Bose-Einstein Gas with Repulsive Interactions: General Theory

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The properties of a Bose-Einstein gas with repulsive interparticle interactions are determined at low temperature. It is shown that the contribution to the energy arising from particle excitation with small momentum transfers computed in conventional perturbation theory is divergent, but that this difficulty can be avoided by an alternative procedure. An exact method is developed for dealing with that part of the Hamiltonian which gives rise to the perturbation divergence and an exact solution is obtained. The treatment of the region of large momentum transfers is then carried out by introducing the concept of the scattering length of the interaction. The energy is given by the well-known result of the optical theorem corrected by a series in powers of $(\rho a^3)^{\frac{1}{2}}$, where ρ is the density and a the scattering length. Examination of the processes contributing to the energy shows that 95.8% of the correction of order $(\rho a^3)^{\frac{1}{2}}$ results from a simple alteration of the perturbation energy denominators which takes into account the interaction energy of excited pairs with the unexcited pairs of the medium. The remaining 4.2% arises from multiple particle excitation. These methods also predict the existence of phonon excitation with phonon energies that are linear in the phonon momentum for small excitation and approach $q^2/2M$ for large momentum. The detailed consideration of this spectrum forms part of the following paper.

The results are compared with the theory of fermion systems with strong interactions, where again the largest correction to the first-order "optical" energy arises from alteration of the two-particle propagator which is required to take into account interactions with the many unexcited particles of the medium. The propagator corrections in the fermion and boson systems are similar except for a characteristic difference arising from the statistics. The theory for bosons is shown to be essentially identical with that given by Brueckner and Levinson in their general formulation of the theory of many-body systems with strong interactions.

Systems with attractive but saturating interactions are also considered and some new difficulties are shown to arise which cannot be treated by a straightforward application of the methods of this paper.

I. INTRODUCTION

RECENTLY the theory of many-body systems with strong interactions has received considerable impetus from work carried out on bosons with hard-sphere interactions,[1,2] on the electron gas,[3,4] and on nuclear matter.[5–8] In this paper we shall discuss a system of bosons at low temperature and develop methods appropriate to the study of strong interactions both at low and at high density. In this we shall show first how the formalism developed by Brueckner and Levinson[5] and applied extensively to the nuclear many-body problem gives in first approximation essentially the result obtained by Yang and Lee[2] using their "binary collision approximation method." As a more important result we shall show how in good approximation this method can be applied in the high-density region where the Lee-Yang procedure, which is based on the introduction of the concept of pseudopotentials and uses a low-density expansion, probably cannot be used.

The principal difficulty encountered in any simple theory of the ground state wave function and energy of a many-body system of bosons is that a perturbation evaluation of the interaction energy leads to a divergent result. This difficulty occurs even if the interactions are weak and repulsive. The divergence does not occur at extremely low densities; it is in fact a consequence of the special features of the system at finite density which result from the Bose statistics. The divergence of the perturbation series is discussed in Sec. II where it is shown that the divergence is intimately associated with the large excitation energy required to remove particles from the ground state.[9] The occurrence of this "energy gap" is the origin of the divergence difficulty which results from the attempt to expand the energy in powers of the ratio of the finite interaction energy to the very small kinetic energy. An alternative procedure is developed in Sec. II to deal with the region of low excitation where the usual perturbation theory fails. It is shown that not only is an exact treatment possible of this restricted region but also that the transformation leading to the solution predicts a phonon excitation spectrum. This spectrum is discussed in more detail in the following paper. The existence of the phonon spectrum is a consequence in part of the finite energy gap for simple particle excitation and hence is intimately associated with the statistics of the particles.

The method developed in Sec. II for dealing with low excitation is extended in Sec. III to include the high excitations. This is most simply carried out by introducing the concept of the scattering matrix and the scattering length of the interaction. It is then shown that the ground state energy is given as the result of the elementary "optical theorem" corrected by a series

[1] K. Huang and C. N. Yang, Phys. Rev. **105**, 1119 (1957).
[2] T. D. Lee and C. N. Yang (private communication). Their results were first presented in preliminary form at the International Congress on Theoretical Physics in Seattle, Washington, (September 17–21, 1956).
[3] M. Gell-Mann and K. Brueckner, Phys. Rev. **106**, 364 (1957).
[4] K. Sawada, Phys. Rev. **106**, 372 (1957).
[5] K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955); K. A. Brueckner, Phys. Rev. **100**, 36 (1955).
[6] R. J. Eden and N. C. Francis, Phys. Rev. **98**, 1445 (1955); R. J. Eden, Proc. Roy. Soc. (London) **A235**, 408 (1956).
[7] H. A. Bethe, Phys. Rev. **103**, 1353 (1956).
[8] J. Goldstone, Proc. Roy. Soc. (London) (to be published).
[9] The importance of this feature has also been emphasized by Huang and Yang (see reference 1) and by R. P. Feynman, Phys. Rev. **91**, 1291 (1953).

in powers of $(\rho a^3)^{\frac{1}{2}}$, where ρ is the density and a the scattering length.[10] This result is then analyzed in Sec. III where it is shown that almost all of the corrections to the simplest approximation to the energy are the result of a simple modification of the perturbation energy denominators which includes the interaction energy of excited particles with the unexcited particles of the medium. The further corrections to the energy are the consequence of multiple excitation of pairs of particles all carrying the same momentum. These processes, although they alter the ground state energy by only 4%, are the origin of the phonon spectrum, as is shown in Sec. III.

The simplified method of Secs. II and III is generalized in Sec. IV where it is shown that the procedure of the earlier section is very similar to that followed in the study of fermion systems with strong interactions.[5] The particular features of the boson system resulting from the statistics and simplicity of the ground state lead, however, to a considerably simpler formulation of the general problem than is possible in the case of fermions. Some difficulties are shown to remain in the boson system which are the result of the complicated propagation properties of bosons in excited states. Arguments are given to show that the approximation to the excited state propagator (suggested in Sec. IV) can introduce only a small change in the properties of the system.

In Sec. V the results of Sec. IV are extended to the determination of the corrections to the energy of the ground state and the phonon spectrum. It is shown that the general features are similar to those deduced in the simple theory of Secs. II and III although the phonon motion must represent much more complicated particle motion than in the simplified case. A weak phonon-phonon interaction is also shown to exist in the more exact treatment.

In Sec. VI some difficulties are discussed which arise in the case of potentials which are repulsive at small distances but have longer-ranged regions of attraction. It is shown that some of the features of systems with such interactions are likely to be markedly different from those of systems with only repulsive forces.

