Analysis of the Bogoliubov Method Applied to a Simple Boson Model*

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A simple model of a boson system is considered for which the exact Schrödinger equation reduces to a difference equation which can be solved numerically. Application of the Bogoliubov method and comparison of its results with the numerical results then yield some insight into the validity of the Bogoliubov approximations. The simple model considered has, in the absence of interactions, only a zero energy state and two states of unit energy available to each boson. Initially there is assumed to be no interaction between bosons in the degenerate excited states and all existing interactions are assumed to be repulsive. The ground-state energy is calculated in the Bogoliubov approximation, with and without the depletion effect considered, and in another numerical approximation. These results and the results of the numerical solution of the exact Schrödinger equation converge to the Bogoliubov result with depletion ignored when the number of particles in the system approaches infinity. It is surprising to note that, for the interaction strengths considered, the Bogoliubov result is within 3% of the numerical result for as few as 32 particles in the system, and within 10% for only 4 particles. A modification of the above system is considered in which there exists an additional two-body interaction between particles in the degenerate excited states which may be attractive or repulsive. It is shown that the ground-state energy, with this additional interaction present, deviates from the Bogoliubov value linearly with the strength of the added interaction, i.e., $W=W_{\text{Bog}}+\alpha F$ (with F the strength parameter of the interaction). The factor α is found to be small and constant over a wide range of F and in this range the deviation of W from the Bogoliubov value is small. There is, however, a transition point F_T, beyond which α is constant and large and the usual Bogoliubov approximation is invalid for interactions more attractive than that characterized by F_T. A Bogoliubov-like approximation is shown to be quite accurate in this region. It is then shown that F_T^{-1} is a linear function of the number of particles in the system.

INTRODUCTION

IN order to supply motivation for the following analysis of a simple model of a boson system consider a system of particles constrained to a ring of radius L. If there were no interaction between the particles, each particle would be described by the Schrödinger equation

$$(-\hbar^2/2mL^2)(\partial^2\psi/\partial\theta^2)=E\psi. \tag{1}$$

The general solution to (1) is

$$\psi=Ae^{ik\theta}+Be^{-ik\theta}, \tag{2}$$

with

$$k=L(2mE)^{1/2}\hbar^{-1}. \tag{3}$$

By virtue of the required periodicity of ψ and its derivative, k and E are quantized according to

$$k=n \tag{4}$$

and

$$E=\hbar^2n^2/(2mL^2) \quad (n \text{ is any integer}). \tag{5}$$

A system of N such Bose-Einstein particles, of equal mass and zero spin, with a two-body interaction present, would be described by

$$H\Phi=W\Phi=i\hbar(\partial/\partial t)\Phi,$$

where

$$H=\sum_{i=1}^{N}\frac{\hbar^2}{2mL^2}\frac{\partial^2}{\partial\theta_i^2}+\sum_{i\neq j}v(\theta_i,\theta_j) \tag{6}$$

and Φ, the many-body wave function, is symmetric with respect to an interchange of coordinates. The solution of such a problem is often more convenient if the theory is formulated in the second quantized representation. This is, in effect, accomplished by introducing a field operator, ϕ, and its Hermitian conjugate which satisfy the usual Bose-Einstein commutation relations. If the ϕ's and $\phi^\dagger$'s are then expanded in a Fourier series, the coefficients of which are the usual creation and destruction operators, one finds for H in the second quantized representation

$$H=\sum_k \hbar^2k^2/(2m)a_k^\dagger a_k + \tfrac{1}{2}\sum_{k_1,k_2,k_3,k_4}\langle k_3k_4|v(\theta_1,\theta_2)|k_1k_2\rangle a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}a_{k_4}, \tag{7}$$

where

$$\langle k_3k_4|v(\theta_1,\theta_2)|k_1k_2\rangle = (2\pi)^{-2}\int\int d\theta_1 d\theta_2 e^{-i(k_1-k_4)L\theta_1-i(k_2-k_3)L\theta_2}v(\theta_1,\theta_2), \tag{8}$$

and $\hbar k$ is the momentum of a particle.

For simplicity let us assume that

$$v(\theta_1,\theta_2)=v(|\theta_1-\theta_2|), \tag{9}$$

in which case

$$\langle k_3k_4|v(\theta_1,\theta_2)|k_1k_2\rangle=u(k_1-k_4)\delta_{k_1+k_2,k_3+k_4}. \tag{10}$$

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Then

$$H=\sum_k \hbar^2k^2/(2m)a_k^\dagger a_k + \tfrac{1}{2}\sum_{k_1,k_2,k_3,k_4} u(k_1-k_4)\delta_{k_1+k_2,k_3+k_4}a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3}a_{k_4}. \quad (11)$$

Suppose one considered the above situation in an approximation where all but the two lowest single-particle energies were neglected. In this case, one would be led to investigate a system with only a zero-momentum state and a degenerate excited state, with equal and opposite momenta, available to the single particles. Setting the kinetic energy of a single particle in the excited state equal to unity and labeling the excited momentum states by + and −, the Hamiltonian becomes, in this approximation

$$\begin{aligned}H=&a_+^\dagger a_+ + a_-^\dagger a_- + \tfrac{1}{2}[u(+)+u(-)]\\ &\times[a_0^\dagger a_0(a_+^\dagger a_+ + a_-^\dagger a_-)+a_0^{\dagger 2}a_+a_- + a_0^2 a_+^\dagger a_-^\dagger]\\ &+\tfrac{1}{2}u(0)[a_0^\dagger a_0(2a_+^\dagger a_+ + a_0^\dagger a_0 + 2a_-^\dagger a_-)\\ &+2a_+^\dagger a_-^\dagger a_+ a_- + a_+^\dagger a_+^\dagger a_+ a_+ + a_-^\dagger a_-^\dagger a_- a_-]. \quad (12)\end{aligned}$$

In the first sections of the following, a Hamiltonian will be considered which is equal to the above, with $u(0)$ assumed to be zero. In the later sections, the effect of scattering of particles in the + state with those in the − state will be investigated. The appropriate Hamiltonian will then be the above with all terms in the last bracket ignored except $a_+^\dagger a_-^\dagger a_+ a_-$.

