Ground State and Low Excited States of a Boson Liquid with Applications to the Charged Boson System*

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The maximum deviation of the radial distribution function $g(r)$ from its asymptotic value, $g(\infty)=1$, is used as an expansion parameter in calculating the properties of a degenerate boson system. The uniform limit, defined by the condition $1-g(0)\ll 1$, holds at low densities under appropriate constraints on the Fourier transforms of the interaction potential and also at high densities for the charged-boson system. In the uniform limit a procedure based on (1) a Jastrow-type trial function, (2) the Wu-Feenberg functional for the kinetic energy, (3) the Kirkwood superposition approximation, or the more accurate Abe form for the three-particle distribution function, yields the Bogoliubov formulas for the ground-state energy and the excitation energies of a degenerate or nearly degenerate boson system. Results for the ground state of the high-density charged-boson system include

$$\frac{\langle \mathrm{KE}\rangle}{N}=-\frac{1}{5}\frac{\langle \mathrm{PE}\rangle}{N}+O(r_s^0),$$

$$\frac{E}{N}\leqq -\frac{0.8031}{r_s^{3/4}}+0.028.$$

Numerical results are also computed at intermediate and moderately low densities ($0.01\leqq r_s\leqq 100$).

1. INTRODUCTION

We study a system of N bosons confined within a cubical box of volume Ω. The particles interact in pairs through radial potentials $v(r_{ij})$. A general constraint on $v(r)$ develops out of the analysis, but for the moment we require only that $v(r)$ possess a well-defined Fourier transform. The Yukawa potential $V_0e^{-r/b}/(r/b)$ is a possible form which includes the Coulomb interaction as a special case ($V_0b=e^2$, $b\to\infty$).

The present study yields a simple derivation in configuration space of Bogoliubov's formulas for the ground-state energy and the excitation energies of a degenerate or nearly degenerate boson gas. Some results going beyond the Bogoliubov approximation are also given. The essential novel points are:

(i) use of the maximum deviation of the radial distribution function from its asymptotic value as a physically meaningful expansion parameter,

(ii) the explicit formulation of the uniform limit (defined in Sec. 4),

(iii) proof of the relation $\langle \mathrm{KE}\rangle=-\frac{1}{5}\langle \mathrm{PE}\rangle$ for the ground state of the charged-boson system at high density,

(iv) evaluation of the kinetic, potential, and total energies of a charged-boson gas at intermediate and low densities.

One way or another, the treatment is related to earlier studies by Bijl,[1] Bogoliubov and Zubarev,[2] Abe,[3] Gaskell,[4] Gross,[5] Foldy,[6] Girardeau,[7] Lieb and Sakakura,[8] and Wu and Feenberg.[9]

2. BASIC RELATIONS

To estimate the expectation value of the Hamiltonian operator in the ground state we introduce a Bijl-Dingle-Jastrow (BDJ) type correlated trial function

$$\Psi_0{}^B=\prod_{i<j}\exp\tfrac{1}{2}\mathfrak{U}(r_{ij})\Big/\left[\int\prod_{m<n}\exp\mathfrak{U}(r_{mn})dv_{12\cdots N}\right]^{1/2}. \quad (1)$$

This function can describe a wide variety of physical states [depending on the choice of correlation function $\mathfrak{U}(r)$] all the way from the short-range order of a quantum liquid (as in liquid He[4]) to the long-range order of a well-defined space lattice (as in the electron system at sufficiently low density). We proceed to the basic definitions and relations needed to complete the calculation of the mean kinetic and potential energies.

Radial Distribution Function

$$g(r_{12})=\frac{N-1}{N}\Omega^2\int\Psi_0{}^{B2}d\mathbf{r}_{34\cdots N}. \quad (2)$$

Three-Particle Distribution Function

$$p(1,2,3)=N(N-1)(N-2)\int\Psi_0{}^{B2}d\mathbf{r}_{45\cdots N}. \quad (3)$$

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[9] F. Y. Wu and E. Feenberg, Phys. Rev. **122**, 739 (1961).

Kirkwood Superposition Approximation (Ref. 10)

$$p_K(1,2,3)=\rho^3 g(r_{12})g(r_{23})g(r_{31}), \tag{4}$$

in which $\rho=N/\Omega$ is the number density.

Bogoliubov-Born-Green-Kirkwood-Yvon Relation (Ref. 10)

$$g(r_{12})\nabla_1\mathfrak{U}(r_{12}) = \nabla_1 g(r_{12}) - (1/\rho^2)\int[p(1,2,3)-\rho^3 g(r_{12})g(r_{13})] \times\nabla_1\mathfrak{U}(r_{13})d\mathbf{r}_3. \tag{5}$$

The substitution of $p_K(1,2,3)$ for $p(1,2,3)$ in Eq. (5) reduces it to the explicit form

$$g(r_{12})\nabla_1\mathfrak{U}(r_{12}) = \nabla_1 g(r_{12}) + \rho\int[1-g(r_{23})]g(r_{12})g(r_{13}) \times\nabla_1\mathfrak{U}(r_{13})d\mathbf{r}_3. \tag{6}$$

Expectation Value of the Kinetic Energy

$$\langle \mathrm{KE}\rangle = N\rho\frac{\hbar^2}{8m}4\pi\int_0^\infty \nabla\mathfrak{U}\cdot\nabla g\, r^2 dr. \tag{7}$$

Expectation Value of the Potential Energy

$$\langle \mathrm{PE}\rangle = 2\pi N\rho\int_0^\infty g(r)v(r)r^2 dr. \tag{8}$$

3. EVALUATION OF THE KINETIC ENERGY

In Secs. 7, 8, and 9, the integral in Eq. (7) is evaluated by a systematic iteration-variation procedure employing Eq. (6) and the functional $J(\nabla\mathfrak{U})$ introduced in Ref. 9. A related, but less accurate, variational method is also used in Sec. 8. In this section we take some steps in the direction of an explicit analytical evaluation of the kinetic energy. First, the radial distribution function is written in the form

$$g(r)=1-\alpha G(\alpha^{1/3}\rho^{1/3}r) \tag{9}$$

subject to the normalization conditions

$$\rho\int[g(r)-1]d\mathbf{r} = -\alpha\rho\int G(\alpha^{1/3}\rho^{1/3}r)d\mathbf{r} = -\int G(s)d\mathbf{s} = -1, \tag{10}$$

$$G(0)=1. \tag{11}$$

A change to the s space of Eq. (10) now proves convenient. Let $s=(\alpha\rho)^{1/3}r$ and

$$\mathcal{Y}(s)=\mathfrak{U}(r). \tag{12}$$

Equation (6) becomes

$$\nabla\left[\mathcal{Y}(s)-\int G(|\mathbf{s}'-\mathbf{s}|)\mathcal{Y}(s')d\mathbf{s}'-\ln\{1-\alpha G(s)\}\right] = -\alpha\int G(|\mathbf{s}'-\mathbf{s}|)G(s')\nabla'\mathcal{Y}(s')d\mathbf{s}'. \tag{13}$$

In terms of the Fourier transforms

$$F(q)=\int e^{i\mathbf{q}\cdot\mathbf{s}}G(s)d\mathbf{s}, \qquad Z(q)=\int e^{i\mathbf{q}\cdot\mathbf{s}}\mathcal{Y}(s)d\mathbf{s}, \tag{14}$$

Eq. (13) assumes the partially solved form

$$Z(q)[1-F(q)]=\int e^{i\mathbf{q}\cdot\mathbf{s}}\ln[1-\alpha G(s)]d\mathbf{s} -\alpha F(q)\left(\frac{1}{2\pi}\right)^3\int\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}F(|\mathbf{q}'-\mathbf{q}|)Z(q')d\mathbf{q}', \tag{15}$$

an inhomogeneous linear integral equation for the unknown function $Z(q)$.