II. GENERAL FEATURES OF THE THEORY

We consider the Hamiltonian for the system

$$H=H_0+H', \tag{1}$$

where the kinetic energy is

$$H_0=\sum_p \eta_p^*\eta_p p^2/2m, \tag{2}$$

and the interaction energy is

$$H'=\tfrac{1}{2}\sum_{ijkl} v_{ij,kl}\eta_i^*\eta_j^*\eta_k\eta_l. \tag{3}$$

The operators η^* and η are the usual creation and annihilation operators. The matrix elements $v_{ij,kl}$ are taken with respect to a basic set of plane wave states, i.e.,

$$v_{ij,kl}=\frac{1}{\Omega^2}\int e^{-i\mathbf{k}_i\cdot\mathbf{r}_1}e^{-i\mathbf{k}_j\cdot\mathbf{r}_2}v(r_{12})e^{i\mathbf{k}_k\cdot\mathbf{r}_1}e^{i\mathbf{k}_l\cdot\mathbf{r}_2}d\mathbf{r}_1 d\mathbf{r}_2$$

$$=\frac{1}{\Omega}\delta_{ij,kl}\int d\mathbf{r}v(r)e^{-i(\mathbf{k}_i-\mathbf{k}_k)\cdot\mathbf{r}}, \tag{4}$$

where Ω is the normalization volume. The interaction $v(r)$ in Eq. (4) is the two-body potential. The Kronecker delta function $\delta_{ij,kl}$ expresses the conservation of total momentum. In the following we shall consider only nonsingular two-body potentials so that perturbation theory can be used. Those features of the theory which we wish to discuss in detail in the next two sections are typical of any repulsive interaction and therefore are first most easily discussed by using a weak potential. To deal with the case of a singular interaction such as a hard-sphere repulsion, it is convenient still to work directly with the matrix elements of the potential which can be defined by considering the potential to be the limit of a repulsion of great but finite strength. In this we depart from the procedure followed by Huang and Yang[1] who introduced the concept of pseudopotential first used by Fermi. We follow this procedure since we wish to maintain the parallelism to the previous theoretical development[5–8] and since the final result we wish to obtain differs radically from that obtained in the pseudopotential approximation. We will return to this point in more detail in Secs. IV and V.

We proceed by first noting the structure of the conventional perturbation theory for the energy. This exhibits certain peculiar features which show that a profound modification of the theory is necessary before a reasonable result can be obtained. We restrict ourselves to a consideration of the energy in the ground state, which we denote by φ_0. We shall also first consider contributions to the energy which comes from transitions to low excited states so that we can regard the matrix elements of v to be independent of the transition. We shall return later to the treatment of the contributions from states far from the ground state.

In this approximation, we make the replacement

$$v_{ij,kl}\rightarrow v_{00,00}=\alpha. \tag{5}$$

The successive orders of the perturbation series for the energy then are:

$$E_1=\tfrac{1}{2}\alpha(\varphi_0,\eta_0^*\eta_0^*\eta_0\eta_0\varphi_0)$$
$$=\tfrac{1}{2}\alpha N(N-1)\underset{N\rightarrow\infty}{\longrightarrow}\tfrac{1}{2}\alpha N^2, \tag{6}$$

where N is the number of particles. The second-order

[10] This structure of the energy expansion is the essential feature of the result obtained by Lee and Yang (reference 2).

energy is

$$E_2=-\frac{\alpha^2}{4}\left(\varphi_0,\ \eta_i^*\eta_j^*\eta_k\eta_l\frac{1}{H_0}\eta_m^*\eta_n^*\eta_r\eta_s\varphi_0\right)$$
$$=-\frac{\alpha^2}{2}\sum_q\left(\varphi_0,\ \eta_0^*\eta_0^*\eta_q\eta_{-q}\frac{1}{q^2/m}\eta_q^*\eta_{-q}^*\eta_0\eta_0\varphi_0\right) \quad (7)$$
$$=-\frac{\alpha^2N^2}{2}\sum_q\frac{1}{(q^2/m)}.$$

For convenience in the following, we here introduce a graphical representation of these processes. In Fig. 1(a), we give the graphical representation of the process giving rise to E_2. In the next order, we first give the graphical representation and then write down the matrix elements by inspection. The process represented in Fig. 1(b) is the excitation of a pair to the state $(\mathbf{q}, -\mathbf{q})$, their scattering to the state $(\mathbf{q}', -\mathbf{q}')$, and final de-excitation. The matrix element is

$$E_3{}^b=N^2\frac{\alpha^3}{2}\sum_q\sum_{q'}\left(\frac{m}{q^2}\right)\left(\frac{m}{q'^2}\right). \quad (8)$$

The next diagram, [Fig. 1(c)], represents the excitation of a pair to the state $(\mathbf{q}, -\mathbf{q})$, the interaction of both of these particles with the unexcited particles, and final deexcitation. The matrix element is

$$\frac{N^3\alpha^3}{2}\sum_q\left(\frac{m}{q^2}\right)^2\times 4, \quad (9)$$

the factor of 4 coming from the direct and exchange interactions of both particles. We now note a feature of these contributions to the energy. Each term is formally proportional to N multiplied by a power of the density, since each power of α gives a factor of Ω^{-1} and each summation over $\mathbf{q}$ or $\mathbf{q}'$, when replaced by an integration, gives a factor of Ω. The two terms, however, are of very different magnitude for small q; the contribution arising from Fig. 1(b) depends on

$$\frac{1}{\Omega^2}\sum_q\sum_{q'}\frac{1}{q^2}\frac{1}{q'^2}\rightarrow\frac{1}{(2\pi)^6}\int\frac{d\mathbf{q}}{q^2}\int\frac{d\mathbf{q}'}{q'^2}, \quad (10)$$

and hence is nonsingular at small values of $\mathbf{q}$, $\mathbf{q}'$. The other term, however, varies as

$$\int\frac{d\mathbf{q}}{q^4}, \quad (11)$$

and hence diverges at the lower limit. Thus, unless a cutoff is introduced for long wavelengths, the third-order energy is infinite. This feature was already implicit in the work of Huang and Yang.[1] Such a result, is, of course, physically meaningless and hence represents a breakdown in the approximation rather than a physical effect. A similar divergence (although of different physical order) occurs in second order in the Coulomb interaction; its exact treatment has recently been given by Gell-Mann and the authors.[3,4]

To proceed, we note that in higher orders, the most divergent terms are always associated with the excitation of one or more pairs to the state $(\mathbf{q}, -\mathbf{q})$ and their interaction (with exchange) with the unexcited particles. If more momentum transfers occur, the multiple integral over the momentum transfer will lead to a lower degree of divergence. Such contributions will be considered separately. In this approximation, the diagrams which interest us are shown in Fig. 2.