A SIMPLE BOSON SYSTEM

We consider a model boson system in which there are only three states available to each boson. In the absence of interactions between the bosons these states are a zero-energy state and two states of unit energy. We designate the creation and destruction operators for the zero-energy state by $a_0^\dagger$, a_0 and for the degenerate excited states by $a_+^\dagger$, a_+, $a_-^\dagger$, a_-. The interaction is such that it destroys (creates) a pair of particles in the zero-energy state while creating (destroying) a particle in each of the degenerate energy states. The Hamiltonian is then

$$\begin{aligned}H=&a_+^\dagger a_+ + a_-^\dagger a_- + g[a_0^\dagger a_0(a_+^\dagger a_+ + a_-^\dagger a_-)\\ &+a_0^{\dagger 2}a_+a_- + a_0^2 a_+^\dagger a_-^\dagger]. \quad (13)\end{aligned}$$

The total number of particles

$$N=a_0^\dagger a_0 + a_+^\dagger a_+ + a_-^\dagger a_- \quad (14)$$

is a constant of the motion, and so also is

$$\Delta=a_+^\dagger a_+ - a_-^\dagger a_-. \quad (15)$$

EXACT SOLUTION

A procedure for obtaining exact eigenvalues for this problem is the following. Let $|N,\Delta,n\rangle$ be an eigenfunction of $a_0^\dagger a_0$, $a_+^\dagger a_+$, and $a_-^\dagger a_-$ belonging to the eigenvalues N for $a_0^\dagger a_0 + a_+^\dagger a_+ + a_-^\dagger a_-$, Δ for $a_+^\dagger a_+ - a_-^\dagger a_-$, and n for $a_-^\dagger a_-$. We assume $\Delta \geq 0$. This then corresponds to the eigenvalues

$$a_0^\dagger a_0 = N-\Delta-2n, \quad a_+^\dagger a_+ = \Delta+n, \quad a_-^\dagger a_- = n. \quad (16)$$

Then we can write an eigenfunction of H in the form

$$\Psi=\sum_{n=0}^{(N-\Delta)/2} C_n|N,\Delta,n\rangle, \quad (17)$$

provided $N-\Delta$ is even (which we shall assume for the present) or with the upper limit $(N-\Delta-1)/2$ if $N-\Delta$ is odd. The equation $H\Psi=W\Psi$ then takes the form

$$\begin{aligned}&\sum_n[(\Delta+2n)+g(N-\Delta-2n)(\Delta+2n)-W]C_n|N,\Delta,n\rangle\\ &+\sum_n g[(N-\Delta-2n)(N-\Delta-2n-1)\\ &\times(\Delta+n+1)(n+1)]^{1/2}C_n|N,\Delta,n+1\rangle\\ &+\sum_n g[(N-\Delta-2n+1)(N-\Delta-2n+2)\\ &\times(\Delta+n)n]^{1/2}C_n|N,\Delta,n-1\rangle=0, \quad (18)\end{aligned}$$

or

$$\begin{aligned}&g[(N-\Delta-2n+2)(N-\Delta-2n+1)(\Delta+n)n]^{1/2}C_{n-1}\\ &+[\Delta+2n+g(N-\Delta-2n)(\Delta+2n)-W]C_n\\ &+g[(N-\Delta-2n-1)(N-\Delta-2n)\\ &\times(\Delta+n+1)(n+1)]^{1/2}C_{n+1}=0. \quad (19)\end{aligned}$$

This is a set of difference equations that uncouples at $n=(N-\Delta)/2$. We thus set

$$C_{-1}=C_{(N-\Delta)/2+1}=C_{(N-\Delta)/2+2}\cdots=0. \quad (20)$$

The $n=(N-\Delta)/2$ equation will be a redundant one and must be satisfied by the C_n's generated previously if W is to be an eigenvalue.

The C_n's must of course satisfy the normalization condition

$$\sum_n C_n^2=1 \quad (21)$$

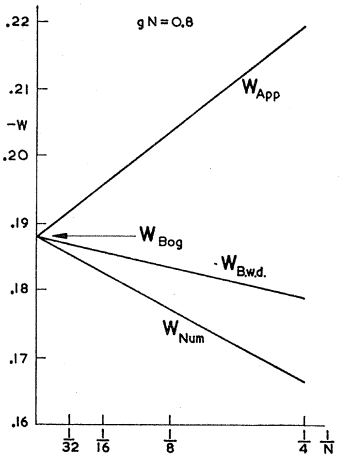

FIG. 1. A typical graph of the ground-state energies, plotted versus $1/N$, as calculated by the various methods. W_{App} is the energy calculated using the "better" approximation, W_{Bog} the Bogoliubov energy with depletion ignored, $W_{\text{B.w.d.}}$ the Bogoliubov energy with depletion considered, and W_{Num} the result of the computer calculation with the exact Schrödinger equation.

