Charged Boson Gas at High Density*

KEITH A. BRUECKNER
Institute for Radiation Physics and Aerodynamics, University of California, San Diego, La Jolla, California

(Received 31 October 1966)

The ground-state energy of a charged boson gas at high density is evaluated exactly to second order in the density expansion, making use of complete sums of one- and two-ring diagrams. The result agrees numerically with Feenberg's variational calculation of the energy, although the methods appear to be substantially different. The presence of logarithmic terms in the energy, which are absent in the exact result, is shown to be a result of truncation of the Hamiltonian in the pair approximation or of inadequacies of variational wave functions which omit interpair correlations.

THE ground-state energy of a charged boson gas has been considered by several authors using various techniques for determining the ground-state energy. The leading term in the energy at high density was first evaluated exactly by Foldy,[1] who realized that this term arose from the ring diagrams (involving only a single momentum transfer) which could be exactly summed by the Bogoliubov transformation. The structure of the expansion for the energy in powers of the density was also briefly discussed by Foldy and considered in more detail by Girardeau and Arnowitt,[2] Girardeau,[3] Lee and Feenberg,[4] and Wright.[5] They showed that the series is the form of

$$\frac{E}{N}=\frac{c_0}{r_s^{3/4}}+(c_1+c_2\ln r_s)+O(r_s^{3/4})+\cdots, \tag{1}$$

with r_s, the spacing per particle, measured in units of $\hbar^2/me^2$. The various authors have, however, given different values for the constant c_1 in Eq. (1) and, more important, have disagreed on the existence of the logarithmic term which dominates the correction to the lowest-order energy at high density. It is the purpose of this paper to give an exact evaluation of the constant term in the energy and to show that the logarithmic term is absent.

The Hamiltonian is

$$H=\sum_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}\frac{q^2}{2m}+\frac{1}{2}\sum_{\mathbf{q}\mathbf{q}'\mathbf{q}''} v(\mathbf{q}-\mathbf{q}'')a_{\mathbf{q}}^\dagger a_{\mathbf{q}'}^\dagger a_{\mathbf{q}''}a_{\mathbf{q}+\mathbf{q}'-\mathbf{q}''} \tag{2}$$

with

$$v(q)=\frac{4\pi e^2}{\Omega q^2}, \quad q\neq 0$$
$$=0, \quad q=0. \tag{3}$$

The vanishing of the $q=0$ matrix element of v is due to an assumed fixed positive charge background giving charge neutrality. The Hamiltonian may now be separated into

$$H=H_p+H_3+H_4 \tag{4}$$

with (we set the ground-state operators a_0 and $a_0^\dagger$ equal to $\sqrt{N_0}$)

$$H_p=\sum_{\mathbf{q}}\left\{\left[\frac{q^2}{2m}+N_0v(q)\right]a_{\mathbf{q}}^\dagger a_{\mathbf{q}}+\tfrac{1}{2}N_0v(q)(a_{\mathbf{q}}^\dagger a_{-\mathbf{q}}^\dagger+a_{\mathbf{q}}a_{-\mathbf{q}})\right\},$$
$$H_3=\tfrac{1}{2}N_0^{1/2}\sum_{\mathbf{q}\mathbf{q}'\neq 0}(a_{\mathbf{q}}^\dagger a_{\mathbf{q}'}a_{\mathbf{q}-\mathbf{q}'}+a_{\mathbf{q}'}^\dagger a_{\mathbf{q}-\mathbf{q}'}^\dagger a_{\mathbf{q}})\times[v(\mathbf{q}-\mathbf{q}')+v(q')],$$
$$H_4=\tfrac{1}{2}\sum_{\mathbf{q}\mathbf{q}'\neq 0}v(\mathbf{q}-\mathbf{q}')[a_{\mathbf{q}}^\dagger a_{-\mathbf{q}}^\dagger a_{\mathbf{q}'}a_{-\mathbf{q}'}+a_{\mathbf{q}}^\dagger a_{\mathbf{q}}a_{\mathbf{q}'}^\dagger a_{\mathbf{q}'}]$$
$$+\tfrac{1}{2}\sum_{\mathbf{q}\mathbf{q}'\mathbf{q}''\neq 0}v(\mathbf{q}-\mathbf{q}'')a_{\mathbf{q}}^\dagger a_{\mathbf{q}'}^\dagger a_{\mathbf{q}''}a_{\mathbf{q}+\mathbf{q}'-\mathbf{q}''}. \tag{5}$$