We now make use of this result to simplify the Hamiltonian. Since we evaluate the energy for a fixed momentum transfer $\mathbf{q}$ and then sum over $\mathbf{q}$ to get the total energy, we can break up the Hamiltonian into

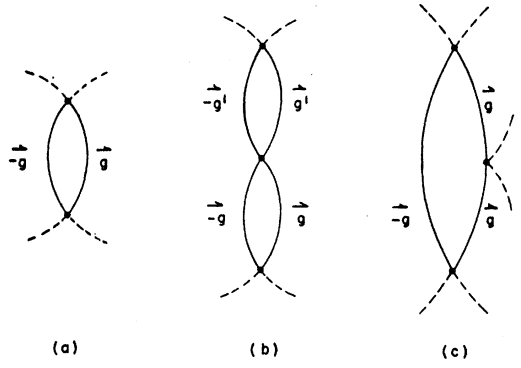

FIG. 1. Excitations contributing to the second and third order of the perturbation energy. In these diagrams the excited particles are indicated by solid lines, the unexcited particles by dashed lines. The diagrams are to be read in the sense of time proceeding from below to above; they therefore do not have the same meaning as a Feynman diagram.

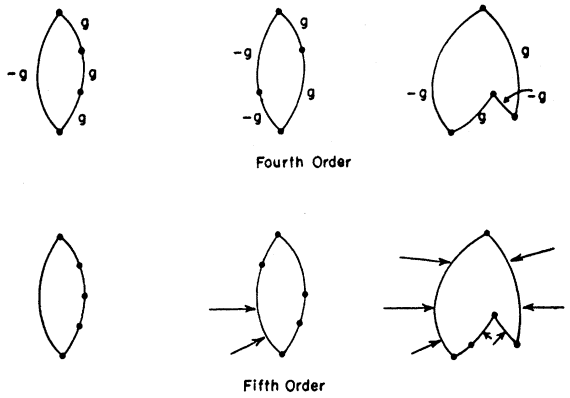

FIG. 2. Connections to the energy in fourth and fifth order. The paths of the unexcited particles are not explicitly indicated, but at each vertex indicated by a closed circle, a number of dashed lines must be added to make the total number of attached lines equal to four. In the diagrams of fifth order, the additional possibilities which arise from different functions of the diagonal interaction are indicated by arrows. These all correspond to different time sequences of interaction.

terms referring to a single $\mathbf{q}$. A typical term we call h_q. The structure of h_q is very simple: the kinetic energy term is

$$h_q^{(0)}=\frac{q^2}{2m}(\eta_q^*\eta_q+\eta_{-q}^*\eta_{-q}). \tag{12}$$

The interaction term is also very simple. The terms arising from interaction between the excited particles and the ground-state particles are:

$$\alpha[\eta_q^*\eta_{-q}^*\eta_0\eta_0+\eta_q\eta_{-q}\eta_0^*\eta_0^* +2\eta_q^*\eta_q\eta_0\eta_0^*+2\eta_{-q}^*\eta_{-q}\eta_0^*\eta_0]. \tag{13}$$

In this the first two terms are pair creation and annihilation; the second two represent forward scattering and exchange (giving a factor of 2). We also must take into account the variation of the expectation value of the interaction energy of the unexcited particles which is

$$\tfrac{1}{2}N_0(N_0-1)\alpha. \tag{14}$$

This we write in terms of the occupation numbers of the excited states by replacing N_0 by

$$N_0=N-\textstyle\sum_q(N_q+N_{-q}). \tag{15}$$

Combining this with the interaction term of Eq. (13), we find for the total interaction term (writing $N_q=\eta_q^*\eta_q$, etc.)

$$h_q'=\alpha[\eta_q^*\eta_{-q}^*\eta_0\eta_0+\eta_q\eta_{-q}\eta_0^*\eta_0^*+2\eta_q^*\eta_q\eta_0^*\eta_0 +2\eta_{-q}^*\eta_{-q}\eta_0^*\eta_0-N\eta_q^*\eta_q-N\eta_{-q}^*\eta_{-q}], \tag{16}$$

where we have dropped some terms which are of order N_q/N_0 and $1/N_0$.

We now further simplify this result by observing that in the terms involving the η_q's, we can replace η_0^* and η_0 by $\sqrt{N}$, where N is the total number of particles. This introduces an error of only order N_q/N in the result. Making this simplification, we obtain

$$h_q=h_q^{(0)}+h_q'=\beta(\eta_q^*\eta_q+\eta_{-q}^*\eta_{-q}) +\alpha N(\eta_q^*\eta_{-q}^*+\eta_q\eta_{-q}), \tag{17}$$

where

$$\beta=(q^2/2m)+\alpha N. \tag{18}$$

This result is remarkable in that it shows that the excitation energy of a pair,

$$\Delta E=(q^2/m)+2\alpha N, \tag{19}$$

may be very much larger than the kinetic energy alone. The consequence is that there is an energy gap (equal to αN in this approximation) between the ground state and any particle excited state.[9] This feature is not only decisive in determining the ground state energy but also leads, as we shall show, to a quite different class of low-lying states which cannot be described simply in terms of particle excitation. It must be emphasized that the gap in energy is a unique consequence of the Bose statistics.

The simple form of the Hamiltonian of Eq. (17) allows us to obtain an exact solution.* We introduce the transformation, assuming $A_q^2<1$,

$$\begin{aligned}\eta_q&=(1-A_q^2)^{-\frac{1}{2}}(A_q\mu_{-q}^*+\mu_q),\\ \eta_q^*&=(1-A_q^2)^{-\frac{1}{2}}(A_q\mu_{-q}+\mu_q^*),\end{aligned} \tag{20}$$

to new operators μ_q^* and μ_q which are easily shown to have the same commutation relations as the η's. In terms of these operators, the Hamiltonian becomes

$$h_q=\frac{2\beta A+\alpha N(1+A^2)}{1-A^2})(\mu_q^*\mu_{-q}^*+\mu_q\mu_{-q}) +\frac{\beta(1+A^2)+2\alpha NA}{1-A^2}(\mu_q^*\mu_q+\mu_{-q}^*\mu_{-q}) +\frac{2\beta A^2+2\alpha NA}{1-A^2}. \tag{21}$$

The nondiagonal terms can be eliminated by choosing

$$2\beta A+\alpha N(1+A^2)=0, \tag{22}$$

or

$$A=\frac{-\beta+(\beta^2-\alpha^2N^2)^{\frac{1}{2}}}{\alpha N}, \tag{23}$$

the positive square root being taken. Inserting this result into h_q, we obtain for the transformed Hamiltonian

$$h_q^T=-\beta\left[1-\left(1-\frac{\alpha^2N^2}{\beta^2}\right)^{\frac{1}{2}}\right] +(\beta^2-\alpha^2N^2)^{\frac{1}{2}}(\mu_q^*\mu_q+\mu_{-q}^*\mu_{-q}). \tag{24}$$