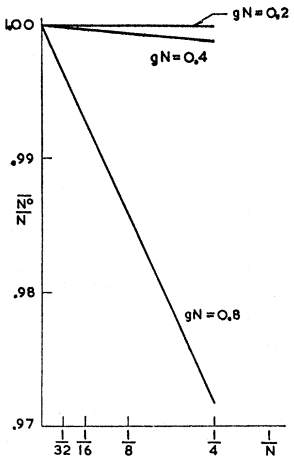

FIG. 2. The average fractional occupation of the ground state for various gN values, plotted versus $1/N$.

in order to have the usual probabilistic interpretation.

For $\Delta=0$, the equation simplifies to

$$gn[(N-2n+2)(N-2n+1)]^{1/2}C_{n-1}+[2n+2gn(N-2n)-W]C_n+g(n+1)[(N-2n-1)(N-2n)]^{1/2}C_{n+1}=0. \quad (22)$$

This set of equations can readily be solved using a computer. This was done for various values of g and N. The results are displayed graphically in Figs. 1 and 2. (See Appendix for summary of program procedure.) The results will be discussed in a later section.

BOGOLIUBOV APPROXIMATION

The Bogoliubov[1] approximation consists of replacing a_0 and $a_0^\dagger$ in Eq. (13) by a c number $N^{01/2}$, so that

$$H_B=a_+^\dagger a_+ + a_-^\dagger a_- + gN^0[a_+^\dagger a_+ + a_-^\dagger a_- + a_+ a_- + a_+^\dagger a_-^\dagger]. \quad (23)$$

As a result N is no longer a constant of the motion, though Δ still is. The Hamiltonian H_B can be diagonalized by the canonical transformation

$$a_+=c\alpha_+ - s\alpha_-^\dagger, \quad a_-=c\alpha_- - s\alpha_+^\dagger,$$
$$a_+^\dagger=c\alpha_+^\dagger - s\alpha_-, \quad a_-^\dagger=c\alpha_-^\dagger - s\alpha_+, \quad (24)$$
$$c^2-s^2=1,$$

with

$$c=[(1+gN^0+\epsilon)/2\epsilon]^{1/2}, \quad s=[(1+gN^0-\epsilon)/2\epsilon]^{1/2},$$
$$\epsilon=[1+2gN^0]^{1/2}, \quad (25)$$
$$cs=gN^0/2\epsilon, \quad c^2+s^2=(1+gN^0)/\epsilon.$$

Then

$$H_B=\epsilon-1-gN^0+\epsilon(\alpha_+^\dagger\alpha_+ + \alpha_-^\dagger\alpha_-). \quad (26)$$

Thus the lowest eigenvalue is

$$W_0=\epsilon-1-gN^0. \quad (27)$$

To determine N^0, one requires

$$N^0+\langle a_+^\dagger a_+ + a_-^\dagger a_-\rangle = N^0+2s^2 = N, \quad (28)$$

where N is the number of particles in the system. Thus

$$N=N^0-1+(1+gN^0)/(1+2gN^0)^{1/2}. \quad (29)$$

To fix the relationship between the Bogoliubov approximation and the exact solutions, we let $|n\rangle$ represent an eigenstate of $a_+^\dagger a_+$ and $a_-^\dagger a_-$ belonging, for each, to the eigenvalue n. Then letting

$$\Psi=\sum_{n=0}^{\infty} C_n|n\rangle, \quad (30)$$

we have, from $H_B\Psi=W\Psi$,

$$gnN^0C_{n-1}+[2n+2gnN^0-W]C_n+g(n+1)N^0C_{n+1}=0; \quad (31)$$

and this, we see, corresponds to approximating $[(N-2n+2)(N-2n+1)]^{1/2}$, $[(N-2n-1)(N-2n)]^{1/2}$, $N-2n$, all by N^0 for all n.

Let us now solve Eq. (31). To do this, let

$$\Phi=\sum_{n=0}^{\infty} C_n x^n. \quad (32)$$

Then

$$\Phi'=\sum_{n=1}^{\infty} nC_n x^{n-1}=\sum_{n=0}^{\infty}(n+1)C_{n+1}x^n, \quad (33)$$

$$x\Phi'=\sum_{n=1}^{\infty} nC_n x^n=\sum_{n=0}^{\infty} nC_n x^n,$$

$$(x\Phi)'=(\sum_{n=0}^{\infty} C_n x^{n+1})'=\sum_{n=1}^{\infty}(n+1)C_n x^n, \quad (34)$$

$$x(x\Phi)'=\sum_{n=1}^{\infty}(n+1)C_n x^{n+1}=\sum_{n=0}^{\infty} nC_{n-1}x^n.$$

Multiplying (31) by x^n and summing,

$$gN^0x(x\Phi)'+2(1+gN^0)x\Phi'-W\Phi-gN^0\Phi'=0, \quad (35)$$

or

$$\Phi'/\Phi=[W-gN^0x]/[gN^0(1+x^2)+2x]. \quad (36)$$

This leads to

$$\Phi=\frac{A[x+(gN^0+1-\epsilon)/gN^0]^{[(W+gN^0+1)/2\epsilon-\frac{1}{2}]}}{[x+(gN^0+1+\epsilon)/gN^0]^{[(W+gN^0+1)/2\epsilon+\frac{1}{2}]}}.$$