To determine the leading term in the energy, it is sufficient to evaluate the sum of the ring diagrams involving a single momentum $\mathbf{q}$. The ring diagrams may be represented as indicated in Fig. 1 or in the more compact notation of Fig. 1. These diagrams contribute to the energy in order $\rho^{1/4}$ and unity, the structure of a term of order n being [with momenta measured in

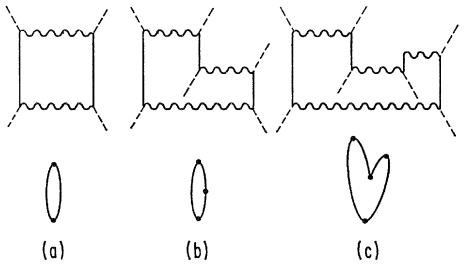


FIG. 1. Diagrammatic representation of the ring diagrams. In the upper diagrams, the condensate lines are shown as dashed lines and the interactions as wavy lines. In the lower diagrams, the condensate lines are suppressed and the interaction lines (which may include exchange) replaced by dots.

* This research was supported by the Advanced Research Projects Agency (Project DEFENDER) and was monitored by the U. S. Army Research Office (Durham) under Contract No. DA-31-124-ARO-D-257, and the U. S. Atomic Energy Commission.

[1] L. L. Foldy, Phys. Rev. **124**, 649 (1961).
[2] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).
[3] M. Girardeau, Phys. Rev. **127**, 1809 (1962).
[4] D. K. Lee and E. Feenberg, Phys. Rev. **137**, A731 (1965).
[5] D. Wright, Phys. Rev. **143**, 91 (1966).

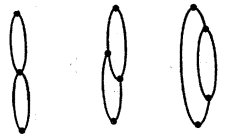
units of $(4\pi me^2\rho_0)^{1/4}$]

$$\frac{\rho_0^{5/4}}{\rho}\sum_n C_n\int dp\frac{1}{p^{4n}}, \tag{6}$$

with C_n a numerical factor resulting from the number of diagrams of a given order but with different sequences of vertices. This sum may be evaluated by the Bogoliubov transformation applied to the pair Hamiltonian H_p.

We now consider from the same viewpoint the diagrams contributing to the next term in the density expansion for the energy. These are given in Fig. 2. The density dependence of these terms is fixed in order n by the n factors of $1/\Omega$ coming from the interaction, the two factors of Ω arising from the integrals over the two momenta appearing in the two rings, and the factor $N_0{}^{n-1}$ arising from the ground-state operators at each vertex. The remaining dependence on density enters from introducing the momenta scaled in units of $(4\pi\rho_0 me^2)^{1/4}$, which give factors $(\rho_0)^{3/2}$ from the integrals over the two momenta and $\rho_0{}^{1/2-n}$ from the matrix elements of the interaction and the energy denominators. Collecting these factors gives

FIG. 2. Two-ring diagrams. In the general perturbation expansion, each closed ring is replaced by the sum of all single-ring diagrams.



$$\frac{E(2\text{ ring})}{N}\sim\frac{\Omega^2}{\Omega^n}\frac{N_0{}^{n-1}}{N}\frac{1}{\rho_0{}^{n-2}}\times(\text{dimensionless integrals over two momenta})$$

$$=\frac{\rho_0}{\rho}\times(\text{dimensionless integrals over two momenta}). \tag{7}$$

This argument does not, of course, determine the possible dependence of the energy in this order on $\ln\rho$.