The mean kinetic energy can now be expressed in terms of F and Z:

$$\frac{\langle \mathrm{KE}\rangle}{N} = -(\alpha\rho)^{2/3}\frac{\hbar^2}{8m}\int\nabla\mathcal{Y}(s)\cdot\nabla G(s)d\mathbf{s} = -\frac{\hbar^2(\alpha\rho)^{2/3}}{(4\pi)^3 m}\int q^2 Z(q)F(q)d\mathbf{q} = -\frac{\hbar^2(\alpha\rho)^{2/3}}{(4\pi)^3 m}\left[\int q^2\frac{F(q)}{1-F(q)}\int e^{i\mathbf{q}\cdot\mathbf{s}}\ln\{1-\alpha G(s)\}d\mathbf{s}d\mathbf{q}-\alpha\left(\frac{1}{2\pi}\right)^3\int\mathbf{q}\cdot\mathbf{q}'\frac{F^2(q)}{1-F(q)}F(|\mathbf{q}'-\mathbf{q}|)Z(q')d\mathbf{q}d\mathbf{q}'\right]. \tag{16}$$

The dependence of $\mathcal{Y}(s)$, $Z(q)$, and $\langle \mathrm{KE}\rangle$ on α can be made completely explicit by introducing the power

[10] H. S. Green, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1960), Vol. 10.

series expansions

$$\mathcal{Y}(s)=\sum_{n=1}^{\infty}\alpha^n\mathcal{Y}_n(s),$$

$$Z(q)=\sum_{n=1}^{\infty}\alpha^n Z_n(q), \tag{17}$$

$$\int e^{i\mathbf{q}\cdot\mathbf{s}}\ln[1-\alpha G(s)]d\mathbf{s}=-\sum_{n=1}^{\infty}\frac{\alpha^n}{n}F_n(q),$$

in which

$$Z_n(q)=\int e^{i\mathbf{q}\cdot\mathbf{s}}\mathcal{Y}_n(s)d\mathbf{s},$$

$$F_n(q)=\int e^{i\mathbf{q}\cdot\mathbf{s}}G^n(s)d\mathbf{s} \tag{18}$$

$$=\left(\frac{1}{2\pi}\right)^3\int F_1(|\mathbf{q}'-\mathbf{q}|)F_{n-1}(q')d\mathbf{q}',$$

and Eq. (16) becomes

$$\frac{\langle\mathrm{KE}\rangle}{N}=-\frac{\hbar^2(\alpha\rho)^{2/3}}{(4\pi)^3 m}\sum_{n=1}^{\infty}\alpha^n\left[\frac{1}{n}\int q^2 Z_1(q)F_n(q)d\mathbf{q}\right.$$
$$+\left(\frac{1}{2\pi}\right)^3\int\mathbf{q}\cdot\mathbf{q}'F_1(|\mathbf{q}'-\mathbf{q}|)F_1(q)$$
$$\left.\times Z_1(q)Z_{n-1}(q')d\mathbf{q}d\mathbf{q}'\right]. \tag{19}$$

Equation (19) involves two approximations, the BDJ form of the trial wave function and the Kirkwood superposition form for the three-particle distribution function. The first is unavoidable in the present context, but the second can be replaced by a better approximation. Abe[11] derives the form

$$p_A(1,2,3)=\rho^3 g(r_{12})g(r_{23})g(r_{31})$$
$$\times\exp\left[\rho\int\{g(r_{14})-1\}\{g(r_{24})-1\}\right.$$
$$\left.\times\{g(r_{34})-1\}d\mathbf{r}_4+\cdots\right] \tag{20}$$

for the three-particle distribution function generated by the classical partition function describing equilibrium states of a gas of interacting particles at low density. The complete argument of the exponential factor in Eq. (20) is a power series in the density with coefficients which are functionals of $g(r)-1$.

The identity in mathematical structure of the classical N-particle equilibrium distribution function and the BDJ trial function has the consequence that Abe's derivation of p_A applies also to the three-particle distribution function generated by the BDJ trial function (under a suitable limiting condition on the density—in the Coulomb problem $\rho\to\infty$). The application of Eq. (20) to study the ground state of a charged-boson gas at high density is developed in Sec. 6.

[11] R. Abe, Progr. Theoret. Phys. (Kyoto) **21**, 421 (1959).

4. THE UNIFORM LIMIT

The mean potential energy of Eq. (8) can be expressed simply in terms of $F(q)$ and the Fourier transform of $v(r)$. The latter quantity is

$$h(k)=\int e^{i\mathbf{k}\cdot\mathbf{r}}v(r)d\mathbf{r}. \tag{21}$$

Note that $k=(\alpha\rho)^{1/3}q$. Then

$$\frac{\langle\mathrm{PE}\rangle}{N}=\tfrac{1}{2}\rho h(0)-\frac{\alpha\rho}{4\pi^2}\int_0^{\infty}F(q)h(\alpha^{1/3}\rho^{1/3}q)q^2dq. \tag{22}$$

Suppose now that the correct value of α is small ($\alpha\ll 1$) so that only the leading term need be retained in the mean kinetic energy represented by Eq. (19). This condition defines the uniform limit in the sense that the radial distribution function is nearly constant. A physical basis for the uniform limit may be found in low density and weak interaction as in the usual statement of conditions for the validity of the Bogoliubov approximation.

Also, as pointed out by Foldy[6] and Lieb,[12] the uniform behavior is produced by high density in conjunction with some weak constraints on the potential. In all cases, the assumption that the potential possesses a Fourier transform rules out comparison of the present development with calculations based on a hard core or strongly singular potential. Under the assumed condition ($\alpha\ll 1$) the energy formula reduces to

$$\frac{E-\frac{1}{2}\rho h(0)}{N}=\alpha^{5/3}\frac{\hbar^2\rho^{2/3}}{16\pi^2 m}\int_0^{\infty}\frac{q^4F^2(q)}{1-F(q)}dq$$
$$-\frac{\alpha\rho}{4\pi^2}\int_0^{\infty}F(q)h(\alpha^{1/3}\rho^{1/3}q)q^2dq. \tag{23}$$

Inspection of Eq. (23) reveals that the optimum function $F(q)$ can depend on α only through the combination $k=(\alpha\rho)^{1/3}q$. Consequently Eq. (23) can be expressed simply in terms of the variable k and the liquid structure function

$$S(k)=1+\rho\int e^{i\mathbf{k}\cdot\mathbf{r}}[g(r)-1]d\mathbf{r}$$
$$=1-F(q). \tag{24}$$

[12] E. H. Lieb, Phys. Rev. **130**, 2518 (1963).

The new form is

$$\frac{E-\frac{1}{2}\rho h(0)}{N}=\frac{\hbar^2}{16\pi^2 m\rho}\int_0^\infty \frac{[1-S(k)]^2}{S(k)}k^4dk$$
$$-\frac{1}{4\pi^2}\int_0^\infty [1-S(k)]h(k)k^2dk. \quad (25)$$

The supplementary conditions

$$G(0)=\left(\frac{1}{2\pi}\right)^3\int F(q)d\mathbf{q}=1,$$
$$\int G(s)d\mathbf{s}=F(0)=1, \quad (26)$$

become

$$\int_0^\infty [1-S(k)]k^2dk=2\pi^2\alpha\rho$$
$$S(0)=0. \quad (27)$$

The optimum liquid-structure function is determined by the condition for minimum energy:

$$\int_0^\infty \delta S(k)\left[\frac{\hbar^2}{4m\rho}k^2\left(1-\frac{1}{S^2(k)}\right)+h(k)\right.$$
$$\left.+\frac{\hbar^2}{4m\rho}k^2\frac{\delta S(k)}{S^3(k)}\right]k^2dk\geqq 0 \quad (28)$$

or

$$S(k)=\left[1+\frac{4m\rho h(k)}{\hbar^2k^2}\right]^{-1/2}, \quad (29)$$

provided that

$$2\rho h(k)+(\hbar^2k^2/2m)>0. \quad (30)$$

The supplementary conditions are satisfied without need for terms associated with Lagrangian multipliers. Equation (30) requires $h(0)>0$; in addition, Eq. (27) defines α as a function of ρ for given $S(k)$:

$$\alpha=\frac{1}{2\pi^2\rho}\int_0^\infty\left[1-\left\{1+\frac{4m\rho h(k)}{\hbar^2k^2}\right\}^{-1/2}\right]k^2dk. \quad (31)$$

The Bijl-Feynman formula[1,13] for the energy of an elementary excitation

$$\epsilon(k)=\hbar^2k^2/2mS(k) \quad (32)$$

now yields

$$\epsilon(k)=[(\hbar^2k^2/2m)^2+2(\hbar^2k^2/2m)\rho h(k)]^{1/2} \quad (33)$$

in agreement with Bogoliubov and Zubarev.[2] Notice that the right-hand member of Eq. (13) is not involved in the derivation of Eqs. (23)–(33). This means that the approximate (or incorrect) features of $p_K(1,2,3)$ do not enter into the derivations.