If the exponent of the numerator is nonintegral, the C_n's are not normalizable. If we choose

$$W=\epsilon-gN^0-1+2n\epsilon,$$

[1] N. N. Bogoliubov, J. Phys. (USSR) **11**, 23 (1947).

then the C_n's are normalizable. For $n=0$,

$$\Phi=A[x+(gN^0+1+\epsilon)/gN^0]^{-1}$$
$$=A\sum_{n=0}^{\infty}\frac{gN^0}{gN^0+1+\epsilon}\left(\frac{-gN^0x}{gN^0+1+\epsilon}\right)^n. \quad (37)$$

Thus,

$$C_n=\frac{AgN^0}{gN^0+1+\epsilon}\left(\frac{-gN^0}{gN^0+1+\epsilon}\right)^n,$$

$$\sum_{n=0}^{\infty}C_n^2=\sum_{n=0}^{\infty}A^2\left(\frac{gN^0}{gN^0+1+\epsilon}\right)^{2n+2}=1,$$

$$A=\left[1-\left(\frac{gN^0}{gN^0+1+\epsilon}\right)^2\right]^{1/2}\left[\frac{(gN^0+1+\epsilon)}{gN^0}\right],$$

and

$$C_n=\left[1-\left(\frac{gN^0}{gN^0+1+\epsilon}\right)^2\right]^{1/2}\left(\frac{-gN^0}{gN^0+1+\epsilon}\right)^n. \quad (38)$$

A "BETTER" APPROXIMATION

We have seen that the Bogoliubov approximation corresponds to the replacement by N^0 of $[(N-2n+2)\times(N-2n+1)]^{1/2}$, $[(N-2n-1)(N-2n)]^{1/2}$, and $N-2n$. It was thought that perhaps a more accurate energy would result from the approximations

$$[(N-2n+2)(N-2n+1)]^{1/2}\rightarrow N-2n+2,$$
$$[(N-2n-1)(N-2n)]^{1/2}\rightarrow N-2n, \quad (39)$$

and

$$N-2n\rightarrow N-2n.$$

The difference equation now becomes

$$gn(N-2n+2)C_{n-1}+[2n+2gn(N-2n)-W]C_n+g(n+1)(N-2n)C_{n+1}=0. \quad (40)$$

This set of equations was also solved using a computer. The results are displayed in Figs. 1 and 2. It is surprising to note that this improved approximation leads to a correction in the wrong direction.

RESULTS

A typical graph of the ground-state energies, for a given value of gN, is plotted versus $1/N$ in Fig. 1. The point marked W_{Bog} is the Bogoliubov-approximate energy calculated with the depletion of the number of particles in the ground-state ignored, i.e.,

$$W=\epsilon-gN-1. \quad (41)$$

It is therefore a constant for fixed gN. The line labeled $W_{\text{B.w.d.}}$ is calculated by the above formula with N replaced by N^0 which was found by solving (29) by iteration. W_{App} is the energy calculated using the presumably improved treatment of the square roots in the difference equation. W_{Num} is, of course, the result of the computer calculation with the exact Schrödinger equation. The calculated values did not fall exactly on the straight lines shown. There was a small deviation for the lowest N value. The straight lines were drawn through the calculated points for the higher N values so that the asymptotic behavior is as shown. The deviation for $N=4$ is in the fifth significant figure. We note the following general features from the graph: The extrapolated values for the energy, with an infinite number of particles in the system, converge to the Bogoliubov-approximate energy for all three methods of calculation. Taking the depletion effect into consideration corrects the energy in the direction of the exact value, the amount of the correction being the greatest for the largest value of the effective coupling constant gN. The "better" approximation method adds a correction to the Bogoliubov-approximate energy which goes as $1/N$ as does the exact result. The coefficient of this correction term is, however, of the wrong sign!

In Fig. 2 will be found a graph of the fraction of particles in the ground state, for various gN values, plotted, again versus $1/N$. These values for N^0 were taken from the numerical solution for the distribution weighting factors but the iterated solution of Eq. (29) gives almost exactly the same values. The calculated values fall to the limit of visual accuracy on the straight lines shown. We see that, as would be expected, the deviation of this fraction from unity increases as gN increases. It is perhaps surprising that the deviation for small numbers of particles is quite small. We see that in the limit of an infinite number of particles the fraction, in all cases, becomes unity. This explains the virtual exactness of the Bogoliubov-approximate energy with depletion ignored in this limit.

In the following section the fluctuation in the number of particles in the ground state is calculated for this system. We see that for small values of gN the value of the fractional number of particles in the ground state will not be appreciably altered by fluctuations.

FLUCTUATIONS

The root-mean-square fluctuations in the ground state were calculated for this simple gas using the Bogoliubov-approximate distribution. The result is

$$R=\left(\frac{\langle n_0^2\rangle_{\text{av}}-\langle n_0\rangle_{\text{av}}^2}{\langle n_0\rangle_{\text{av}}^2}\right)^{1/2}$$
$$=\frac{b}{4N^2(1-b)^2-4Nb(1-b)+b^2}, \quad (42)$$

where

$$b=gN^0/(gN^0+1+\epsilon). \quad (43)$$

Thus

$$\lim_{b\rightarrow 0}R\rightarrow 0 \quad [\text{From (43) } b\rightarrow 0 \text{ implies } gN^0\rightarrow 0], \quad (44)$$

$\lim_{b\to 1} R \to 1$ (Of course, $b \to 1$ implies $gN^0 \to \infty$). (45)

We may conclude that there are situations where the quantity gN^0 is sufficiently small so that the fluctuations do not make the approximation of N^0 by a c number invalid.