The energy therefore is given by a constant together with a term proportional to the number of "particles" present. The ground state energy is, when one replaces β by $q^2/2m+\alpha N$,

$$E_0(q)=-\left(\frac{q^2}{2m}+\alpha N\right)\left\{1-\left[1-\frac{\alpha^2N^2}{[(q^2/2m)+\alpha N]^2}\right]^{\frac{1}{2}}\right\}, \tag{25}$$

and the total energy, when one replaces the sum over $\mathbf{q}$ by an integral, is

$$E_0=-\frac{1}{2}\frac{\Omega}{(2\pi)^3}\int d\mathbf{q}\left(\frac{q^2}{2m}+\alpha N\right)\times\left\{1-\left[1-\frac{\alpha^2N^2}{[(q^2/2m)+\alpha N]^2}\right]^{\frac{1}{2}}\right\}+\frac{\alpha}{2}N^2, \tag{26}$$

* *Note added in proof.*—It has been pointed out to us by Dr. R. Brout that the following method is very similar to that used by Bogolubov in his theory of superfluidity; J. Phys. U.S.S.R. **11**, 23 (1947).

including the constant term contributed by the unexcited particles. (The factor of $\frac{1}{2}$ compensates for the separation in h_q of the sum over $\mathbf{q}$ into positive and negative $\mathbf{q}$.)

The excited state energies are

$$E_N=E_0+\sum_q \omega_q N_q. \tag{27}$$

We shall here tentatively identify the excited states as phonon states[11]; the phonon energy is

$$\omega_q=\left[\frac{q^2}{2m}\left(\frac{q^2}{2m}+2\alpha N\right)\right]^{\frac{1}{2}}, \tag{28}$$

which, for small q is

$$\omega_q=q(\alpha N/m)^{\frac{1}{2}}, \quad q^2\ll 4m\alpha N. \tag{29}$$

The low excitation energy of these states is in marked contrast to the large energy gap for particle excitation. The linear dependence of ω_q on q is also a consequence of the energy gap since it follows from $q^2/2m\ll 2\alpha N$. Only for excitation large compared to the energy gap does the excitation energy take on the normal form $\omega_q\approx q^2/2m$. We shall not discuss this "phonon" spectrum here in more detail; the detailed discussion and extension of this result forms part of the content of the following paper.

Now returning to the ground state energy, before evaluating Eq. (26) we shall analyze the contributions to the energy using a direct evaluation of the nontransformed Hamiltonian h_q of Eq. (17). We shall again use a graphical representation of the perturbation terms. The interaction

$$h_q'=\alpha N(\eta_q^*\eta_{-q}^*+\eta_q\eta_{-q}) \tag{30}$$

can only create or annihilate pairs; the unperturbed energy

$$h_q^{(0)}=(q^2/2m)+\alpha N \tag{31}$$

describes particle propagation in a medium with a constant potential term of interaction with the medium. The term in $N\alpha$ in the propagator

$$\frac{1}{E_0-h_q^{(0)}}=-\frac{1}{[(q^2/2m)+\alpha N](\eta_q^*\eta_q+\eta_{-q}^*\eta_{-q})}, \tag{32}$$

if expanded as a perturbation, gives rise to an infinite number of interactions via the diagonal interaction term

$$N\alpha(\eta_q^*\eta_q+\eta_{-q}^*\eta_{-q}) \tag{33}$$

which simply arises from the forward and exchange scattering of a particle with the unexcited particles of the medium. Thus, along any propagation line in a diagram, the potential of interaction acts an infinite number of times to give simple propagation.

[11] The validity of this identification is demonstrated in the following paper [K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1128 (1957)].

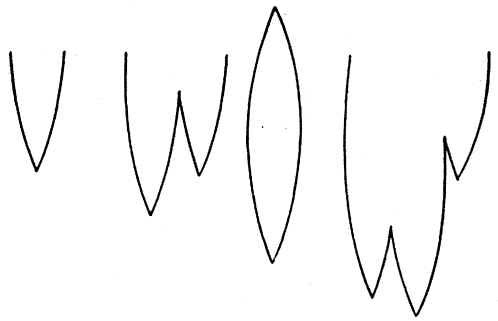

FIG. 3. Correction for self-energy. The pair annihilation operator acting on excited pairs can annihilate one pair to give a closed and separated loop or a self-energy process.

Let us now examine the structure of the perturbation arising from the interaction term. Each term in this series has the form

$$\left(\varphi_0, h_q'\frac{1}{h_q^{(0)}}h_q'\frac{1}{h_q^{(0)}}\cdots\frac{1}{h_q^{(0)}}h_q'\frac{1}{h_q^{(0)}}h_q'\varphi_0\right). \tag{34}$$

To evaluate this matrix element, we consider the effect of the operation

$$\frac{1}{h_q^{(0)}}h_q'\varphi(n), \tag{35}$$

where $\varphi(n)$ is the wave function for n excited pairs. The creation operators in h_q' give

$$\frac{1}{h_q^{(0)}}\eta_q^*\eta_{-q}^*\varphi(n)=\frac{1}{h_q^{(0)}}(n+1)\varphi(n+1)=\frac{1}{2\beta}\varphi(n+1), \tag{36}$$

since

$$h_q^{(0)}\varphi(n+1)=2(n+1)\beta\varphi(n+1). \tag{37}$$

In operating with the annihilation operator, we must avoid including the self-energy which results if the pair annihilated forms a separable closed loop, as shown in Fig. 3. This term occurs only once in operating with $\eta_q\eta_{-q}$ which can close only one loop out of n. Consequently, the matrix element is

$$\begin{aligned}\frac{1}{h_q^{(0)}}\eta_q\eta_{-q}\varphi(n)&=\frac{1}{h_q^{(0)}}[n\varphi(n-1)\\&\quad-\varphi(n-1)(\text{self-energy correction})] \\&=\frac{1}{2\beta}\varphi(n-1).\end{aligned} \tag{38}$$

Thus, the operator $h_q^{(0)-1}h_q'$ multiplies the wave function by $1/2\beta$ and changes the number of pairs by ± 1. The number of contributions to a given order of perturbation theory is therefore the number of ways of going from a no-pair state to a no-pair state multiplied by $N\alpha/2\beta$ raised to the order of the diagram. This

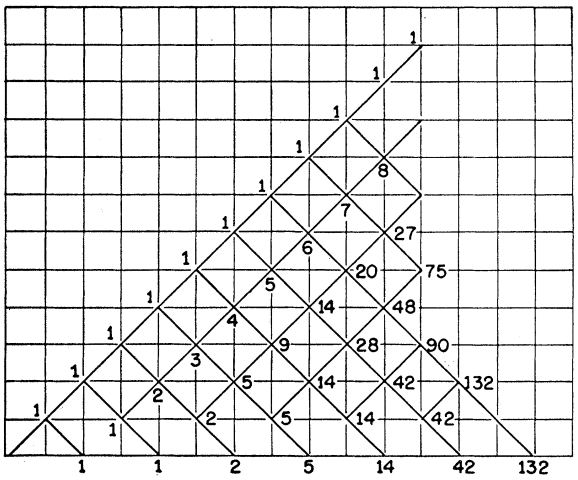

FIG. 4. Number of contributions to each order of perturbation theory with the pair interaction operator. Starting from the lower left, each point in the diagram can be reached in an increasing variety of ways as indicated at each vertex. The sequence of numbers along the lower axis then gives the number of ways of going from a no-pair state (the origin) to a final no-pair state without reaching the axis along the way.

counting is easily carried by inspection of the diagram of Fig. 4 which gives at each vertex the number of ways that vertex can be reached starting at the left. The series is, with $(N\alpha/2\beta)^2=x$,

$$-\frac{N^2\alpha^2}{4\beta}[1+x+2x^2+5x^3+14x^4+42x^5+132x^6+\cdots], \quad (39)$$

which is the expansion of Eq. (25). We shall return to the contribution of the successive terms in this series after evaluating the energy.