[13] R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).

5. THE YUKAWA POTENTIAL

$$v(r)=(Ze)^2e^{-k_0r}/r, \quad (34)$$
$$h(k)=4\pi(Ze)^2/(k_0^2+k^2). \quad (35)$$

To simplify the notation, introduce

$$r_s=(3/4\pi\rho)^{1/3},$$
$$t=\left[\frac{1}{12Z^2}\frac{\hbar^2}{me^2}r_s^3\right]^{1/4}k,$$
$$t_0=\left[\frac{1}{12Z^2}\frac{\hbar^2}{me^2}r_s^3\right]^{1/4}k_0, \quad (36)$$

and measure r_s and k_0^{-1} in Bohr units of length ($\hbar^2m^{-1}e^{-2}=0.5292\times10^{-8}$ cm if m and e are identified with the mass and charge of the electron). Equation (31) for α becomes

$$\alpha=r_s^{3/4}Z^{3/2}\frac{4}{\pi}\left(\frac{4}{3}\right)^{1/4}\int_0^\infty\left[1-\frac{t(t_0^2+t^2)^{1/2}}{(1+t^2(t_0^2+t^2))^{1/2}}\right]t^2dt$$
$$\leqq r_s^{3/4}Z^{3/2}\frac{4}{\pi}\left(\frac{4}{3}\right)^{1/4}\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]t^2dt. \quad (37)$$

The equality in the second line of Eq. (37) holds only in the limiting case of charged bosons ($k_0\rightarrow 0$) already investigated by Foldy[6] using the Bogoliubov approximation and by Girardeau[7] using the pair approximation. Our formalism is adapted to the charged boson gas by omitting $h(0)$ in Eq. (25) and introducing the limit $k_0\rightarrow 0$ into Eqs. (25), (29), and (31).

Using the notation of Eq. (36), the energy formula for the charged-boson system reduces to

$$\frac{E}{N}=\frac{2}{\pi}(12)^{1/4}\frac{Z^{5/2}}{r_s^{3/4}}\left[\int_0^\infty\left\{1-\frac{t^2}{(1+t^4)^{1/2}}\right\}^2(1+t^4)^{1/2}t^2dt\right.$$
$$\left.-\int_0^\infty\left\{1-\frac{t^2}{(1+t^4)^{1/2}}\right\}dt\right] \quad (38)$$

with energy in Ry ($2^{-1}me^4\hbar^{-2}=13.60$ eV) and length in Bohr units.

We show in Appendix A that the three integrals appearing in Eqs. (37)–(38) can be reduced to beta functions and have the values

$$\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]t^2dt=0.6180, \quad (39)$$

$$\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]dt$$
$$=5\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]^2(1+t^4)^{1/2}t^2dt=0.8472. \quad (40)$$

Equations (A3a) and (A3b) verify the surmise that the second integral in Eq. (38) is five times as large as the first one. This surmise is based on Eq. (23) giving E as a function of α following the replacement of $h(\alpha^{1/3}\rho^{1/3}q)$ by $4\pi(Ze)^2(\alpha\rho)^{-2/3}q^{-2}$. With $\langle\mathrm{KE}\rangle$ proportional to $\alpha^{5/3}$ and $\langle\mathrm{PE}\rangle$ to $\alpha^{1/3}$ the condition for minimum energy with respect to α has the consequence

$$\langle\mathrm{KE}\rangle=-\tfrac{1}{5}\langle\mathrm{PE}\rangle. \tag{41}$$

The derivation of Eq. (41) calls for a brief comment. The function $F(q)$ is treated as given and only α is varied. Observe the contrast with Eq. (28) where α does not appear explicitly and $F(q)=1-S(k)$ is varied. The explicit development of this derivation [and the proof that it yields a formula for α consistent with Eqs. (37)] appears in Appendix D. Final results for α and E are

$$\alpha=0.8456Z^{3/2}r_s^{3/4}, \tag{42}$$

$$E/N=-(0.8031Z^{5/2}/r_s^{3/4}). \tag{43}$$

The exact value of the numerical coefficient in Eq. (43) is

$$(8(12)^{1/4}/5\pi^{3/2})\Gamma^2(\tfrac{3}{4})=0.8030786\cdots.$$

The same value is given by Lieb and Sakakura.[8] Girardeau[7] gives 0.8037 because of small errors in the evaluation of the integrals occurring in his calculation.

With $Z=1$, $r_s<\frac{1}{16}$ Bohr units appears to be safely within the range of useful accuracy of Eqs. (29), (33), (42), and (43) and the corresponding Bogoliubov and pair approximations.

With $S(k)$ known as an explicit function of k, the inverse Fourier transform of Eq. (24) serves as an integral representation for the radial distribution function $g(r)$. Plots of $g(r)$ against r, computed by numerical integration, appear in Fig. 1 for $r_s=0.01$, 0.03, and 0.06 Bohr units.

We have not used the notion of single-particle orbital. However, the occupation number N_0 of the ground-state orbital in the problem of the charged-boson system is related to the density through Foldy's equation[6]

$$(N-N_0)/N\cong 0.2114Z^{3/2}r_s^{3/4}. \tag{44}$$

Equations (37) and (39) yield immediately the connection

$$(N-N_0)/N\cong\alpha/4, \quad \alpha\ll 1. \tag{45}$$

A general translational formula (for arbitrary interaction potential) connecting α and N_0 is not apparent in the general integral relations defining α and N_0.

Consider now a general potential $v(r)$ with Fourier transform $h(k)$ subject to the inequality of Eq. (30). Suppose a parameter Ze can be chosen so that $h(k)$ is dominated by $4\pi(Ze)^2k^{-2}$. Equation (37) then applies with the inequality holding more or less strongly. In this case, uniform limiting behavior occurs at sufficiently high density.

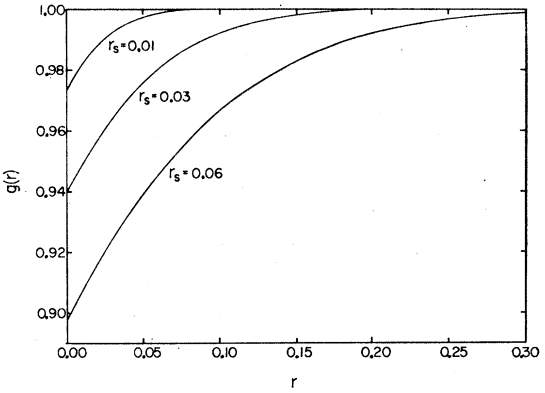

FIG. 1. Radial distribution function $g(r)$.