A MODIFIED SIMPLE BOSON SYSTEM

We can consider here the simplified boson system investigated in the previous sections with the modification that there will now exist a two-body interaction between particles of opposite momenta, i.e., between particles in the + and − states. The Hamiltonian for the system in second quantization is

$$H=a_+^\dagger a_+ + a_-^\dagger a_- + g[a_0^\dagger a_0(a_+^\dagger a_+ + a_-^\dagger a_-) + a_0^2 a_+^\dagger a_-^\dagger + a_0^{\dagger 2} a_+ a_-] + h a_+^\dagger a_+ a_-^\dagger a_-, \quad (46)$$

where h is the two-body potential in the momentum-space representation for the interaction of a particle in the + state with one in the − state.

Application of the Bogoliubov approximations to this Hamiltonian will yield exactly the same results as in the preceding sections because the additional interaction does not contain any creation or destruction operators for the zero-momentum state and will thus be ignored. We can now perhaps gain some insight into the effect of such ignored terms in the Hamiltonian for an actual system by solving this modified problem numerically and examining the effect here of the additional term.

Proceeding as in the previous case, we write

$$\Psi = \sum_{n=0}^{\infty} C_n |N,\Delta,n\rangle, \quad (47)$$

and upon substitution of this and H from Eq. (46) into

$$H\Psi = W\Psi, \quad (48)$$

we find the following difference equation (for $\Delta=0$):

$$gn[(N-2n+2)(N-2n+1)]^{1/2}C_{n-1} + [2n+2gn(N-2n)+hn^2-W]C_n + g(n+1)[(N-2n-1)(N-2n)]^{1/2}C_{n+1}=0. \quad (49)$$

This set of equations with the boundary conditions (20) was solved using the computer and the same technique as is described in the Appendix. The results are displayed graphically in Figs. 3–6. The value of h used in the calculations was varied from

$$h=g$$

to

$$h=-4g.$$

It was anticipated that the fractional occupation number of the ground state would be increased when h was positive, with a corresponding increase in the energy, and would be decreased when h was negative, with an accompanying decrease in the energy.

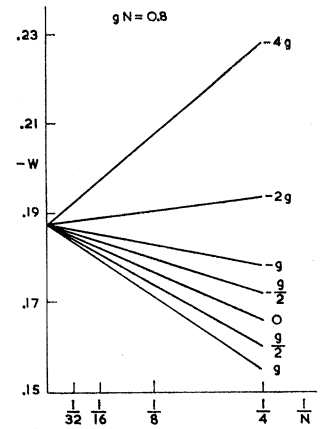

FIG. 3. The ground-state energy plotted versus $1/N$ for various values of h, with constant gN.

In Fig. 5 the fractional occupation number of the ground state is plotted against $1/N$ for constant gN and various values of h. The Bogoliubov result with depletion ignored is given by the asymptotic result for $h=0$ in the limit of infinite N. The Bogoliubov result with depletion considered is again virtually identical with the $h=0$ result. We see that the predicted behavior is indeed present. It is perhaps surprising that in the limit of infinite N the fractional occupation numbers approach unity, the Bogoliubov value, for all values of h. This verifies the Bogoliubov assumption that the interactions of excited particles amongst themselves, i.e., multiple scatterings, is negligible, at least in this simple case for this value of gN. It is shown in the next section that, if the value of h were increased further, an appreciable depletion would take place by virtue of the lower potential energy of particles in states of higher kinetic energy. In order for an effect to persist in the limit of infinite N, however, much larger values of the effective coupling constant, gN, would have to be considered.

In Fig. 6 the fractional occupation of the ground state is plotted against h for constant gN and N. Again we see the diminution of the depletion as N increases (or g decreases). These results also indicate that a more pronounced effect would occur if larger values of h were considered. At least for small numbers of particles we see a hint of the assumed inversion of energy states as h is made increasingly negative.

In Fig. 3 the energy is plotted versus $1/N$ for various values of h again with constant gN. Again we see that the Bogoliubov energy is virtually exact, even for negative h, in the limit of infinite N. The energy is also seen to follow the predicted pattern. We see from the graph of the energy versus h for constant gN and various values of N (Fig. 4) that, as the number of particles approaches infinity, the presence of the added interaction produces no effect. We note further that the neglect of such interaction terms yields poor results

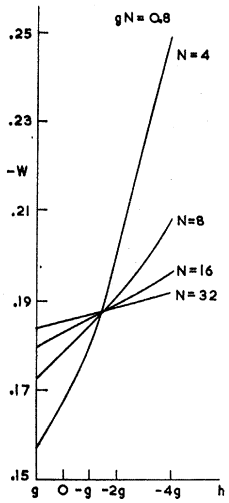

FIG. 4. The ground-state energy plotted versus h for various values of N, with constant gN.

for very small numbers of particles but, that for even as few as 16 particles, the error involved for these values of h is at worst of the order of 10%, and for 32 particles the largest error is of the order of 5%.

In the next section the effect of the added interaction for larger values of h will be studied. Of course from the fluctuation calculation it seems obvious that for large enough values of gN the Bogoliubov approximations will be invalid because of the fluctuations in the occupation number of the ground state.

THE "PHASE TRANSITION"

The modified system, considered in the previous section, was studied for a fixed number of particles in order to understand more completely the effect of the added interaction. The graph in Fig. 7 shows the behavior of the ground-state energy as a function of F, where $F=-h/g$. This graph, which has $N=64$ and $g=0.01$, shows the characteristic behavior of the energy, since the results were of the same form for a wide range of N and g.

