi/4})\}+R_\pm(y). \tag{C18}$$

$$|R_\pm(y)|\leqslant e^{-y/\sqrt{2}}\int_0^\infty e^{-ys/\sqrt{2}}s^{1/2}(1+s)^3(6s+4s^2+s^3)ds$$
$$=e^{-y/\sqrt{2}}\left\{6\Gamma\left(\frac{5}{2}\right)\Psi\left(\frac{5}{2},\frac{13}{2};\frac{y}{\sqrt{2}}\right)+4\Gamma\left(\frac{7}{2}\right)\Psi\left(\frac{7}{2},\frac{15}{2};\frac{y}{\sqrt{2}}\right)+\Gamma\left(\frac{9}{2}\right)\Psi\left(\frac{9}{2},\frac{17}{2};\frac{y}{\sqrt{2}}\right)\right\}. \tag{C19}$$

Since the asymptotic behavior of the confluent hypergeometric function is

$$\Psi(a,b;x)=x^{-a}+O(x^{-a-1}), \tag{C20}$$

it follows that

$$F_\pm(y)=8\Gamma(3/2)(ye^{\mp i\pi/4})^{-3/2}\exp[-ye^{\mp i\pi/4}]+O(e^{-y/\sqrt{2}}y^{-5/2})$$
$$=4\sqrt{\pi}y^{-3/2}\exp\left[-\frac{y}{\sqrt{2}}\pm i\left(\frac{y}{\sqrt{2}}+\frac{3\pi}{8}\right)\right]+O(e^{-y/\sqrt{2}}y^{-5/2}). \tag{C21}$$

Finally,

$$u(z)=r_s^{3/4}\frac{8(12)^{1/8}}{3\sqrt{\pi}}\frac{\exp(-{}^4\sqrt{3}z)}{z^{5/2}}\cos\left[({}^4\sqrt{3}z)+\frac{3\pi}{8}\right]+r_s^{3/4}O\left[\frac{\exp(-{}^4\sqrt{3}z)}{z^{7/2}}\right]. \tag{C22}$$