To find a sufficient condition for associating uniform behavior with low density let h_m denote the maximum value of $|h(k)|$. Assume also that $h(k)$ vanishes outside of a spherical region in k space $[h(k)=0,\ k>k_1]$. Equation (27) implies

$$\alpha<\frac{1}{2\pi^2\rho}\int_0^{k_1}\left[1-\left\{1+\frac{4m\rho h_m}{\hbar^2k^2}\right\}^{-1/2}\right]k^2dk. \tag{46}$$

In the low-density limit, Eq. (46) reduces to

$$\alpha<\frac{mh_mk_1}{\pi^2\hbar^2}=\frac{1}{2\pi^2}\frac{2m}{\hbar^2k_1^2}h_mk_1^3. \tag{47}$$

A sufficient condition for $\alpha\ll 1$ in the low-density limit is

$$h_mk_1^3\ll 2\pi^2(\hbar^2k_1^2/2m). \tag{48}$$

Note also that Eq. (48) implies

$$|v(r)|<\frac{1}{(2\pi)^3}\frac{4\pi}{3}k_1^3h_m\ll\frac{1}{3}\frac{\hbar^2k_1^2}{2m}. \tag{49}$$

These relations illustrate how low density and weak interaction together produce a special case of the uniform limit.

6. FIRST-ORDER CORRECTIONS IN THE UNIFORM LIMIT

In the uniform limit, Abe's form for the three-particle distribution function [Eq. (20)] reduces to

$$\begin{aligned}p_A(1,2,3)&=\rho^3(1-\alpha G(s_{12}))(1-\alpha G(s_{23}))(1-\alpha G(s_{31}))\\&\times\left[1-\alpha^2\int G(s_{14})G(s_{24})G(s_{34})d\mathbf{s}_4+\cdots\right].\end{aligned} \tag{50}$$

The sequential relation

$$1-\alpha G(s_{12})=\frac{1}{(N-2)\alpha\rho^3}\int p(1,2,3)d\mathbf{s}_3 \tag{51}$$

may be used to test the accuracy of Eq. (50) with the

result that the relation fails by terms of order α^2 (the Kirkwood form gives an error term of order α). We have verified that the neglected terms in the exponential factor of Eq. (20) do not contribute to the term in α^2 in Eq. (50).

Using $p_A(1,2,3)$, Eq. (13) is replaced by

$$\nabla\Big[\mathcal{Y}(s)-\int G(|\mathbf{s}'-\mathbf{s}|)\mathcal{Y}(s')d\mathbf{s}'-\ln\{1-\alpha G(s)\}\Big]$$
$$=-\alpha\int G(|\mathbf{s}'-\mathbf{s}|)G(s')\nabla'\mathcal{Y}(s')d\mathbf{s}'+\alpha\int G(s'')G(|\mathbf{s}''-\mathbf{s}|)G(|\mathbf{s}''-\mathbf{s}'|)\nabla'\mathcal{Y}(s')d\mathbf{s}'d\mathbf{s}''+\cdots. \quad (52)$$

The corresponding replacement for Eq. (15) is

$$Z(q)(1-F_1(q))=\int e^{i\mathbf{q}\cdot\mathbf{s}}\ln\{1-\alpha G(s)\}d\mathbf{s}-\alpha\frac{F_1(q)}{(2\pi)^3}\Big[\int\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}F_1(|\mathbf{q}'-\mathbf{q}|)Z(q')d\mathbf{q}'$$
$$-\int\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}F_1(|\mathbf{q}'-\mathbf{q}|)F_1(q')Z(q')d\mathbf{q}'+\cdots\Big]. \quad (53)$$

Equation (53) yields

$$Z_1(q)=-\frac{F_1(q)}{1-F_1(q)},$$
$$Z_2(q)=-\frac{F_2(q)}{1-F_1(q)}+\frac{F_1(q)}{1-F_1(q)}\left(\frac{1}{2\pi}\right)^3\Big[\int\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}F_1(|\mathbf{q}'-\mathbf{q}|)\frac{F_1(q')}{1-F_1(q')}d\mathbf{q}'-\int\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}F_1(|\mathbf{q}'-\mathbf{q}|)\frac{F_1^2(q')}{1-F_1(q')}d\mathbf{q}'\Big]. \quad (54)$$

These functions in Eq. (19) generate the mean kinetic energy per particle:

$$\frac{\langle\mathrm{KE}\rangle}{N}=\frac{\hbar^2(\alpha\rho)^{2/3}}{(4\pi)^3m}\Big[\alpha\int\frac{q^2F_1^2(q)}{1-F_1(q)}d\mathbf{q}$$
$$+\alpha^2\Big\{\frac{1}{2}\int\frac{q^2F_1(q)F_2(q)}{1-F_1(q)}d\mathbf{q}-\left(\frac{1}{2\pi}\right)^3\int\mathbf{q}\cdot\mathbf{q}'\frac{F_1^2(q)}{1-F_1(q)}F_1(|\mathbf{q}'-\mathbf{q}|)F_1(q')d\mathbf{q}'d\mathbf{q}\Big\}+\cdots\Big]. \quad (55)$$

In the k, $S(k)$ notation, the first-order correction to the mean energy per particle is

$$\frac{\delta E}{N}=\frac{\hbar^2}{(8\pi^2)^3m\rho^2}\Big[\frac{1}{2}\int k^2\left(\frac{1}{S(k)}-1\right)(1-S(k'))(1-S(|\mathbf{k}'-\mathbf{k}|))d\mathbf{k}'d\mathbf{k}$$
$$-\int\mathbf{k}\cdot\mathbf{k}'\frac{1}{S(k)}(1-S(k))^2(1-S(k'))(1-S(|\mathbf{k}'-\mathbf{k}|))d\mathbf{k}'d\mathbf{k}\Big]. \quad (56)$$

The zeroth-order $S(k)$ of the Coulomb problem from Eqs. (29) and (36) gives

$$\frac{\delta E}{N}=\left(\frac{Z}{\pi}\right)^4\Big[\frac{1}{2}\int((1+t^{-4})^{1/2}-1)(1-(1+t'^{-4})^{-1/2})(1-(1+|\mathbf{t}'-\mathbf{t}|^{-4})^{-1/2})t^2dt'dt$$
$$-\int(1+t^{-4})^{1/2}(1-(1+t^{-4})^{-1/2})^2(1-(1+t'^{-4})^{-1/2})(1-(1+|\mathbf{t}'-\mathbf{t}|^{-4})^{-1/2})\mathbf{t}\cdot\mathbf{t}'dt'dt\Big] \quad (57)$$

in Ry. The integrals in Eq. (57) have been evaluated by numerical integration with the result

$$\delta E/N=(Z/\pi)^4[\tfrac{1}{2}\times 7.6096-(1.8812-0.8061^A)]$$
$$=0.02802Z^4 \quad (58)$$

and

$$E/N=-(0.8031/r_s^{3/4})Z^{5/2}+0.02802Z^4+O(r_s^{3/4}). \quad (59)$$

The superscript A in Eq. (58) designates the correction generated by the Abe form of the three-particle distribution function. While the correction is not large it is essential to the interpretation of Eq. (59) as placing an upper limit on the true energy at high density.

We may characterize the numerical value of the constant term in Eq. (59) as the best possible within the

TABLE I. Numerical values of $\beta(p)$.

p	1	2	4	8	∞
$\beta(p)$	0.909	1.241	1.406	1.471	1.500

range of BDJ-type trial functions. With inclusion of the remainder $O(r_s^{3/4})$ Eq. (59) is an exact expectation value leaving only the limitations of the BDJ trial function to introduce error into the computed energy. A better trial function may reduce the coefficient of the constant term and/or possibly generate a term $C \ln r_s$ in the energy (with $C>0$ so that $C \ln r_s<0$ for $r_s<1$).

At this point an informative comparison can be made with results obtained by Girardeau[7] and by Lieb and Sakakura[8] in the high-density limit. The former, using a pairing-type trial function, finds

$$(E/N)_G=-(0.8031/r_s^{3/4})Z^{5/2}-\tfrac{1}{8}\ln r_s+O(r_s^0). \quad (60)$$

Notice that the logarithmic term raises the energy (since $r_s \ll 1$). Girardeau's calculation is completed by a demonstration that the leading nonpair corrections are of higher order than the logarithmic. This appears to establish the logarithmic term as the correct second term in an exact formula for E/N. For sufficiently small r_s our formula gives a lower energy than Girardeau's. Since our result is obtained by the accurate evaluation of an expectation value it should lie above the correct energy. There is a contradiction here between two apparently rigorous procedures.