III. EVALUATION OF THE ENERGY AT LOW DENSITY

To evaluate the energy, we must first return to the consideration of the high momentum contributions. For large momentum transfers, Eq. (26) for the energy reduces to

$$\Delta E'=\frac{N^2}{2}\left[\alpha+\sum_q \alpha\frac{1}{-(q^2/m)}\alpha\right] \quad (40)$$

which is the low-momentum approximation to

$$\Delta E''=\frac{N^2}{2}\left[v_{00,00}+\sum_q v_{00,q-q}\frac{1}{-(q^2/m)}v_{q-q;00}\right]. \quad (41)$$

These are the first two terms in the expansion of the diagonal element of the scattering operator at zero momentum, which is defined for general momentum transfer by the integral equation

$$S_{q-q,00}=v_{q-q,00}+\sum_{q'} v_{q-q;q'-q'}\frac{1}{-(q'^2/m)}S_{q'-q',00}. \quad (42)$$

The diagonal element is defined in terms of the scattering length a, i.e.,

$$S_{00,00}=(4\pi/m\Omega)a. \quad (43)$$

Thus $\Delta E''$ is the second-order approximation to the scattering length,

$$\Delta E''=(4\pi/m\Omega)a^{(2)}N^2/2. \quad (44)$$

We make use of these results to write the energy in terms of the scattering length, and a convergent integral over $\mathbf{q}$, i.e.,

$$\Delta E=\frac{N^2}{2}\left\{\frac{4\pi}{m\Omega}a^{(2)}+\sum_q[\alpha G(q)\alpha]+\sum_q v_{00,q-q}\frac{m}{q^2}v_{q-q,00}\right\}, \quad (45)$$

where the Green's function $G(q)$ is defined in Eq. (25). We finally shall assume that the integral over $\mathbf{q}$ converges rapidly so that we can replace in the second term $v_{00,q-q}$ by α.

We now return to the evaluation of the energy. Inserting the explicit form for $G(q)$, we find

$$\Delta E=\frac{4\pi N^2}{2m\Omega}a^{(2)}-\frac{1}{2}\frac{\Omega}{(2\pi)^3}\int d\mathbf{q}\left\{\left(\frac{q^2}{2m}+\alpha N\right)\times\left[1-\frac{\alpha^2N^2}{[(q^2/2m)+\alpha N]^2}\right]^{\frac{1}{2}}-\frac{\alpha^2N^2}{(q^2/m)}\right\}. \quad (46)$$

To evaluate the integral, we make the change in variable $q=(2\alpha Nm)^{\frac{1}{2}}S$, which gives

$$\Delta E=\frac{4\pi N^2}{2m\Omega}a^{(2)}-\frac{4\pi\Omega}{(2\pi)^3}\frac{(2\alpha mN)^{\frac{5}{2}}}{4m}\times\int^{\infty}S^2dS\left\{1+S^2-[(1+S^2)^2-1]^{\frac{1}{2}}-\frac{1}{2S^2}\right\}. \quad (47)$$

To bring this to final form, we write

$$\alpha=4\pi a^{(1)}/m\Omega, \quad (48)$$

where by $a^{(1)}$ we mean the first approximation to the scattering length, and write

$$N/\Omega=\rho, \quad (49)$$

where ρ is the density. The integral over S gives $-8\sqrt{2}/15$. Collecting these results, we find

$$\Delta E=N\frac{2\pi\rho}{m}\left\{a^{(2)}+\frac{128}{15\sqrt{\pi}}(a^{(1)})^{\frac{5}{2}}\rho^{\frac{1}{2}}\right\}=N\frac{2\pi\rho a}{m}\left\{1+\frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}\right\}\{1+O(\rho a^3)^{\frac{1}{2}}\}, \quad (50)$$

where the higher order correction terms in ρa^3 arise

from processes we have not yet considered. The coefficient of $(\rho a^3)^{\frac{1}{2}}$ in Eq. (50) agrees with that first obtained by Lee and Yang (private communication) and also that obtained independently by Watson and Riesenfelt [Phys. Rev. (to be published)].

This result gives exactly the first correction to the leading term in a. It is interesting to note, however, that almost all of the correction arises from an exceedingly simple class of diagrams. To show this, we notes that expansion of the integrand of Eq. (47) over S in powers of $(1+S^2)^{-1}$ is equivalent to the expansion of Eq. (39) in powers of the numbers of operations of the pair interaction. The character of this expansion is most easily seen if we write the integral in an alternative form which is obtained by using the identity

$$1+S^2-[(1+S^2)^2-1]^{\frac{1}{2}} = \{1+S^2+[(1+S^2)^2-1]^{\frac{1}{2}}\}^{-1}. \quad (51)$$

Consequently the integral of Eq. (47) can be written

$$\int_0^\infty dS\left\{\frac{S^2}{1+S^2+[(1+S^2)^2-1]^{\frac{1}{2}}}-\frac{1}{2}\right\}. \quad (52)$$

Expansion in powers of $1/S^2$ yields the divergent perturbation series; expansion in $(1+S^2)^{-1}$ is equivalent to the series with the simple propagator modification in which $q^2/2m$ is replaced by $(q^2/2m)+\alpha N$. We note that to a very good approximation, we can make the replacement

$$\frac{S^2}{1+S^2+[(1+S^2)^2-1]^{\frac{1}{2}}} \doteq \frac{1}{2}\left(\frac{S^2}{1+S^2}\right), \quad (53)$$

since $[(1+S^2)^2-1]^{\frac{1}{2}}$ can be accurately replaced by $1+S^2$ except for small S (where the integrand vanishes). To verify this result, we expand the integral to obtain the previously considered series of Eq. (39):

$$\int_0^\infty dS\left\{\frac{S^2}{2(1+S^2)}\left[1+\frac{1}{[2(1+S^2)]^2}+\frac{2}{[2(1+S^2)]^4}+\frac{5}{[2(1+S^2)]^6}+\cdots\right]-\frac{1}{2}\right\} = -\frac{\pi}{4}\left[1-\frac{1}{32}-\frac{5}{1024}-\cdots\right]. \quad (54)$$

Thus the corrections from higher powers of $(1+S^2)^{-1}$ are only about 4%, and it is a very good approximation to compute the energy with the simple correction to the propagator alone. We discuss this feature further in the next section and extend our results to a more general approach.