The energy at $F=0$ is essentially the value obtained from the Bogoliubov method, with or without the depletion effect taken into consideration. From the graph we see that for negative F and positive F smaller than 6.23 the Bogoliubov approximation remains virtually exact. At this transition point, F_T, the Bogoliubov approximation completely breaks down. The energy is a linear function of F, as it is in the "normal" region, but the constant of proportionality is a much larger number.

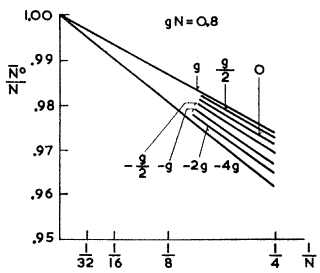

FIG. 5. The average fractional occupation of the ground state plotted versus $1/N$ for various values of h, with constant gN.

This transition can be partially understood from the graph in Fig. 8. Here C_0 is the square root of the probability of finding all of the particles in the zero-energy state. The value of C_0 in the normal range of F is a good measure of the relative probability of finding any particle in the zero-energy state because the distribution of C_n's decreases monotonically and sharply from the value at $n=0$. C_0 in this range is approximated quite well by the Bogoliubov value (see Fig. 2), and since $C_0 \simeq 0.98$ nearly all the particles are in the zero state. The transition region was examined as closely as the computer accuracy would permit and the apparent discontinuity in C_0 remained. Beyond the transition point C_0 decreases exponentially, with the first C_0 beyond F_T being of order 10^{-15}. The distribution of C_n's now rises monotonically and sharply from the $n=0$ value. There is thus an inversion in the population beyond and this region will be called the inverted region.

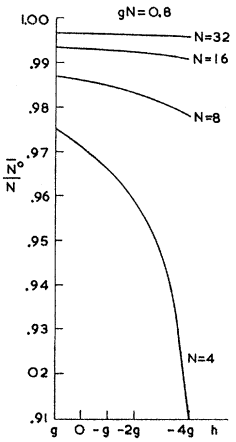

FIG. 6. The average fractional occupation of the ground state plotted versus h for various values of N, with constant gN.

The variation of the reciprocal of the transition value of F with N, as numerically computed, is shown in Fig. 9. Perhaps the most interesting feature of this graph is that F_T is infinite for $N=2$. For $N=2$ there can be only one $+$, $-$ pair present, implying perhaps the presence of one pseudoparticle. Thus one might conclude that the transition phenomenon is a result of pseudoparticle scattering.

The transition value of F is plotted, for fixed N, as a function of g in Fig. 10. This graph is of the nature of a phase diagram with the normal and inverted regions separated by the $F_T(g)$ curve. The numerically computed values of F_T and those obtained from Eq. (60) were almost equal.

A DIAGONALIZING TRANSFORMATION IN THE INVERTED REGION

We have seen that in the modified model boson system considered in the previous sections there is a

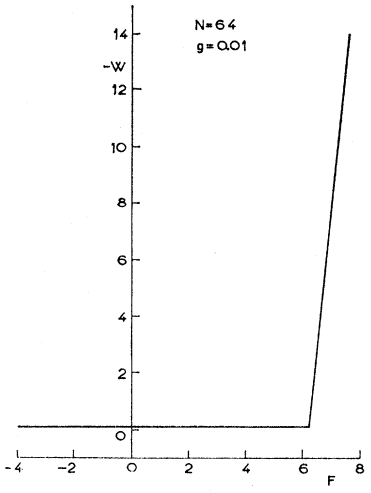

FIG. 7. The ground-state energy plotted versus F, where $h=-Fg$, with constant g and N.

critical value of the interaction strength parameter beyond which there is a population inversion between the two energy levels and that in this inverted region the Bogoliubov method is inapplicable. Because the + and − levels are now "macroscopically occupied" and the zero state is almost empty, one is naturally led to apply a Bogoliubov-like method in the inverted region where $a_+^\dagger$, a_+, $a_-^\dagger$, and a_- are treated as c numbers and only $a_0^\dagger$ and a_0 are treated as operators. We thus set

$$a_+^\dagger=a_+=a_-^\dagger=a_-=(\bar{N}/2)^{1/2} \tag{50}$$

with the restriction

$$\langle a_0^\dagger a_0\rangle+\bar{N}=N. \tag{51}$$

The Hamiltonian (45) in this approximation is

$$H=\bar{N}+\tfrac{1}{2}g\bar{N}[2a_0^\dagger a_0+a_0^2+a_0^{\dagger 2}]+\tfrac{1}{4}h\bar{N}^2. \tag{52}$$

Introducing pseudoparticle operators as in the usual transformation we have

$$\alpha_0=ca_0+sa_0^\dagger, \tag{53}$$

where

$$c^2-s^2=1 \tag{54}$$

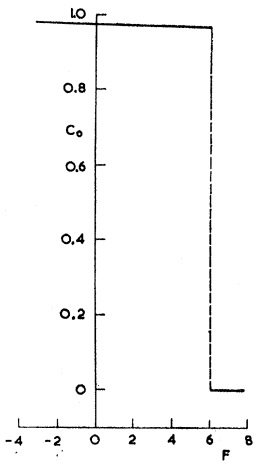

FIG. 8. C_0, the square root of finding all of the particles in the zero-energy state, plotted versus F.

in order that the transformation be canonical. The transformed Hamiltonian is

$$H=\bar{N}+\tfrac{1}{4}h\bar{N}^2+g\bar{N}s(s-c)+g\bar{N}(c-s)^2\alpha_0^\dagger\alpha_0 +\tfrac{1}{2}g\bar{N}(c-s)^2(\alpha_0\alpha_0+\alpha_0^\dagger\alpha_0^\dagger) \tag{55}$$

In order to diagonalize this Hamiltonian one would ordinarily set $c-s=0$. However (54) could then only be satisfied if $c+s$ were infinite. Thus, the transformation is singular and invalid in addition to which such a transformation would not give the excitation spectrum since the coefficient of $\alpha_0^\dagger\alpha_0$ is equal to that of the nondiagonal part H.