Lieb and Sakakura[8] obtain

$$(E/N)_{LS}=-(0.8031/r_s^{3/4})Z^{5/2}+0.0597Z^4. \quad (61)$$

Again our energy is lower (a smaller constant term) showing that the procedure used in Ref. 8 to evaluate the energy is accurate only for the leading term in the energy formula.

7. VARIATIONAL FORMULATION OF THE CHARGED-BOSON PROBLEM

A family of radial distribution functions

$$g_B(s)=1-\alpha e^{-(s/a)^p} \quad (62)$$

are used to compute the expectation values of the kinetic and potential energy operators. The normalization condition of Eq. (10) requires

$$a=[3/4\pi(3/p)!]^{1/3}. \quad (63)$$

In atomic units the mean potential energy per particle is

$$\langle \mathrm{PE}\rangle/N=-[\beta(p)/r_s]\alpha^{1/3} \quad (64)$$

$$\beta(p)=\tfrac{3}{2}(2/p)!/[(3/p)!]^{2/3}. \quad (65)$$

Numerical values of $\beta(p)$ appear in Table I.

For given p and sufficiently low density ($r_s \gg 1$) the kinetic energy becomes negligible (even with $\alpha=1$) and the minimum value of $\langle H\rangle$ with respect to α occurs at $\alpha=1$. It is clear that the best value of p is then a monotonic increasing function of r_s so that $p=\infty$ (a rectangular distribution) is associated with $r_s=\infty$. Equation (64) and Table I give the proof. The limiting value of β, $\beta(\infty)=1.5$, falls short by 20% of the correct value 1.792 derived from Wigner's static body-centered crystal model.[14] This discrepancy points to the need for an oscillatory behavior of $g(s)-1$ for large r_s at low densities. Preliminary studies have shown that great care is needed in choosing oscillatory forms of $g(s)$ to avoid conflict with necessary conditions implied by the definition [Eq. (2)] relating $g(s)$ to a many-particle state function. We believe that reasonable approximations to the monatonic functions $g(s)$ defined by Eq. (62) can be generated by many-particle trial functions of the Jastrow type.

To compute the kinetic energy we employ the Wu-Feenberg functional[9]

$$\begin{aligned} &J=2J_1-J_{2a}-J_{2b},\\ &J_1=4\pi\int_0^\infty \frac{dg}{ds}\frac{d\mathcal{Y}}{ds}s^2ds,\\ &J_{2a}=4\pi\int_0^\infty g\left(\frac{d\mathcal{Y}}{ds}\right)^2 s^2ds, \qquad (66)\\ &J_{2b}=\frac{1}{\alpha}\int[g(s_{23})-1]g(s_{12})g(s_{13})\frac{d\mathcal{Y}(s_{12})}{ds_{12}}\frac{d\mathcal{Y}(s_{13})}{ds_{13}}\\ &\qquad\times\cos(12,13)d\mathbf{s}_2d\mathbf{s}_3, \end{aligned}$$

in which $s=(\alpha\rho)^{1/3}r$. One verifies easily that the requirement that J be stationary with respect to variations in $\mathcal{Y}(s)$ yields Eq. (6) [with $\mathcal{Y}(s)=u(r)$] as the appropriate Euler-Lagrange equation. Also, if $\mathcal{Y}$ satisfies Eq. (6), J reduces to J_1. In atomic units [as in Eq. (38)] the expectation value of the kinetic energy per particle is

$$\frac{\langle \mathrm{KE}\rangle}{N}=\frac{1}{16}\left(\frac{6}{\pi}\right)^{2/3}\frac{1}{r_s^2\alpha^{1/3}}J_{\text{extremum}}. \quad (67)$$

Any trial function $\mathcal{Y}(s)$ in J may be replaced by $\mathcal{Y}(s)$ and γ determined to give J an extreme value:

$$\gamma=J_1/J_2, \quad J_2=J_{2a}+J_{2b}, \quad J=J_1^2/J_2. \quad (68)$$

The BBGKY relation was first applied to a pure state by Ryuzo Abe[3] in a study of the ground state of liquid He^4. Wu and Feenberg[9] introduced the functional J and found by numerical trials that the extreme value is a maximum in physical problems. The proof that J_{extremum} is a maximum is trivial in the special case

[14] E. P. Wigner, Trans. Faraday Soc. 34, 678 (1938).

$g(s)\leqq 1$. We find

$$|J_{2b}|\leqq\int g^2(s)\left(\frac{d\mathcal{Y}}{ds}\right)^2 d\mathbf{s}\leqq J_{2a}. \tag{69}$$

Consequently J_2 is positive and the extreme value in Eq. (67) is a maximum. Spurious solutions may occur using the homogeneous form of Eq. (68). These have $J_1=0$ and need not concern us.

A slight modification in notation proves helpful in evaluating J_{2b}. Let

$$dW(s)/ds=g(s)[d\mathcal{Y}(s)/ds], \tag{70}$$

and fix $W(s)$ by requiring $W(\infty)=0$. This defines a function which can be characterized in a qualitative manner on the strength of Eq. (6) as generally resembling $g(s)-1$. The integrals making up J now become

$$\begin{aligned} J_1&=4\pi\int_0^\infty \frac{1}{g}\frac{dg}{ds}\frac{dW}{ds}s^2ds,\\ J_{2a}&=4\pi\int_0^\infty \frac{1}{g}\left(\frac{dW}{ds}\right)^2 s^2ds,\\ J_{2b}&=\frac{1}{\alpha}\int \nabla_1 W(s_{12})\cdot\nabla_1 W(s_{13})[g(s_{23})-1]d\mathbf{s}_2 d\mathbf{s}_3. \end{aligned} \tag{71}$$

The last integral can be expressed simply in terms of the Fourier transforms of $g-1$ and W: $S(q)$ and

$$R(q)=\int e^{i\mathbf{q}\cdot\mathbf{s}}W(s)d\mathbf{s} \tag{72}$$

lead to

$$J_{2b}=\frac{1}{2\pi^2\alpha}\int_0^\infty q^4R^2(q)[S(q)-1]dq. \tag{73}$$

8. APPROXIMATE EVALUATION OF THE KINETIC ENERGY

With $g(s)$ given by Eq. (62) a suitable trial function for $W(s)$ is

$$W(s)=-\gamma e^{-z(s/a)^p}. \tag{74}$$

The amplitude parameter γ disappears from the homogeneous form of J [Eq. (68)] leaving the scale factor z as the only free parameter.

The function

$$K_p(\alpha,z)=\sum_{n=0}^{\infty}\frac{\alpha^n}{(n+1+z)^{2+1/p}} \tag{75}$$

occurs in both J_1 and J_{2a}. We find

$$\begin{aligned} J_1&=4\pi z\alpha a(p+1)(1/p)!K_p(\alpha,z),\\ J_{2a}&=4\pi z^2a(p+1)(1/p)![\alpha K_p(\alpha,2z)+(2z)^{-2-1/p}]. \end{aligned} \tag{76}$$

The function J_{2b} is evaluated in Appendix B. Explicit forms are given for the special cases $p=1$ and 2 and $p\gg 2$. Explicit formulas for J at $p=1$, 2, and $p\gg 2$ follow:

$p=1$

$$J=32\pi^{2/3}\alpha^2\{K_1(\alpha,z)\}^2\Big/\left[8\alpha K_1(\alpha,2z)+\frac{1}{z(z+1)^2}+\frac{2}{z(z+1)^3}+\frac{3}{z(z+1)^4}+\frac{4}{z(z+1)^5}\right]; \tag{77}$$

$p=2$

$$J=6\pi\alpha^2\{K_2(\alpha,z)\}^2\Big/\left[\alpha K_2(\alpha,2z)+\left(\frac{1}{2z}\right)^{5/2}-\left(\frac{1}{z(z+2)}\right)^{5/2}\right]; \tag{78}$$

$p\gg 2$

$$J=(p+1)4\pi(3/4\pi)^{1/3}J',\quad J'=\frac{\alpha^2\{K_\infty(\alpha,z)\}^2}{\alpha K_\infty(\alpha,2z)+1/(2z)^2}. \tag{79}$$

These functions vanish at $z=0$ and $z=\infty$ and attain a single maximum at some intermediate value $z_m(\alpha)$. The same behavior is expected at $p=4$. Numerical calculations verify this expectation. Plots of $J/\alpha^{1/3}$ against z (for $p=2$) are exhibited in Fig. 2. Values of $z_m(\alpha)$ and associated numerical results appear in Table II.