IV. STRUCTURE OF THE CORRECTION TERMS; RELATION TO FERMION MANY-BODY THEORY

The result of the last section shows that in computing the ground state energy, it is sufficient to a very good approximation to correct the propagator for the excited pairs to take into account their interaction with the medium but to neglect the effects of the simultaneous excitation of many particles. (This procedure is not precise enough, however, to describe properly the phonon excitations which will be treated separately.) To generalize this result we now remove the approximations of the previous sections. As in the theory of the fermion systems with strong interactions, we introduce operators which take into account the repeated interaction of each pair of particles. In this we shall follow closely the formal results given by Brueckner and Levinson[5] in their general theory of fermion and boson systems in strong interaction.

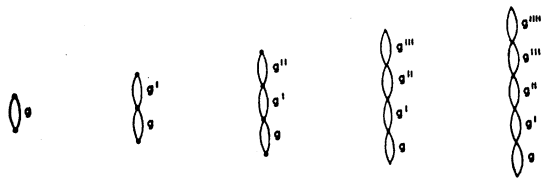

FIG. 5. The succession of transitions summed in the t matrix.

If the particle-particle interactions are strong, we expect that a pair of particles excited from the ground state will interact many times before returning to the ground state. In terms of diagrams, this multiple interaction is shown in Fig. 5 which shows a pair of particles being excited to the state $(\mathbf{q}, -\mathbf{q})$, then interacting and going to the state $(\mathbf{q}', -\mathbf{q}')$, etc., and finally returning to the ground state. In scattering terminology, we expect that the pair-wise interaction will be given by the elements of the scattering matrix which is defined by the integral equation[12]

$$t=v+vGt. \quad (55)$$

We wish to emphasize the fact that this matrix is equal to the free-particle scattering matrix S of Eq. (42) only in the limit of zero density. In this limit, the t-matrix formalism reduces essentially to the pseudopotential formalism used by Yang and Huang.[1] The difference at finite density appears through the many-body effects included in the propagator. In contrast to the scattering case, the Green's function G describes propagation in the presence of the unexcited ground state particles. It is the effects of the propagator alteration, particularly because of the energy gap against particle excitation, which cannot be treated by perturbation methods at high density and which we wish to evaluate in closed form.

The interaction of the excited particles with the unexcited particles can as before be represented as an infinite number of direct and exchange interactions along each propagation line. In contrast to the previous

[12] This integral equation was first used extensively in scattering theory by B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950). Equations of similar structure from the basis of the multiple scattering theory of K. M. Watson, Phys. Rev. **89**, 575 (1953) and of the many-body theory discussed in references 5–8.

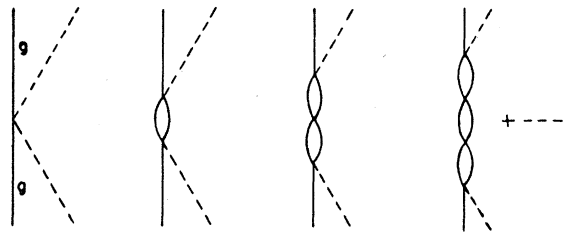

FIG. 6. The diagrams contributing to the interaction between a propagating particle and an unexcited particle. This sequence is summed by introducing the t matrix at the vertex instead of the two-body potential of interaction.

calculation, however, where only the first-order interaction was taken into account, we now include the multiple interactions with the ground state particles. This is equivalent to replacing the first-order interaction v by the t matrix in taking account of the interaction between the excited and unexcited particles. Diagrammatically this is shown in Fig. 6. It is to be emphasized, however, that along each line of any diagram the interation via the t matrix occurs an infinite number of times, while in computing the t matrix itself, the internal propagation lines again include the multiple interactions. Thus a graphical representation is not directly possible, at least in terms of the perturbation interaction.

To determine the Green's function, following the results of Brueckner and Levinson[5] and of the previous sections, we need the excitation energy of a pair taken from the ground state. The propagator for the pair with momenta $\mathbf{q}$, $-\mathbf{q}$ is

$$(\mathbf{q},-\mathbf{q}|G|\mathbf{q},-\mathbf{q})=[E(0,0)-E(q,-q)]^{-1}. \quad (56)$$

The ground state energy is

$$E(0,0)=\tfrac{1}{2}[N(N-1)]t_{00,\,00} \quad (57)$$

and the excited state energy is

$$E(q,-q)=\tfrac{1}{2}(N-2)(N-3)t_{00,\,00}+N(t_{0q,\,0q}+t_{0q,\,q0}+t_{0-q,\,0-q}+t_{0-q,\,-q0})+q^2/m. \quad (58)$$

In the interaction term we have included the exchange contribution. The energy difference then is, if one sets $t_{0q,\,0q}=t_{0-q,\,0-q}$, etc.,

$$E(0,0)-E(q,-q)=-\{(q^2/m)+2N(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00})\}. \quad (59)$$

In the low-momentum limit where all t elements are equal, we see that this reduces to the simple-energy denominator we previously obtained, except that α has been replaced by $t_{00,\,00}$. The corrections to this propagator are, as before, the contributions of multiple excitation of particles through the nondiagonal elements of the t matrix.

It is interesting now to compare this result with the result previously obtained for the fermion case.[5] There, as in this problem, the interaction energy in first approximation is expressed in terms of the scattering operators computed with the Green's function appropriate to propagation in the many-body medium. In that case the corrections to the energy occurred as a series of "linked clusters" which appeared first in third order. These corrections take account of the fluctuations in the average potential seen by a given pair of particles due to their interaction while excited with a third particle of the medium. The transitions of particles in that case were with (i, j, k states in the Fermi gas)

$$\begin{aligned} i+j &\rightarrow i'+j', \\ i'+k &\rightarrow i+k', \\ j'+k' &\rightarrow j+k. \end{aligned} \quad (60)$$

This sequence is the interaction of unexcited particles i and j with excitation to the states i' and j' above the Fermi surface, the interaction of the excited ith particle with the unexcited kth particle of the Fermi gas followed by return to the ith particle to its initial state and excitation of the kth particle, and final interaction of the excited jth and kth particles with transition back to their initial states. These transitions cannot be easily included in the definition of the propagation function and hence were treated as a perturbation in the fermion case. In the boson case such terms are very much simpler and can in fact be easily included in the propagator of an excited pair. To see this, we set $i=j=k=0$ since all unexcited particles are in the same state. The sequence of transitions then is

$$\begin{aligned} 0+0 &\rightarrow q+(-q), \\ q+0 &\rightarrow \left\{\begin{matrix} q+0 \\ 0+q \end{matrix}\right\}, \\ q+(-q) &\rightarrow 0+0, \end{aligned} \quad (61)$$

which has already been included in the definition of the propagator for the excited pair. This feature also persists into the higher order cluster terms and allows the most important class of corrections of the fermion problem to be very simply incorporated in the boson system into the general propagator for the excited pairs.

