

the behavior of $g(1.0)$ from Eq. (6) as a function of r_c . Also shown for comparison are $g^{\text{CHNC}}(1.0)$, $g^{\text{PY}}(1.0)$, and $g^{\text{DH}}(1.0)$. The labels CHNC and PY on the lowest curves in Fig. 2 indicate the results obtained with Eq. (6) when g^{SR} is calculated with the CHNC and PY equations, respectively.

Any errors in g from Eq. (6) might be expected to vary with r_c . When these errors are negligible, g will be independent of r_c . For this reason, we believe that the flat region of g in Fig. 2 (where the CHNC and PY equations are producing almost the same g^{SR}) may be very close to the exact value of g . This value compares much more favorably with g^{PY} than with g^{CHNC} (with $r_c = \infty$).

In conclusion then, we are lead to believe that

the PY equation is superior to the CHNC equation for long-range potentials as well as short-range at the temperatures and densities we have investigated. In addition, the procedure described here may provide a means of determining a nearly exact g in cases where it shows a region independent of r_c .

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EXACT SOLUTION OF THE PERCUS-YEVICK INTEGRAL EQUATION FOR HARD SPHERES*

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An increasing body of numerical computations has given strong evidence for the adequacy, over an extensive range of parameters, of various approximate integral equations for the radial distribution function of a classical fluid. The simplest, and on the basis of comparisons thus far made, the most satisfactory of these, is due to Percus and Yevick (PY).¹ Despite its simplicity, this equation until now has not been solved rigorously in any special situation, so that its basic properties have not been ascertained. It is the purpose of this Letter to obtain in closed form the pair distribution and equation of state of the PY equation for the prototype of interacting hard spheres.

The PY equation¹ for hard spheres is given by

$$\begin{aligned} \tau(\vec{r}) = 1 + n \int_{|\vec{r}'| < R} \tau(\vec{r}') d\vec{r}' \\ - n \int_{\substack{|\vec{r}'| < R, \\ |\vec{r} - \vec{r}'| > R}} \tau(\vec{r}') \tau(\vec{r} - \vec{r}') d\vec{r}', \end{aligned} \quad (1)$$

where R is the hard-sphere diameter, n is the particle density. The function $\tau(\vec{r})$ of PY¹ is related to the pair distribution function $g(\vec{r})$ and the direct correlation function $C(\vec{r})$ of Ornstein and Zernike² by

$$\begin{aligned} g(\vec{r}) &= 0 & (r < R), \\ g(\vec{r}) &= \tau(\vec{r}) & (r > R), \\ C(\vec{r}) &= -\tau(\vec{r}) & (r < R), \\ C(\vec{r}) &= 0 & (r > R). \end{aligned} \quad (2)$$

If we take the one-side Laplace transform of (1), defining

$$F(t) = R^{-2} \int_0^R r \tau(r) \exp(-sr) dr,$$

$$G(t) = R^{-2} \int_R^\infty r \tau(r) \exp(-sr) dr,$$

$$K = R^{-3} \int_0^R \tau(r) r^2 dr,$$

$$\eta = \frac{1}{8} n R^3, \quad sR = t,$$

we obtain

$$\begin{aligned} t[F(t) + G(t)] = t^{-1}[1 + 24 \eta K] \\ - 12 \eta [F(-t) - F(t)]G(t), \end{aligned} \quad (3)$$

where the real part of s must be greater than zero.

On expanding the PY equation in powers of the density, one finds that in second order $C(r)$ retains the functional form obtained in first order, namely, a cubic polynomial with quadratic term absent. This suggests trying a solution of the form

$$-C(x) = \alpha + \beta x + \gamma x^2 + \delta x^3, \quad (4)$$

where $x = (r/R)$, computing $F(t)$ and $F(-t)$ and solving Eq. (3) for $G(t)$. One can show directly from (1) that $\tau^{(n)}(r)$, with the superscript denoting differentiation, is continuous at $r = R$ for $n = 0, 1, 2$, and that $\tau(0) = 1 + 24 \eta K$. The values of