TABLE II. Values of z_m and associated numerical values of $J/\alpha^{1/3}$.

p	α	$\ll 1$	0.2	0.4	0.6	0.8	1.0
1	z_m	0.65	0.65	0.66	0.67	0.68	0.70
	$J/\alpha^{1/3}$	$1.432\alpha^{5/3}$	0.1024	0.3423	0.7168	1.256	2.065
2	z_m	0.60	0.60	0.60	0.60	0.60	0.60
	$J/\alpha^{1/3}$	$5.895\alpha^{5/3}$	0.4163	1.379	2.874	5.055	8.644
4	z_m	0.77	0.77	0.77	0.77	0.77	0.77
	$J/\alpha^{1/3}$	$12.58\alpha^{5/3}$	0.8958	3.001	6.350	11.44	20.90
∞	z_m						1.02
	$J'/\alpha^{1/3}$						0.6450

In the extreme case $p\gg 2$, the parameter p can be determined as a function of $z_m(\alpha)$, α, and r_s. First of all an explicit formula for $\beta(p)$ as a function of p can be derived from[15,16]

$$\begin{aligned} x!&=[(1-x)\pi x/(1+x)\sin\pi x]^{1/2}e^{\Lambda(x)}\\ \Lambda(x)&=c_1x-c_3x^3+\cdots \end{aligned} \tag{80}$$

[15] Jahnke-Emde-Lösch, *Tables of Higher Functions* (McGraw-Hill Book Company, Inc., New York, 1960), 6th ed., p. 5, p. 298.
[16] N. Nielsen, *Handbuch der Theorie der Gammafunktion* (Teubner, Leipsig, 1906), p. 38.

valid for $x \ll 1$. We find

$$\beta(p)=\frac{3}{2}\left(1-\frac{\pi^2}{6p^2}+\cdots\right), \quad p\gg 2. \tag{81}$$

The total energy is now an explicit function of p: in atomic units

$$\frac{E_0}{N}=\frac{3pJ'}{4r_s^2}-\frac{3}{2}\left(1-\frac{\pi^2}{6p^2}\right)\frac{\alpha^{1/3}}{r_s}. \tag{82}$$

Minimum energy with respect to p and α is found at $\alpha=1$ with

$$p=(2\pi^2 r_s/3J')^{1/3}=2.169 r_s^{1/3} \tag{83}$$

and has the value

$$\begin{aligned}\frac{E_0}{N}&=-\frac{3}{2}\left(1-\frac{\pi^2}{2p^2}\right)\frac{1}{r_s}\\&=-\frac{3}{2r_s}+\frac{1.574}{r_s^{5/3}}.\end{aligned} \tag{84}$$

Equations (81)–(83) are valid provided that Eq. (83) determines p in agreement with the initial premise $p\gg 2$. This requires $r_s\gg 1$ (in Bohr units).

The exact energy formula at low densities, incorporating the potential energy of the body-centered electron lattice and the associated zero-point vibrational energy[6,14] is

$$\frac{E}{N}=-\frac{1.792}{r_s}+\frac{2.65}{r_s^{3/2}}. \tag{85}$$

Our formula [Eq. (84)] exhibits a certain family resemblance to Eq. (85); however, the differences are important (20% deficiency in the potential energy and $r_s^{-10/6}$ instead of $r_s^{-9/6}$ in the vibrational energy) and indicate the difficulty in generating a quantitative description of the low-density system starting from the BDJ trial function.

$p=4$

$$J=\frac{20\pi^{2/3}(\frac{1}{4})!\alpha^2}{[\frac{4}{3}(\frac{3}{4})!]^{1/3}}\times\frac{\{K_4(\alpha,z)\}^2}{\alpha K_4(\alpha,2z)+(1/2z)^{9/4}-(32/5\sqrt{2}\pi^2 z^{7/2})I(z)} \tag{86}$$

with $I(z)$ defined and tabulated in Appendix B.

9. EVALUATION OF THE ENERGY AT INTERMEDIATE AND LOW DENSITIES

Equations (64) and (67) give the total energy per particle

$$\frac{E}{N}=\frac{1}{16}\left(\frac{6}{\pi}\right)^{2/3}\frac{1}{r_s^2\alpha^{1/3}}J_{\rm ext}-\frac{\beta(p)\alpha^{1/3}}{r_s}. \tag{87}$$

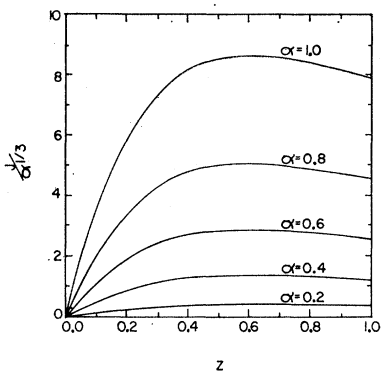

FIG. 2. Plots of $J/\alpha^{1/3}$ against z for $p=2$. The maximum value of J is attained at $z=0.60$ for each value of α.

The approximate procedure based on Eqs. (62) and (74) can be tested in the high-density region where the energy is known accurately. In this region

$$J_{\rm ext}\cong\alpha^2 L(p) \tag{88}$$

and hence minimum energy as a function of α occurs at

$$\alpha=(\pi/6)^{1/2}[16\beta(p)r_s/5L(p)]^{3/4} \tag{89}$$

with the value

$$\begin{aligned}(E/N)_{\rm min}&=-A(p)/r_s^{3/4}\\A(p)&=\tfrac{4}{5}(\pi/6)^{1/6}[16\beta(p)/5L(p)]^{1/4}\beta(p).\end{aligned} \tag{90}$$

Numerical results appear in Table III. For $p=2$, $A(p)$ exceeds the correct value 0.8031. This is possible because the approximate evaluation of $J_{\rm ext}$ underestimates the mean kinetic energy. The actual closeness to the correct value offers support for the view that the approximate procedure is at least moderately accurate in the intermediate and near low-density range. Numerical results over the range $0.01\leqq r_s\leqq 100$ for $p=1$, 2, 4 and $p\gg 2$ are plotted in Fig. 3.

The use of a specific trial function $W(s)$ in evaluating $J_{\rm ext}$ is an unnecessary approximation. We obtain a

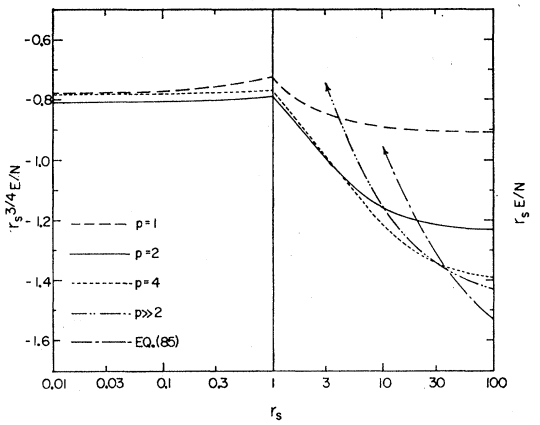

FIG. 3. Ground-state energies computed by the approximate method. Values of $r_s^{3/4}E/N$ and r_sE/N are shown over the ranges $0.01\leqq r_s\leqq 1$ and $1\leqq r_s\leqq 100$, respectively. The exact low-density formula [Eq. (85)] is also plotted.