The first boson correction of double pair creation and annihilation corresponds to a certain class of the fourth order linked cluster terms in the fermion case. The smallness of the 3-body cluster correction in the fermion case arose from the statistics which entered in the high zero-point energy and suppressed multiple excitation. In the boson case, the terms are small for a different reason which is simply the nearly-negligible statistical weight of the diagrams associated with multiple excitation.

Although these corrections to the ground state energy are relatively small, it is still desirable to be

able to evaluate them precisely. The phonon energy spectrum is also sensitive to the precise contributions of the multiple excitations. Both of these problems are considered in detail in the next section.

V. CORRECTIONS TO THE GROUND STATE ENERGY AND PHONON ENERGIES

To determine the corrections to the ground state energy computed from the t matrices defined in the last section, we next determine the remaining processes contributing to the energy which have not yet been included. We again use a graphical representation of the interactions. The most obvious omission is that arising from multiple excitations as shown in Fig. 7. These are the same as those considered in Sec. II except that now the vertex operators are the nondiagonal elements of the t matrix and the propagation lines include infinitely repeated interactions with the unexcited particles of the medium. All of these diagrams are generated by the interaction term

$$\sum_q(\eta_q^*\eta_{-q}^*\eta_0\eta_0 t_{q-q,\,00}+\eta_q\eta_{-q}\eta_0^*\eta_0^* t_{00,\,q-q}), \qquad (62)$$

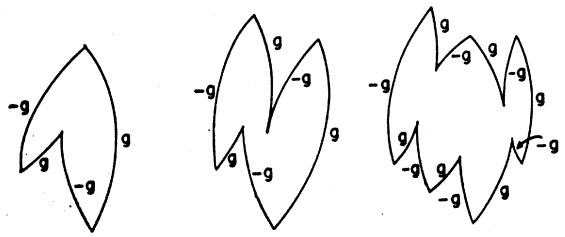

FIG. 7. Diagrams not summed in the t matrices. These represent excitation of more than one pair with the same momentum transfer.

which also determines the phonon energies, as will be shown in the following.

Another class of omitted diagrams is shown in Fig. 8. These represent particle propagation with complicated interactions among the excited particles brought about by excitation of the medium. These alter the definition of the propagation function somewhat but do not lead to an appreciable quantitative change in the t matrices. Their complete inclusion must be considered at the same time the very complicated question of the exact structure of the "off-the-shell" propagators is discussed. These problems also occur in the fermion system where they have been discussed by Brueckner[5] and by Bethe.[7] Such terms can have only a small quantitative effect on the system properties and will not be considered further here.

Finally, the last type of interaction not included in the t matrices is shown in Fig. 9(a). This gives the simplest process involving successive multiple excitation of pairs. It is important to note that the other diagrams of Fig. 9(b) which might seem to contribute in a manner similar to the diagrams of Fig. 9(a) have already been included in the t matrices which include all successive

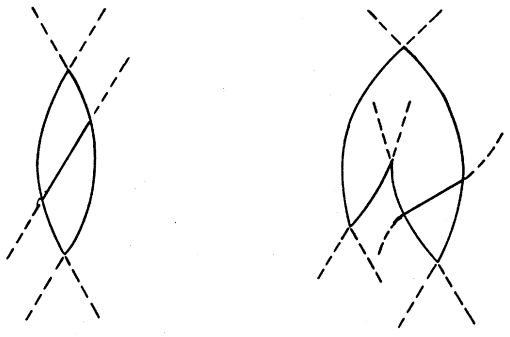

FIG. 8. Complicated interparticle couplings brought about by interaction via the unexcited particles. The unexcited particles are shown explicitly.

interactions at any vertex. The transition of Fig. 9(a) are brought about by the interaction.

$$\sum_q\sum_{q'} t_{q-q,\,q'-q'}\eta_q^*\eta_{-q}^*\eta_{q'}\eta_{-q'}, \qquad (63)$$

which, however, can never act on the ground state and can only be allowed to act between successive multiple excitations. This term leads to phonon-phonon interactions and hence has a very small effect at low phonon densities.

One final effect, which has been mentioned above in connection with the corrections represented by Fig. 8, arises from the approximations which must be made in computing the excited state propagators. We assume that the propagator for an excited particle does not depend on the energy states of other simultaneously excited particles. More explicitly, in computing the matrices such as which determine the excited state propagators, we use the integral equation

$$t_{q'q'',\,0q}=v_{q'q'',\,0q}+\sum_{mn} v_{q'q'',\,mn}(2E_0-E_m-E_n)^{-1}t_{mn,\,0q}, \qquad (64)$$

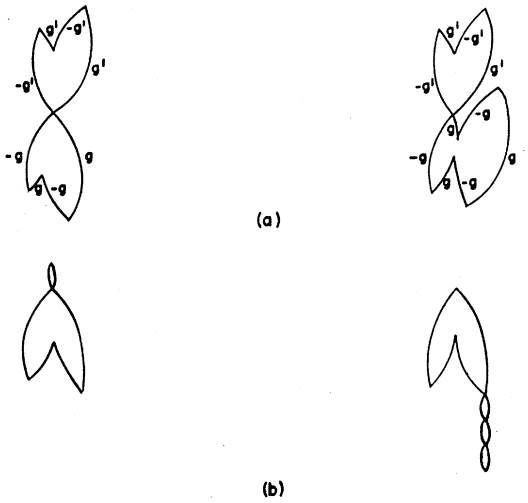

FIG. 9. Interactions between multiple excitations are labeled (a). The diagrams labeled (b) are already included in Fig. 7 since the vertex operator already includes all repeated interactions.

with the propagator not a function of the state of other particles which may be simultaneously excited. This "decoupling" of the energy denominators is already familiar in the fermion case where it forms the essential part of the proof of the noncontribution of the so-called "unlinked clusters" to the energy. The interconnections of the energy denominators which appears in a connected diagram, however, are much more complicated and it has not yet been possible to prove the rigorous independence of the propagation of two excited particles which form the part of a connected diagram.

The assumption of independence or a similar approximation must be made, however, to reduce the formal equation for the reaction matrix to a soluble form. The error introduced by this approximation is not at present well known, but the quantitative effect on the energy seems to be small. Also, as in the case of the contributions of Fig. 8, the effect of this approximation can only slightly alter the quantitative features of the phonon spectrum and will almost certainly not affect the qualitative features. This question is being further investigated at present and will be separately discussed.