These difficulties can be circumvented by writing (52) as

$$H=\bar{N}+\tfrac{1}{2}g\bar{N}[a_0^\dagger a_0+a_0a_0^\dagger+a_0^2+a_0^{\dagger 2}]-\tfrac{1}{2}g\bar{N}+\tfrac{1}{4}h\bar{N}^2 =\bar{N}-\tfrac{1}{2}g\bar{N}+\tfrac{1}{4}h\bar{N}^2+\tfrac{1}{2}g\bar{N}(a_0+a_0^\dagger)^2. \tag{56}$$

This Hamiltonian is already diagonal in the operator

$$A=a_0+a_0^\dagger, \tag{57}$$

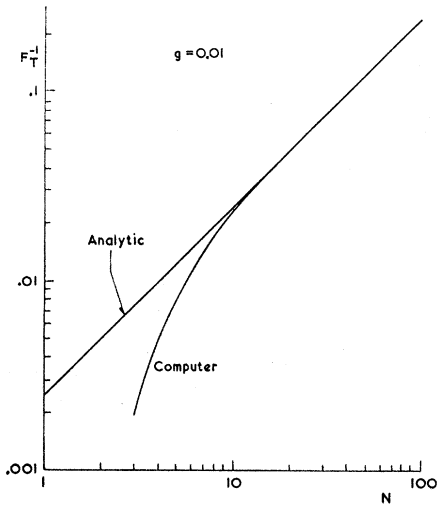

FIG. 9. The variation of the reciprocal of the transition value of F as a function of N as calculated from Eq. (60) and the computer results.

which has the character of a field operator (or more precisely a position or momentum operator) and has a continuous spectrum extending from $-\infty$ to ∞. Because it is the quantity A^2 that enters in H the excitation spectrum will consist of the continuum of positive numbers.

Thus, the ground-state energy in the inverted region should be given by

$$W=\bar{N}-\tfrac{1}{2}g\bar{N}+\tfrac{1}{4}h\bar{N}^2. \tag{58}$$

The values of W, ignoring any "depletion effect," as a function of F in the region beyond F_T are virtually identical with the computer values shown in Fig. 7. Of course this approximation (50) is invalid for $F<F_T$. From (27) and (58) one should be able to predict at

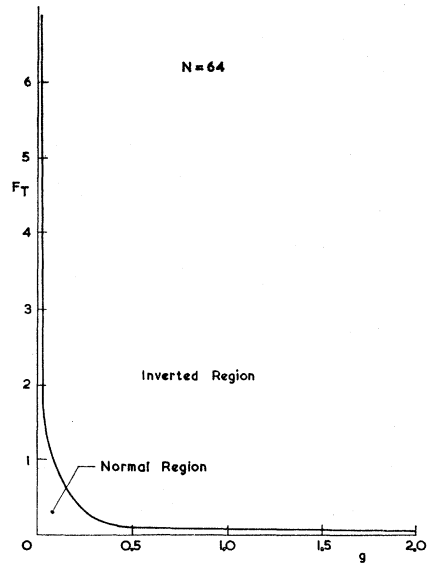

FIG. 10. The transition value of F plotted versus g for fixed N.

what value of F the transition will occur for any N and g. Equating the two expressions for W at the transition point we find, ignoring both depletion effects

$$[1+2gN]^{1/2}-1-gN=N-\tfrac{1}{2}gN-\tfrac{1}{4}F_TgN^2 \quad (59)$$

or

$$F_T=\frac{1+\frac{1}{2}gN+N-[1+2gN]^{1/2}}{\frac{1}{4}gN^2}. \quad (60)$$

The value of F_T^{-1} for $g=0.01$ as a function of N is shown in Fig. 9 along with the actual computer values. The large fractional errors for small N are partially attributable to the inaccuracy of the usual Bogoliubov approximation for small N. The values of F_T^{-1} for $N=64$ and various values of g were calculated from (60) and compared with the computer values. The agreement is again very good with the error increasing as g increases with less than 3% error for g as large as 2 (Fig. 10).

THE FIRST EXCITED STATE

In the previous sections it has been shown that the ground-state energy of a system of simple bosons can be very well approximated by the usual Bogoliubov method in the normal region and by a Bogoliubov-like method in the inverted region. We now consider the first excited state. The Bogoliubov value for the energy of the first excited state is, as given in Eq. (26)

$$W_1=[1+2gN]^{1/2}-1-gN+2[1+2gN]^{1/2}, \quad (61)$$

the coefficient 2 of the last term being a result of our choosing $\Delta=0$. The results of the previous sections lead one to anticipate that this approximation will be valid only in the normal region and that for F beyond F_T, W_1 must be obtained from Eq. (56).