A characteristic of the double-ring diagrams is the restricted appearance of the three vertex types at which a momentum transfer occurs, as indicated in Fig. 3. The X vertex occurs only once with no accompanying Y or λ vertex, and the Y and λ vertices must appear together, but only once. The other vertices associated with the operators v_{11}, v_{02}, and v_{20} may, however, appear an arbitrary number of times. The terms in the Hamiltonian giving v_{11}, v_{02}, and v_{20} must therefore be evaluated exactly, but perturbation theory in first order may be applied to the X vertex and in second order to the Y and λ vertices. This may be readily carried out by making the Bogoliubov transformation and then evaluating the nondiagonal terms in the transformed Hamiltonian by first- and second-order perturbation theory in the Bogoliubov representation. The result of this calculation may be obtained from the results given by Girardeau for the X vertex in Eqs. (7) and (8) of Ref. 3 and for the $Y\lambda$ vertices from Eq. (C1) of Ref. 3. He did not, however, correctly note certain features of the results.

The various terms for the energy per particle, in Ry, are

$$\mathcal{E}(1\text{ ring})=\frac{2(3)^{1/4}}{\pi}\frac{f^{5/4}}{r_s^{3/4}}\int_0^\infty p^2dp\left[\left(1+\frac{p^4}{4}\right)^{1/2}-\frac{p^2}{2}-\frac{1}{p^2}\right] \tag{8}$$

with

$$f=\frac{\rho_0}{\rho}=1-f\frac{r_s^{3/4}}{\pi(3)^{1/4}}\int_0^\infty p^2dp\left[\frac{p^2/2+1/p^2}{(1+p^4/4)^{1/2}}-1\right]. \tag{9}$$

Combining these results and introducing the numerical values for the integrals given by Foldy,[1] we find

$$\mathcal{E}(1\text{ ring})=-\frac{0.8031}{r_s^{3/4}(1+0.2114r_s^{3/4})^{5/4}}. \tag{10}$$

The terms from two rings are

$$\mathcal{E}_X=\frac{f}{4\pi^4}\int\frac{d\mathbf{p}d\mathbf{p}'}{(p'')^2}$$

$$\times[AA'(A^2-1)^{1/2}(A'^2-1)^{1/2}+(A^2-1)(A'^2-1)],$$

$$\mathcal{E}_{Y\lambda}=\frac{-f}{4\pi^4}\int\frac{d\mathbf{p}d\mathbf{p}'}{\omega+\omega'+\omega''}F(p,p',p'')$$

$$\times[F(p,p',p'')+F(p',p,p'')+F(p'',p,p')], \tag{11}$$

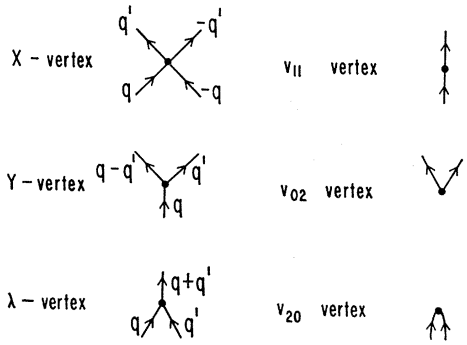


FIG. 3. Elementary vertices contributing to the two-ring diagrams.

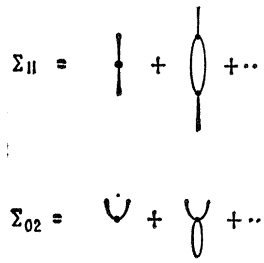


FIG. 4. Contribution to the reduced vertex operators.

with

$$\mathbf{p}''=(\mathbf{p}-\mathbf{p}'),$$

$$\omega=(1+p^4/4)^{1/2},$$

$$A=\left[\frac{p^2/2+1/p^2}{2\omega}+\frac{1}{2}\right]^{1/2},$$

$$F(p,p',p'')=\frac{A-(A^2-1)^{1/2}}{p^2}$$

$$\times[(A'^2-1)^{1/2}A''+(A''^2-1)^{1/2}A']. \quad (12)$$

The integrals in Eq. (11) are both singular for small momenta, where

$$A\rightarrow 1/(2^{1/2}p),$$

$$F(p,p',p'')\rightarrow 1/(2^{1/2}pp'p''). \quad (13)$$

The contribution in the small-momentum limit is

$$\mathcal{E}_X=-\mathcal{E}_{Y\lambda}$$

$$=\frac{f}{8\pi^4}\int\frac{d\mathbf{p}d\mathbf{p}'}{p^2(p')^2(p'')^2}. \quad (14)$$

