Simplified Approach to the Ground-State Energy of an Imperfect Bose Gas. III. Application to the One-Dimensional Model

ELLIOTT H. LIEB*
Belfer Graduate School of Science, Yeshiva University, New York, New York

AND

WERNER LINIGER
IBM—Watson Research Center, Yorktown Heights, New York

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We continue the study of the integrodifferential equation proposed previously for the evaluation of the ground-state energy of an imperfect Bose gas. We apply it here to the one-dimensional delta-function gas where the exact result is known for all values of the coupling constant γ. The results are: (i) For small γ, the equation gives the correct first two terms in an asymptotic series; (ii) a numerical solution of the equation shows that the maximum relative error occurs for $\gamma=\infty$ in which case it is 19%; (iii) for $\gamma=\infty$ we are able to compare the exact two-particle distribution function with that given by the equation. The agreement is quite good.

I. INTRODUCTION

IN a previous paper[1] (hereafter referred to as I) one of us proposed a nonlinear, integrodifferential equation whose solution, hopefully, yielded the ground-state energy E_0 of a gas of bosons interacting via pairwise forces. We have so far established the validity of this equation to the following extent:

(i) In I we verified that for short-range forces and low density (weak-coupling constant). The equation yields the "correct" first two terms for an expansion of E_0 in the density. By the word "correct" we mean that our result agreed with that obtained by numerous other authors, although it must be admitted that no one has yet succeeded in giving a rigorous proof of these terms. An important advantage of our equation in this case is that one is not obliged to introduce a pseudopotential in order to handle a potential with a hard core.

(ii) In the second paper in this series[2] it was shown that the equation also gives the correct result for the charged Bose gas in the limit of weak coupling (in this case high density). Once again, "correctness" has not been rigorously established, but our result agreed with all published calculations on the subject.[3,4] It was also pointed out in this paper that the equation would at least give the correct functional dependence of E_0 on the coupling constant in the limit of large-coupling constant, although the exact coefficient must await a numerical computation.

It is our ultimate aim to apply this equation to the real problem of liquid helium—clearly, not a weak-coupling problem. Prior to this we are obliged to search for as many examples—however, academic—where something is known about the intermediate and strong-coupling constant regions, and to establish the validity of the equation in those cases. Two problems that come to mind in this connection are the hard-sphere Bose gas and the charged Bose gas; these will be investigated in due course.

For the present we turn to the only model problem for which E_0 is exactly known for all values of the coupling constant—the gas of one-dimensional bosons interacting via a repulsive delta-function potential.[5] We wish to report here the following results of a numerical comparison between the solution to the equation and the exact E_0:

(i) In the limit of weak-coupling constant γ, the two agree precisely up to the second term in an expansion in γ.

(ii) The case of maximum relative error occurs for infinite γ, when the error is 19%.

(iii) For infinite γ we are able to evaluate the exact two-particle distribution function and compare it with that given by the numerical solution to the nonlinear equation. The comparison, shown in Fig. 2, is quite good. Assuming that the largest error in the distribution function occurs for infinite γ, as it does for the energy, we may conclude that the equation gives a good approximation to the distribution function as well as to the energy.

Two points are to be noted. Firstly, since the relative error is already quite small, it seems likely that an improved version of the integrodifferential equation (to be obtained by invoking higher correlation functions than the second) will reduce the error still further. Secondly, that the equation gives the first two terms correctly for small γ parallels the results for the three-dimensional gases so far investigated. This fact would seem to support the assertion made in II that this one-dimensional gas is not basically pathological, but has many features in common with real gases.

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[3] M. Girardeau, Phys. Rev. **127**, 1809 (1962).

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In Sec. II we outline the problem at hand and present an analytic solution of the nonlinear equation valid for small γ. In Sec. III we discuss the numerical procedures employed for the general γ and present a numerical comparison with the exact E_0. In Sec. IV we discuss the two-particle distribution function for $\gamma=\infty$.

II. WEAK COUPLING

The Hamiltonian of the problem[6] is

$$H=-\sum_1^N(\partial^2/\partial x_i^2)+2c\sum_{(i,j)}\delta(x_i-x_j), \quad (2.1)$$

where $2c\geq 0$ is the strength of the delta function. The line (on which periodic boundary conditions are satisfied) is of length L. There are N particles, with $\rho=N/L$ being the density. It was shown in II that for a large system E_0 was of the form

$$E_0=N\rho^2 e(\gamma) \quad (2.2)$$

with $\gamma=c/\rho$ being the dimensionless coupling constant. The function $e(\gamma)$ was obtained by solving the integral equation, II (3.18), and inserting the result into II (3.19) and II (3.20). The numerical result was plotted in II Fig. 3. The function $e(\gamma)$ has the following properties: (a) $\lim_{\gamma\to\infty}e(\gamma)=\pi^2/3$; (b) $e(\gamma)$ is monotonically increasing; (c) for small γ

$$e(\gamma)=\gamma-(4/3\pi)\gamma^{3/2}. \quad (2.3)$$

The first term in Eq. (2.3) was obtained directly from the integral equation, II (3.18). The second term is that given by Bogoliubov's perturbation theory which, while we unfortunately could not derive it directly, appeared to agree quite well with the numerical results.