Consider the value of W_1 calculated according to (56) at the transition point.

$$W_1=N-\tfrac{1}{2}gN-\tfrac{1}{4}F_TgN^2. \quad (62)$$

The A^2 term of course giving no contribution. Using (60) for F_T this becomes, of course,

$$W_1(F_T)=W_0=[1+2gN]^{1/2}-1-gN. \quad (63)$$

Equations (61) and (63) thus lead us to believe that, while the ground-state energy is continuous with a discontinuous derivative at F_T, the energy of the first excited state is itself discontinuous, with a discontinuity of magnitude $2[1+2gN]^{1/2}$. Furthermore, for the values of g and N considered ($g=0.01$ and $N=64$), Eq. (61) is

$$W_1=+2.8899 \quad (64)$$

and Eq. (63)

$$W_1(F_T)=-0.13002. \quad (65)$$

A program was designed to compute the energy of the first excited state and the corresponding distribution of C_n's. In the normal region the computing method was quite accurate and the resulting excited state energies were, for $g=0.01$ and $N=64$,

F	W_1
0.0	2.8757,
1.0	2.8603,
3.0	2.8302,
5.0	2.7994,
6.2	2.7807.

The distribution of C_n's was now found to be peaked at $n=1$ and was relatively level until $n=2$ at which point it began to decrease sharply. This perhaps indicates the presence of two pseudoparticles.

In the inverted region the behavior of the excited state energy as computed was essentially as predicted There is a discontinuity at F_T of magnitude 2.9128 as

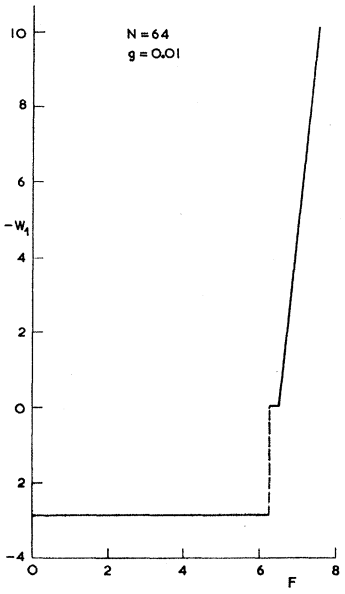

FIG. 11. The energy of the first excited state plotted as a function of F with constant g and N.

compared with the predicted 3.019934. The energy then follows the Bogoliubov ground-state energy over a small range in F and then decreases linearly with F in the same manner as the ground-state energy. The energy of the first excited state as a function of F, for $g=0.01$ and $N=64$, is shown graphically in Fig. 11. The computer program was not entirely dependable in the inverted region and perhaps the quantitative features of Fig. 11 are not to be relied upon there.

The first excited state energy as given by Eq. (56) thus is qualitatively all right but is quantitatively quite inaccurate.

CONCLUSIONS

The results of this analysis can be summarized as follows:

(1) For the model boson system with the h interaction not present, the Bogoliubov method yields quite accurate ground-state and first excited-state energies for a wide range of gN and N.

(2) With the h interaction present, the Bogoliubov method yields accurate ground state and first excited-state energies in the normal region.

(3) There is a transition point F_T beyond which the Bogoliubov method is completely inapplicable. In this region, a Bogoliubov-like method yields quantitatively accurate ground-state energies and describes qualitatively the behavior of the energy of the first excited state as a function of F.

The same procedure as was applied here could be used to investigate the system described by the Hamiltonian (12) with all terms considered. The simple model used in this analysis and the discontinuity in the derivative of its ground-state energy may provide a convenient model for investigating phase transitions.

ACKNOWLEDGMENTS

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APPENDIX: SUMMARY OF COMPUTER PROGRAM

We wished to solve the set of Eqs. (22) with the conditions (20) for the energy W and the distribution weighting factors C_n. We began by setting $C_0=1$, letting W equal the Bogoliubov energy, and using the equations to generate the following C_n's for increasing n. If the energy were too large, i.e., larger than the lowest eigenvalue, a negative C_n would be generated. (This is analogous to the wave function for a hydrogen atom in the ground state having no nodes and for any higher energy having at least one node.) If the energy were too large or too small the $(N/2)$th equation, which is redundant, would not be satisfied. The procedure was then to start with the Bogoliubov energy. If a C_n were negative, we halved the energy and began calculating the C_n's again. We continued this until the C_n's were all positive. If the $(N/2)$th equation were satisfied (within the limits of accuracy of the computer) this energy was considered the eigenvalue. If the equation were not satisfied we raised the energy, half the amount of the last interval. By continuing the process until the C_n's were all positive and the $(N/2)$th equation was satisfied within certain limits, or until two successive energies were equal to some order, we determined the eigenenergy. The C_n's were very sensitive to the value of the energy used with this procedure. Thus, though the energy could be well determined by this method, the C_n's were not. We thus used the calculated energy and solved the set of equations by satisfying the $(N/2)$th equation and generating the C_n's for decreasing n. This procedure was found to give the C_n's to a much greater accuracy. (It should also be noted that when the energy is far from the eigenenergy, the magnitude of the C_n's became too large for the machine to handle. This difficulty was circumvented by calculating the ratio of two successive C_n's.)

In the inverted region it was found that greater accuracy could be obtained by inverting the above process, i.e., searching for the eigenvalue by generating the C_n's for decreasing n and then generating the more accurate C_n's, with this energy, for increasing n. It is hoped that a more efficient and more accurate procedure can be developed, especially since there is some doubt about the validity of the excited-state calculations in the inverted region.