Retaining only the significant terms, we finally obtain the result for the effective Hamiltonian acting through the t matrices:

$$H_t=\sum_q\{[(q^2/2m)+N(t_{0q,\,q0}+t_{0q,\,q0}-t_{00,\,00})]\times(\eta_q^*\eta_q+\eta_{-q}^*\eta_{-q})+Nt_{00,\,q-q}(\eta_q^*\eta_{-q}^*+\eta_q\eta_{-q})\}+\sum_q\sum_{q'}t_{q-q,\,q'-q'}\eta_q^*\eta_{-q}^*\eta_{q'}\eta_{-q'},\quad(65)$$

where, as we have remarked already, the last term must be allowed to act only on the multiply-excited pairs. This effective Hamiltonian, it must be remembered, does not have the simple interpretation of the initial Hamiltonian of Eq. (1). It is the result instead of a transformation carried out on the original Hamiltonian which replaced the two-body interaction potentials by the t-matrices. This transformation is not to be confused with that which can be used to introduce the pseudopotentials of Fermi. As discussed in references 4–8, the t matrix includes the most important many-body effects of high order through the nonlinearity of the defining equations [Eqs. (55), (56), (59), and (64)]. Since the propagator of the integral equation defining any t matrix depends on an infinite set of other t matrices through a sum over their diagonal elements, the defining equations actually form an exceedingly complicated set of coupled nonlinear integral equations. In the nuclear problem it has been possible only recently to obtain accurate detailed solutions of a similar array of equations, using fast computing techniques and applying an iteration procedure of self-consistency.[13] We shall not attempt here to describe the mathematical procedures which can be used to solve the equations, but shall return to these in the case of hard-sphere interactions in the following paper.

[13] K. A. Brueckner and J. Gammel, Phys. Rev. **105**, 1679 (1957).

In the language of the many-body fermion theory,[5–8] the Hamiltonian expressed in terms of the matrices is a "model Hamiltonian" which acts on the states of the transformed or "model" system (which are in this case plane waves). The actual wave function, however, is related to the simple model wave function by the exceedingly complicated correlation function or "model operator." This takes precise account of the strong particle-position correlations which must occur since the interactions are strong. Thus the motion of a "model" particle under the influence of the t matrices as interaction operators represents a very complicated rearrangement of the "bare" particles of the original problem.

The effective Hamiltonian of Eq. (65) is of the same form as the simplified Hamiltonian of Eq. (17) except for the coupling term between the q and the q' pairs. This term cannot be eliminated by an orthogonal transformation and remains, after elimination of the principal coupling terms, as a phonon-phonon interaction. We shall not here consider further the effects of this interpretation except to note that it must be taken into account at appreciable phonon densities where it will lead to finite phon mean free paths.

We can now eliminate the remaining interaction term by an orthogonal transformation of the same form as used in the simplified problem of Sec. II. The result is as given in Eq. (20) except that now the values of α and β as defined in Eqs. (5) and (18) are

$$\alpha=t_{00,\,q-q},$$
$$\beta=(q^2/2m)+N(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00}).\quad(66)$$

The ground state energy is only slightly shifted, with the shift as in the earlier calculation amounting to a few percent. The shift is most easily computed by using a conventional perturbation theory in lowest order. The transitions which give the first correction are, as in the earlier simplified calculation,

$$\begin{aligned}0+0&\rightarrow q+(-q),\\0+0&\rightarrow q+(-q),\\q+(-q)&\rightarrow 0+0,\\q+(-q)&\rightarrow 0+0.\end{aligned}\quad(67)$$

The simpler sequence of transitions,

$$\begin{aligned}0+0&\rightarrow q+(-q),\\q+(-q)&\rightarrow 0+0,\end{aligned}\quad(68)$$

is not to be included since it has already been included in the definition of the t matrix. The result for the first-order energy shift is

$$\Delta E_0=\frac{N^2}{2}\sum_q t_{00,\,q-q}{}^4\left[\frac{q^2}{m}+2N(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00})\right]^{-3}.\quad(69)$$

The phonon energies are now given by

$$\omega_q=\left\{\frac{q^2}{2m}\left[\frac{q^2}{2m}+2N(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00})\right]\right.$$
$$\left.+N^2[(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00})^2-t_{00,\,q-q}{}^2]\right\}^{\frac{1}{2}}. \quad (70)$$

If we assume that t depends only on the momentum transfer (which is not actually true in general), this takes on the simpler form

$$\omega_q\cong\left\{\frac{q^2}{2m}\left[\frac{q^2}{2m}+2Nt_{0q,\,q0}\right]\right\}^{\frac{1}{2}}. \quad (71)$$

This spectrum is discussed in the following paper.

VI. ATTRACTIVE INTERACTIONS

In the previous sections we have considered repulsive interactions only, at least in the sense that we tacitly assumed that the quantity α of Eqs. (5) and (25) or

$$V(q)\equiv N(t_{0q,\,0q}+t_{0q,\,q0}-t_{00,\,00}) \quad (72)$$

of Eq. (59) was positive. If the two-body potential is negative everywhere, then α and $V(q)$ are almost certainly negative and the methods we have used fail. This is most clearly seen in the transformation of Eq. (20), which becomes inapplicable if

$$\beta^2-\alpha^2N^2=[(q^2/2m)+\alpha N]^2-\alpha^2N^2 \quad (73)$$

become negative. This can occur for appropriate values of q if α is negative. This feature, however, is not necessarily surprising since if the interaction is everywhere attractive, the system can find states of much lower energy by collapsing to a small volume in coordinate space and hence to a large volume in momentum space. In other words, the noninteracting Bose system in its ground state is highly unstable against the perturbing effects of an attraction.

The situation is much less clear if the potential is nonmonotonic as, for example, is characteristic of He^4 atoms. In this case, although the strong small-distance repulsion in the interaction makes the diagonal elements of potential positive (in fact infinite), the scattering length of the two-body interaction evaluated for free particles is negative. This is due to the effect of the longer-ranged attraction which is more effective at low relative velocities than is the very strong repulsion. Consequently at very low density the Bose gas with an interaction of this type will be unstable and will tend to collapse into regions of higher density, at least if the temperature is very low. At sufficiently high densities, however, the effect of the relatively weak attraction will be small compared to that of the strong repulsion and the effective "scattering length" at high density will be positive.

At equilibrium density neither of the two extremes is possible. The density is far too high for the free two-body scattering length to be a meaningful measure of the interaction, but also the t matrices are apparently negative since the system has positive binding. The description of this state therefore seems to present certain difficulties which cannot be clearly circumvented by the methods of this paper. This problem will be discussed in a separate paper.