We turn now to the nonlinear integrodifferential equation, I (3.29). It is an equation for the two-particle distribution function, $g(x)$, defined by

$$g(|x_1-x_2|)=L^2\frac{\int_L\psi(x_1,x_2,\cdots,x_N)\prod_3^N dx_i}{\int_L\psi(x_1,x_2\cdots,x_N)\prod_1^N dx_i}, \quad (2.4)$$

where ψ is the ground-state wave function. We also defined $u(x)$, the finite part of $g(x)$, by $u(x)=1-g(x)$. In the present case it is convenient to define the dimensionless variable $y\equiv\rho x$ and $u(y/\rho)\equiv\varphi(y)$, in terms of which [recalling that a delta-function potential is equivalent to a condition on $\dot{\varphi}(0+)$, the derivative of φ at $y=0$] Eq. I (3.29) becomes

$$\ddot{\varphi}=e(1-\varphi)\times\left\{2\varphi-\int\varphi*\varphi+2\int\varphi^2*\varphi-\frac{1}{2}\int\varphi^2*\varphi^2\right\}, \quad (2.5)$$

with

$$\dot{\varphi}(0+)=-\tfrac{1}{2}e, \quad \varphi(\infty)=0, \quad (2.6)$$

and

$$\gamma=e[1-\varphi(0)]^{-1}. \quad (2.7)$$

The convolution integrals are defined by

$$\int f*g\equiv\int_{-\infty}^{\infty}f(x-y)g(y)dy=\int_0^{\infty}[f(x+y)g(y)+f(y)g(x+y)]dy+\int_0^x f(x-y)g(y)dy, \quad (2.8)$$

the last equation being true for symmetric functions. It is to be noted that these equations give γ as a function of e.

For small e we expect $\varphi(y)$ to be small. Thus, it is convenient to define the new variable $z\equiv e^{1/2}y$ and $\varphi(z/e^{1/2})\equiv e^{1/2}\psi(z)$, in terms of which Eqs. (2.5)–(2.7) become

$$\ddot{\psi}=(1-e^{1/2}\psi)\left\{2\psi-\int\psi*\psi+2e^{1/2}\int\psi^2*\psi-\tfrac{1}{2}e\int\psi^2*\psi^2\right\}, \quad (2.5a)$$

$$\dot{\psi}(0+)=-\tfrac{1}{2}, \quad \psi(\infty)=0, \quad (2.6a)$$

and

$$\gamma=e[1-e^{1/2}\psi(0)]^{-1}. \quad (2.7a)$$

To find the first two terms in γ [as in Eq. (2.3)], it is necessary only to find $\psi(0)$ to leading order in e. To this end we can replace Eqs. (2.5a) and (2.6a) by

$$\ddot{\psi}+\delta(z)=2\psi-\int\psi*\psi, \quad (2.8)$$

an equation which can be solved by Fourier transforms. One finds easily that the Fourier transform of ψ is given by

$$\psi(p)=1+\frac{p^2}{2}-\frac{p}{2}[p^2+4]^{1/2}, \quad (2.9)$$

and hence

$$\psi(z)=\frac{1}{2\pi}\int_0^2 p(4-p^2)^{1/2}e^{-pz}dp. \quad (2.10)$$

Equation (2.10) was derived by transforming the inverse Fourier integral from an integral on $(-\infty,\infty)$ to a contour integral around the cut $(-2i, 2i)$ in $\psi(p)$.

Since $\psi(0)=4/3\pi$, Eq. (2.7a) immediately gives the required result, Eq. (2.3). We also note that $\psi(z)$ is montonically decreasing so that $g(x)<1$ for all x and all e as required by Eq. I (3.6d). In fact, it is interesting to note that this simple approximate solution to Eq. (2.5)

[6] To facilitate comparison, we use units in which $\hbar=1$, $2m=1$ as in II.

gives by itself a respectable approximation for $e(\gamma)$. From Eq. (2.7a) we see that e is a monotonically increasing function—a correct result—and that $e(\infty)=\frac{9}{16}\pi^2$. This is greater than the correct result, $\frac{1}{3}\pi^2$, by 69%. As we shall see in the next section, the complete Eq. (2.5) depresses $e(\infty)$, but overcompensates to the extent that the approximate $e(\infty)$ becomes 19% smaller than the correct result.