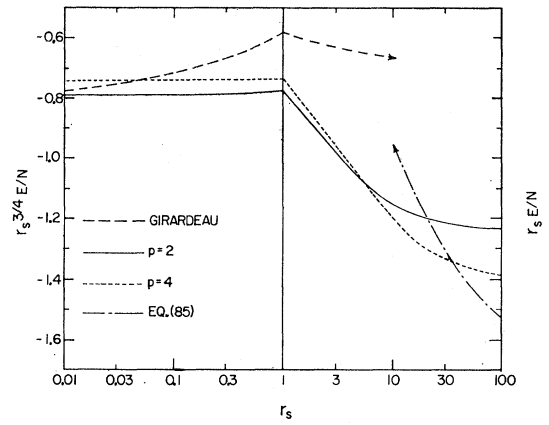

FIG. 4. Ground-state energies computed by the variation-iteration procedure. Values of $r_s^{3/4}E/N$ and r_sE/N are shown over the ranges $0.01 \leqq r_s \leqq 1$ and $1 \leqq r_s \leqq 100$, respectively. The exact low-density formula [Eq. (85)] is also plotted as well as Girardeau's results.

correct numerical evaluation of $J_{\text{ext}}(p,\alpha)$ by a variation-iteration procedure applied to Eq. (6). The iteration process begins with the starting approximation $\mathcal{Y}(s) = \lg(s)$ and continues until two successive values of J_{ext} differ by less than 0.2%. At each stage a best

TABLE III. Numerical values of $L(p)$, $\alpha/r_s^{3/4}$, and $A(p)$.

p	1	2	4
$L(p)$	1.432	5.895	12.58
$\alpha/r_s^{3/4}$	1.231	0.5380	0.3347
$A(p)$	0.7790	0.8072	0.7811

linear combination of all available successive approximations is determined by making the associated J as large as possible. Numerical results appear in Tables IV and V. Figure 4 exhibits the results of these computations. Points computed by Girardeau are also shown as well as the exact low-density behavior [Eq. (85)].

TABLE IV. $\alpha/r_s^{3/4}$ and $-r_s^{3/4}E/N$ for $r_s \ll 1$ by the variation-iteration procedure.

p	2	4	Exact
$\alpha/r_s^{3/4}$	$0.5036Z^{3/2}$	$0.2878Z^{3/2}$	$0.8456Z^{3/2}$
$-r_s^{3/4}E/N$	$0.7897Z^{5/2}$	$0.7427Z^{5/2}$	$0.8031Z^{5/2}$

Our energies fall below those computed by Girardeau. The comparison is between "expectation values" obtained from nearly optimum BDJ-type trial functions

TABLE V. α and $-E/N$ for intermediate density by the variation-iteration procedure ($Z=1$).

	$p=2$		$p=4$		Girardeau
r_s	α	$-E/N$	α	$-E/N$	$-E/N$
0.01	0.016	25.0			24.6
0.03	0.036	11.0			10.5
0.10	0.089	4.44	0.052	4.17	4.05
0.30	0.20	1.94	0.12	1.83	1.65
1.0	0.46	0.776	0.29	0.738	0.582
3.0	0.83	0.327	0.58	0.319	0.211
10.0	1.00	0.115	0.93	0.120	0.0666
30.0	1.00	0.0404	1.00	0.0445	
100.0	1.00	0.0123	1.00	0.0138	

and expectation values with respect to the pair-type trial function of Girardeau. At high densities the quotes on "expectation values" should be omitted [as is clear from the discussion following Eq. (59)]. We hesitate to draw a strong conclusion from the apparent superiority of our method because the use of $p_K(1,2,3)$ in evaluating J_{ext} means that our computed energies are not true expectation values (except at high densities). Nevertheless the behavior at very high and very low densities is consistent with the statement that the use of $p_K(1,2,3)$ in evaluating J_{ext} in conjunction with a family of monatonic trial function for $g(r)$ does not falsify the interpretation of our computed energy as an upper limit on the true eigenvalue (over the entire density range).

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APPENDIX A: EVALUATION OF INTEGRALS OCCURING IN SEC. 5

The integrals in Eqs. (37)–(38) are readily evaluated with the aid of an identity in the theory of beta functions[17]:

$$\int_0^1 \frac{\xi^{x-1}(1-\xi)^{y-1}}{(a+\xi)^{x+y}}d\xi = \frac{B(x,y)}{(1+a)^x a^y}. \tag{A1}$$

With the change of variable

$$\xi = t^2/(1+t^4)^{1/2}$$

the integrals in Eqs. (37)–(38) reduce to

$$\int_0^\infty \left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]t^2dt = \frac{1}{2}\int_0^1 \frac{\xi^{1/2}(1-\xi)^{-3/4}}{(1+\xi)^{7/4}}d\xi = (1/2^{5/2})B(\tfrac{3}{2},\tfrac{1}{4}) = \Gamma^2(\tfrac{1}{4})/12\sqrt{\pi} = 0.6180248\cdots, \tag{A2}$$

[17] W. Magnus and F. Oberhettinger, *Formulas and Theorems for Mathematical Physics* (Chelsea Publishing Company, New York, 1949), p. 4.

$$\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]^2(1+t^4)^{1/2}t^2dt=\frac{1}{2}\int_0^1\frac{\xi^{1/2}(1-\xi)^{-1/4}}{(1+\xi)^{9/4}}d\xi=(1/2^{5/2})B(\tfrac{3}{2},\tfrac{3}{4})=\Gamma^2(\tfrac{3}{4})/5\sqrt{\pi}=0.1694426\cdots, \quad \text{(A3a)}$$

$$\int_0^\infty\left[1-\frac{t^2}{(1+t^4)^{1/2}}\right]dt=\frac{1}{2}\int_0^1\frac{\xi^{-1/2}(1-\xi)^{-1/4}}{(1+\xi)^{5/4}}d\xi=(1/2^{3/2})B(\tfrac{1}{2},\tfrac{3}{4})=\Gamma^2(\tfrac{3}{4})/\sqrt{\pi}=0.8472130\cdots. \quad \text{(A3b)}$$

Note that suitable changes of variable and/or integrations by parts reduce these integrals to those already evaluated by Foldy [Eqs. (A2) and (A3a)], Lieb and Sakakura [Eq. (A3a)], and Girardeau [Eqs. (A3a) and (A3b)].

APPENDIX B

Evaluation of J_{2b} Using Eqs. (72) and (74)

p=1

$$J_{2b}=\pi z^2a\left[-\frac{1}{z^3}+\frac{1}{z(z+1)^2}+\frac{2}{z(z+1)^3}+\frac{3}{z(z+1)^4}+\frac{4}{z(z+1)^5}\right]. \quad \text{(B1)}$$

p=2

$$J_{2b}=-6\pi^{3/2}z^2a[z(z+2)]^{-5/2}. \quad \text{(B2)}$$

p≫2

The substitution

$$-\frac{d}{ds}e^{-z(s/a)^p}\rightarrow\frac{z^{1/p}}{a}\delta\left(z^{1/p}\frac{s}{a}-1\right) \quad \text{(B3)}$$

is a good approximation for large values of p. This yields

$$J_{2b}\rightarrow-8\pi^2\left(\frac{a}{z^{1/p}}\right)^4\int_{-1}^1e^{-z^{-1}[2(1-\mu)]^{p/2}}\mu d\mu \quad \text{(B4)}$$

$$\rightarrow-\frac{9\pi}{4}a.$$

p=4

The Fourier form [Eq. (73)] is convenient in this case, but must be implemented by evaluation of the Fourier transforms of e^{-x^4}. Let

$$\eta_4(q)=\frac{1}{4\pi}\int e^{i\mathbf{q}\cdot\mathbf{x}}e^{-x^4}d\mathbf{x}$$

$$=-\frac{1}{q}\int_0^\infty e^{-x^4}x\sin(qx)dx$$

$$=-\frac{1}{4}\sum_{n=0}^\infty\frac{(-1)^n}{(2n+1)!}\left(\frac{2n-1}{4}\right)!q^{2n}$$

$$=\tfrac{1}{3}(\tfrac{3}{4})!\eta_{4e}(q)-\tfrac{1}{4}(\tfrac{1}{4})!\eta_{40}(q), \quad \text{(B5)}$$

$$\eta_{4e}(q)=1+\frac{1}{5!}\frac{3}{4}q^4+\frac{1}{9!}\frac{3}{4}\frac{7}{4}q^8+\cdots,$$

$$\eta_{40}(q)=\frac{1}{3!}q^2+\frac{1}{7!}\frac{5}{4}q^6+\frac{1}{11!}\frac{5}{4}\frac{9}{4}q^{10}+\cdots. \quad \text{(B6)}$$