This integral is logarithmically singular for small momenta; if a cutoff proportional to $r_s^{1/4}$ is assumed,

$$\mathcal{E}_X=-\tfrac{1}{8}f\ln r_s$$

$$=-\tfrac{1}{8}\ln r_s+O(r_s^{3/4})\ln r_s. \quad (15)$$

This term was first obtained by Girardeau[3] who evaluated the energy variationally in the pair approximation. We see, however, that the contribution $\mathcal{E}_{Y\lambda}$ arising from the nonpair contribution cancels this singularity. The sum of $\mathcal{E}_X$ and $\mathcal{E}_{Y\lambda}$ is then readily seen to be nonsingular for both small and large momenta.

The integrals in Eq. (11) have been evaluated numerically, giving the result

$$\mathcal{E}_X+\mathcal{E}_{Y\lambda}=-0.1842f. \quad (16)$$

Combining this with Eq. (10), we find

$$\mathcal{E}=-0.8031/r_s^{3/4}+0.0280+O(r_s^{3/4}). \quad (17)$$

Girardeau[3] gives numerical results at intermediate density from which the constant term in the expansion may be deduced; his result is

$$\mathcal{E}\cong-0.8031/r_s^{3/4}-\tfrac{1}{8}\ln r_s+0.18. \quad (18)$$

Feenberg's result is

$$\mathcal{E}=-0.8031/r_s^{3/4}+0.0280+O(r_s^{3/4}), \quad (19)$$

which agrees (within the accuracy of the numerical evaluation of the integrals) with the exact result of Eq. (17). This agreement suggests that Feenberg's expression [Eq. (57)] of Ref. 4 might be transformed into our Eq. (11). We have not, however, been able to demonstrate the equivalence of the two forms. The close agreement of Feenberg's result must therefore demonstrate the power and accuracy of his procedure.

The inclusion of nonpair terms, which the above analysis shows markedly affects the ground-state energy, is also important in the excitation spectrum. According to Hugenholtz and Pines,[6] the excitation energy is determined by

$$[\omega-\tfrac{1}{2}\Sigma_{11}(q)+\tfrac{1}{2}\Sigma_{11}(-q)]^2-[\Sigma_0(q)+\tfrac{1}{2}\Sigma_{11}(q)$$

$$+\tfrac{1}{2}\Sigma_{11}(-q)-\mu]^2+\Sigma_{02}^2(q)=0, \quad (20)$$

with

$$\mu=\Sigma_{11}(0)-\Sigma_{02}(0). \quad (21)$$

In Eq. (20), $\Sigma_{11}(q)$ is the sum of all irreducible diagrams with one ingoing and one outgoing line and $\Sigma_{02}(q)$ with two outgoing lines. These include in the leading orders the diagrams shown in Fig. 4, in which the X vertex and the $Y\lambda$ vertices appear together in the second-order term. Obviously a treatment of the excitation energy omitting the nonpair term in the Hamiltonian, and hence the $Y\lambda$ vertices, is correct only in first order, the proper symmetry of the irreducible parts already being lost in second order. The calculation may, however, be carried out with the inclusion of the X and $Y\lambda$ to leading order and the v_{11}, v_{02}, and v_{20} to all orders, maintaining the proper symmetry of Σ_{11} and Σ_{02} and hence satisfying the excitation-energy and self-energy theorems implied by Eqs. (20) and (21).

The author is indebted to Professor Eugene Feenberg for bringing this problem to his attention and to Mrs. Marielle Bryant for programming the integrals in Eq. (11) for CDC 3600 evaluation.

[6] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).