III. NUMERICAL COMPUTATION

For $e\leq 1$, we solved the problem defined by (2.5a)–(2.7a) while for $e>1$, we used Eqs. (2.5)–(2.7) [notice that, for $e=1$, we have $y=z$ and $\varphi(y)=\psi(z)$]. We denote by $\xi[\psi(z)]$ the right side of (2.5a). Unfortunately, Eq. (2.5a) cannot be solved by direct iteration, i.e., by computing a sequence $\psi^{(n)}(z)$, satisfying $\psi^{(n)}=\xi[\psi^{(n-1)}]$, $n=1, 2, \cdots$, with a given first guess, $\psi^{(0)}$, and subject to boundary conditions (2.6). The reason is that these boundary conditions require that

$$\int_0^\infty \xi[\psi^{(n-1)}(z)]dz=\tfrac{1}{2},$$

a condition which will not in general be satisfied. If, instead, we let $\sigma(z)=\psi(z)-\exp(-\lambda z)/2\lambda$, then $\sigma(z)$ satisfies

$$\ddot{\sigma}-\lambda^2\sigma=q \tag{3.1}$$

and boundary conditions $\dot{\sigma}(0)=\sigma(\infty)=0$, where $q(z)=\xi(z)-\lambda^2\psi(z)$. Equation (3.1) can be transformed into a pure integral equation which, if written in terms of $\psi(z)$, is

$$\psi(z)=(1/2\lambda)\left\{e^{-\lambda z}-\int_0^\infty [e^{-\lambda|z-\zeta|}+e^{-\lambda(z+\zeta)}]q(\zeta)d\zeta\right\}, \tag{3.2}$$

and which is amenable to solution by direct iteration. The quantity λ is an arbitrary numerical parameter whose choice will be explained later.

We donate the right side of (3.2) by $f[\psi]$ and define the iteration by $\psi^{(n)}=f[\psi^{(n-1)}]$, $n=1, 2, \cdots$. Each iteration step then involves a number of quadratures, which, for simplicity, were carried out by the trapezoidal rule. The computation was done for an increasing sequence of e values, $e_j=j\Delta e$ $(j=1, 2, \cdots, m)$, $e_m=1$, using the final answer $\psi_j(z)$, associated with e_j, as a first guess, $\psi_{j+1}{}^{(0)}(z)$, of $\psi_{j+1}(z)$. In computing $\psi_1(z)$ the function $\exp(-z/2)$ (which satisfies the boundary conditions) served as a first guess.

In solving the problem for $e>1$, Eq. (2.5) was replaced by

$$\varphi(y)=(1/2\lambda)\left\{(e)e^{-\lambda y}-\int_0^\infty [e^{-\lambda|y-\eta|}+e^{-\lambda(y+\eta)}]r(\eta)d\eta\right\}, \tag{3.3}$$

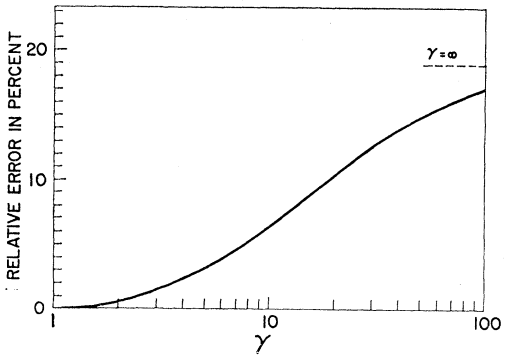

FIG. 1. The relative error, $1-E_0'(\gamma)/E_0(\gamma)$, plotted as a function of the coupling constant γ. $E_0(\gamma)$ is the exact ground-state energy while $E_0'(\gamma)$ is that given by the numerical solution to the integro-differential equation. The dashed line is the asymptotic value, 18.9%.

where $r(y)=\xi[\varphi(y)]-\lambda^2\varphi(y)$, and $\xi[\varphi]$ denotes the right side of (2.5). Equation (3.3) is analogous to (3.2). A program similar to the above was carried out on this equation for $e\geq 1$.

The iterations were stopped when the relative difference between two successive iterations, i.e., $|\psi^{(n)}(z)-\psi^{(n-1)}(z)|/\psi^{(n)}(z)$ in the case of Eq. (3.2), was less than one percent, uniformly in z. Both variables z and y were cut off at a value of 20 and the solution computed on an equidistant grid of 400 points. The truncation error (i.e., the error due to the use of finite difference techniques), could be studied, for $e=0$, by comparison with the known exact solution, Eq. (2.10), and, for larger e's it could be estimated by refining the grid. Similarly, the effect of varying the cutoff was studied. The number of grid points, the cutoff, and the convergence criterion indicated above were found to be adequate.