The useful range of the power series expansion is limited by the accuracy with which the factorial coefficients $(\frac{1}{4})!$ and $(\frac{3}{4})!$ are known. With the factorials given to nine significant figures[15] the power series is useful up to $q=13$. (See Table BI.) The error begins to be considerable at $q=14$. A useful asymptotic formula can be derived by writing

$$q\eta_4(q)=\frac{1}{2i}\int_{-\infty}^\infty e^{-x^4+iqx}xdx. \quad \text{(B7)}$$

The path of integration can be displaced parallel to the real axis until points of maximum amplitude and of stationary phase coincide. A Gaussian-type approximation to the behavior of the integrand in the neighborhood of the points of maximum amplitude then yields approximate evaluation of the integral good for sufficiently large values of q ($q\gg2$). The derivation of the asymptotic formula is somewhat lengthy and here we give only the result:

$$\eta_4(q)\cong\frac{(\pi/6)^{1/2}}{q}e^{-24(q/32)^{4/3}}\left[1+\frac{5}{2304(q/32)^{4/3}}\right]^{1/2}\times\sin\left\{24\sqrt{3}(q/32)^{4/3}+\frac{5\sqrt{3}}{4608(q/32)^{4/3}}\right\}. \quad \text{(B8)}$$

In Table BI numerical results for $\eta_4(q)$ computed using Eqs. (B5) and (B6) are compared with the asymptotic values [Eq. (B8)].

TABLE BI. Numerical values of $\eta_4(q)$.

q	Eqs. (B5), (B6)	Eq. (B8)
2	0.1826	0.1861
3	0.8699×10^{-1}	0.8634×10^{-1}
4	0.2053×10^{-1}	0.2017×10^{-1}
5	-0.7118×10^{-2}	-0.7198×10^{-2}
6	-0.9023×10^{-2}	-0.9019×10^{-2}
7	-0.3140×10^{-2}	-0.3130×10^{-2}
8	0.5628×10^{-3}	0.5655×10^{-3}
9	0.9547×10^{-3}	0.9545×10^{-3}
10	0.2536×10^{-3}	0.2532×10^{-3}
11	-0.1141×10^{-3}	-0.1141×10^{-3}
12	-0.8904×10^{-4}	-0.8901×10^{-4}
13	-0.2158×10^{-5}	-0.2157×10^{-5}
14	0.1704×10^{-4}	0.1697×10^{-4}

TABLE BII. $I(z)$.[a]

z	0.5	0.6	0.7	0.8	0.9	1.0
$I(z)$	0.09269	0.1098	0.1263	0.1419	0.1569	0.1715

[a] The second form of the integral defining $I(z)$ suggests the approximate relation $I(z)\cong z^{5/6}I(1)$ for $|z-1|\ll 1$. In fact, the relation is still moderately good at $z=0.5$.

Equations (63), (73), and (74) combine to yield

$$J_{2b}=\frac{24a}{(\frac{3}{4})!z^{3/2}}I(z)$$
$$I(z)=\int_0^\infty x^4\eta_4{}^2(x/z^{1/4})\eta_4(x)dx \tag{B9}$$
$$=z^{5/6}\int_0^\infty x^4\eta_4{}^2(x/z^{1/12})\eta_4(z^{1/6}x)dx.$$

Numerical results for $I(z)$ are listed in Table BII.

APPENDIX C

Relation between $\delta\Psi_0{}^B$ and $\delta S(k)$ in the Uniform Limit

The freedom in $S(k)$ needed to derive Eq. (28) follows from the direct connection between $S(k)$ and the many-particle trial function $\Psi_0{}^B$. We are not postulating an arbitrary liquid-structure function, but one subject to all the constraints implicit in the connection with the Jastrow-type trial function from which the analysis starts. Thus, with $\alpha\ll 1$, Eqs. (14) and (15) yield

$$Z(q)=\frac{\alpha F(q)}{1-F(q)},$$
$$\mathfrak{U}(r)\equiv\mathfrak{Y}(s)=\alpha\left(\frac{1}{2\pi}\right)^3\int\frac{e^{i\mathbf{q}\cdot\mathbf{s}}F(q)}{1-F(q)}d\mathbf{q}. \tag{C1}$$

The variation $\delta S(k)$ [or $\delta F(q)$] implies

$$\delta\mathfrak{U}(r)\equiv\delta\mathfrak{Y}(s)=\alpha\left(\frac{1}{2\pi}\right)^3\int\frac{e^{i\mathbf{q}\cdot\mathbf{s}}\delta F(q)}{[1-F(q)]^2}d\mathbf{q},$$
$$\alpha\delta F(q)=[1-F(q)]^2\int e^{-i\mathbf{q}\cdot\mathbf{s}}\delta\mathfrak{Y}(s)d\mathbf{s}, \tag{C2}$$

and

$$\delta\Psi_0{}^B=\tfrac{1}{2}\Psi_0{}^B\sum_{i<j}\delta\mathfrak{U}(r_{ij}). \tag{C3}$$

We may start with given $\mathfrak{U}(r)$ (assumed to possess a Fourier transform) and limit $\delta\mathfrak{U}(r)$ to functions possessing a Fourier transform. Equation (C2) determines an allowed class of variations $\delta S(k)$. This class is obviously sufficiently wide to permit the statement of Eq. (29) as a consequence of Eq. (28).

APPENDIX D

Evaluation of E, $\langle\mathbf{KE}\rangle/\langle\mathbf{PE}\rangle$, and α for the High-Density Charged-Boson System

Equation (23) reduces to

$$\frac{E}{N}=\alpha^{5/3}\frac{\hbar^2\rho^{2/3}}{16\pi^2m}\int_0^\infty\frac{q^4F^2(q)}{1-F(q)}dq - (\alpha\rho)^{1/3}\frac{(Ze)^2}{\pi}\int_0^\infty F(q)dq. \tag{D1}$$

Minimum E with respect to α is found at

$$\alpha^{4/3}=\frac{16\pi}{5}\frac{(Ze)^2m}{\hbar^2\rho^{1/3}}\left(\int_0^\infty F(q)dq\Big/\int_0^\infty\frac{q^4F^2(q)}{1-F(q)}dq\right). \tag{D2}$$

The resulting formula for E is

$$\frac{E}{N}=-\frac{4}{5\pi}\rho^{1/4}(Ze)^2\left[\frac{16\pi(Ze)^2m}{5\hbar^2}\right]^{1/4} \times\left[\int_0^\infty F(q)dq\right]^{5/4}\Big/\left[\int_0^\infty\frac{q^4F^2(q)}{1-F(q)}dq\right]^{1/4} \tag{D3}$$

and Eq. (41) follows immediately.

The optimum choice of $F(q)$ as defined by Eqs. (24) and (29) now reduces Eq. (D3) to Eq. (38). Under the same condition the formula for α [Eq. (D2)] reduces to an identity leaving Eq. (37) to determine α. This verification demonstrates the consistency of the two procedures for proving Eq. (41). Notice however that the second procedure [varying α for given and fixed $F(q)$] is more general.