For not too large e, i.e., $e\lesssim 2$, convergence of the direct iteration procedure was achieved with a fixed value of the numerical parameter $\lambda=1$ for all e and all iteration steps. We convinced ourselves that the final answer was independent of λ by carrying out some of the calculations with several values of this parameter. The number of iterations needed was not more than a dozen.

For larger values of e, the iteration did not converge with a fixed λ. Instead, convergence was achieved by using a different λ for each value of e and each iteration step, namely $\lambda_n(e)=e/2\varphi^{(n-1)}(0)$. With this choice of λ, the inhomogeneous term on the right side of (3.3) does not contribute to the change from $\varphi^{(n-1)}(0)$ to $\varphi^{(n)}(0)$, and thus hopefully the over-all change from $\varphi^{(n-1)}(y)$ to $\varphi^{(n)}(y)$ is reduced.

We define the relative error to be $[e(\gamma)-e'(\gamma)]/e(\gamma)$, where $e(\gamma)$ is the exact value and $e'(\gamma)$ is the value given by the integral equation. The relative error is always positive and is shown as a function of γ in Fig. 1. Although we cannot give a rigorous bound on the numerical errors, a pessimistic estimate of them indicates that the relative error for $\gamma=\infty$ is $(18.9\pm 1)\%$.

IV. THE DISTRIBUTION FUNCTION FOR $\gamma=\infty$

We should like to be able to compare the exact $g(x)$, as given by Eq. (2.4), with that given by Eq. (2.5), for this would provide a far more severe test of the equation than a mere comparison of energies. Although the exact wave functions for the problem are known, we unfortunately have been unable to evaluate the N-fold integrals in Eq. (2.4).

We are indebted to Dr. A. Lenard for pointing out that for $\gamma=\infty$ (in which case the gas becomes identical with the Girardeau model[7]) these integrals have been evaluated by Dyson[8] in connection with his work on the statistical theory of energy levels. Dyson in turn relied on the work of Mehta and Gaudin.[9] What we have called $\phi(y)=1-g(y/\rho)$, Dyson[8] denotes by $Y_2(y)$ in his Eq. (51). In Eqs. (54) and (55) he also gives asymptotic expressions for this function for large and small y.

From Eqs. (2.5) and (2.6) we see directly [using the fact that $\phi(0)=1$ in this case] that: $\phi(0)=1$; $\dot{\phi}(0+)=-\frac{1}{2}e=-1.33$; $\ddot{\phi}(0+)=0$; $d^4\phi(0+)/dy^4=-e^3=-18.9$. Unfortunately, we cannot find $d^3\phi(0+)/dy^3$ directly. In the above we have, of course, used the approximate $e(\infty)=2.67$ and not the correct $e(\infty)=\pi^2/3=3.29$. These numbers are to be compared with Eq. (54) of Dyson: $\phi(0)=1$; $\dot{\phi}(0+)=-1.64$, $\ddot{\phi}(0+)=0$;

$$d^4\phi(0+)dy^4=-17.3.$$

For large y we have been unable to find an analytic expression for ϕ from Eq. (2.5). The numerical results, however, indicate that our $\phi(y)$ goes to zero much faster than the correct behavior $(\pi y)^{-2}$. Apparently it goes to zero like $p(y)\exp(-\lambda y)$, where λ is some constant of the order of unity and $p(y)$ is a polynomial. But as we see from Fig. 2, where the exact and approximate functions are plotted up to $y=3.6$, the difference in asymptotic behaviors becomes apparent only when ϕ is numerically small. Beyond $y=3.6$ the approximate ϕ quickly becomes much less than the exact ϕ.

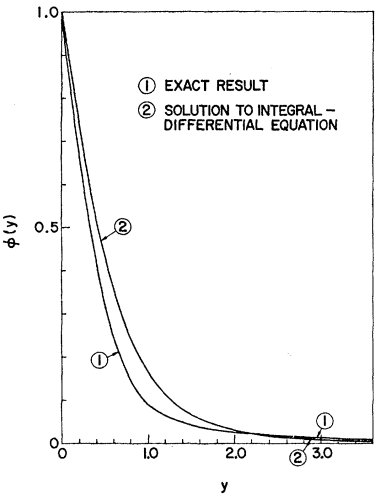

FIG. 2. A comparison plot of the exact $\phi(y)$ and that given by the solution to the nonlinear equation $\phi(y)=1-g(y/\rho)$, where $g(x)$ is the two-particle distribution function defined by Eq. (2.4). These curves are for infinite coupling constant.

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