

This is an equation for w ; for that point on the geodesic w_0 which touches the envelope. The coordinates of this point are found from (35) and (36) after w itself is found. This equation is written out below for the case of space-like geodesics, in the notation

$$\begin{aligned} s &= \sinh w, & c &= \cosh w, \\ s_0 &= \sinh w_0, & c_0 &= \cosh w_0, \\ \bar{s} &= \sinh \bar{w}, & \bar{c} &= \cosh \bar{w}. \end{aligned} \quad (43)$$

Equation (42) for w becomes

$$\frac{-s_0^2 \bar{c}^5}{\bar{s}(\bar{c}^2 - c_0^2)} + \frac{c_0^2 w}{2} - \frac{\frac{3}{2}s_0^2 \bar{w} + c_0^4 \bar{w} - s_0^2 c_0^2 \bar{w} + \frac{c^3 - 3c}{2s} - \frac{c_0^2 \bar{s} \bar{c}}{2} + \frac{c_0^2 \bar{w}}{2} + \frac{\frac{3}{2}s_0^2 \bar{s} \bar{c} - \frac{3}{2}s_0^2 \bar{w} - c_0^4 \bar{w} + s_0^2 c_0^2 \bar{w} + \frac{\bar{s} \bar{c} c_0^4}{\bar{c}^2 - c_0^2}}{2} = 0. \quad (44)$$

No method other than trial and error is evident for solving this equation for w . The envelope of geodesics shown in Fig. 6 was determined, not by solving this equation, but by inspection of the geodesics themselves.

Nonideal Bose Gas at Nonzero Temperatures

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An extension to nonzero temperatures of the Hugenholtz-Pines procedure for the degenerate Bose gas is provided. It is shown that under certain conditions the elementary excitation spectrum must approach zero for zero momentum, at nonzero, as well as at zero temperatures. The apparent discrepancy of this result with the particular case of a charged boson gas with a uniform positive background is discussed. Finally, a suggestion is made for modifying the Bogoliubov approximation, which is particularly relevant at nonzero temperatures.

1. GRAND PARTITION FUNCTION

IT was pointed out by Hugenholtz and Pines¹ that one cannot apply, straightforwardly, field-theoretic techniques to the degenerate gas of interacting Bose particles. Because of the high probability of occupation of the zero-momentum single free-particle state, the cancellation which usually occurs up to terms of order (volume)⁻¹ between disconnected diagrams and renormalization terms in the perturbation series for, say, the ground-state energy per particle no longer takes place. They have also provided a procedure for determining the ground state which is an extension of the Bogoliubov² method for low-density systems. If $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ are the creation and annihilation operators of particles with momentum $\hbar\mathbf{k}$, we replace a_0^\dagger and a_0 by a parameter $\sqrt{N_0}$, and thus obtain a Hamiltonian $H(N_0)$ which is a function of N_0 . One then determines the eigenstate of $H(N_0)$ with the lowest eigenvalue E_0 subject to the subsidiary condition

$$\bar{N}' = N - N_0, \quad (1.1)$$

where $N' = \sum_{\mathbf{k}}' a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$; the prime on the summation symbol indicating the value $k=0$ is to be omitted; the bar indicates a quantum-mechanical average; and N is the total number of particles in the original system.

The parameter N_0 must then be determined in such a way that E_0 is minimal.

Since $H(N_0)$ does not commute with N' , it is insufficient to impose this condition on the unperturbed wave functions. The simplest way of including it is to introduce an undetermined multiplier $\mu_{\text{H.P.}}$, to find the ground state of the Hamiltonian

$$H' = H(N_0) - \mu_{\text{H.P.}} N', \quad (1.2)$$

without any subsidiary condition, and to determine $\mu_{\text{H.P.}}$ from

$$\bar{N}' = N - N_0.$$

N_0 is then again determined by the condition

$$(d/dN_0)(E_0) = 0. \quad (1.3)$$

Although it has not been proved rigorously that this whole procedure leads to correct results, Misawa³ has shown that to third order in the interaction potential it gives correct results for E_0 , and one of us (W.E.P.) has extended this calculation to fourth order, with the same conclusion. We also note that by this method one obtains the same results as Beliaev,⁴ who used a different procedure.

One would next like to extend this idea to the determination of thermodynamic functions at nonzero

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¹ N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

² N. N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947).

³ S. Misawa, Prog. Theoret. Phys. (Kyoto) **24**, 1224 (1960).

⁴ S. T. Beliaev, J. Exptl. Theoret. Phys. (U.S.S.R.) **34**, 417 (1958) [translation: Soviet Phys.—JETP **7**, 289 (1958)].

temperatures. Glassgold *et al.*⁵ have discussed the statistical mechanics of the nonideal Bose gas, but they use Bogoliubov's Hamiltonian in a straightforward way without discussing the replacement of a_0^\dagger and a_0 by $\sqrt{N_0}$.

Their results would seem, therefore, to be true only for low-density systems. However, we shall show that their procedure is correct at all densities.

Suppose that we have found *all* the eigenvectors of $H(N_0)$; that is, taking no account of the subsidiary condition. Let these eigenvectors be $|r, N_0\rangle$, their corresponding eigenvalues $E(r, N_0)$ and the expectation value of $N' = \bar{N}'(r, N_0)$. Now consider the grand partition function (G.P.F.) for the grand canonical ensemble for the actual boson system:

$$\begin{aligned} \text{G.P.F.} &= \text{Tr} \exp[-\beta(H - \mu N_{\text{op}})] \\ &= \sum_{\{\nu, \mathfrak{N}\}} \exp[-\beta(E(\nu, \mathfrak{N}) - \mu \mathfrak{N})], \end{aligned} \quad (1.4)$$

where $N_{\text{op}} = \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ (the $\mathbf{k}=0$ term being included) and $\{\nu, \mathfrak{N}\}$ is some set of states which diagonalize the Hamiltonian in such a way that the total number of particles in the system is \mathfrak{N} . \mathfrak{N} must then be allowed to take all positive integral values. $E(\nu, \mathfrak{N})$ is the eigenvalue of H corresponding to the eigenvector (ν, \mathfrak{N}) . It should be noted that μ is now the chemical potential, and is, therefore, introduced in a very different way from that used to introduce $\mu_{\text{H.P.}}$ at zero temperatures. However, as $T \rightarrow 0$ it can easily be shown that $\mu \rightarrow \mu_{\text{H.P.}}$.

Now, using Hugenholtz and Pines' idea, the energy levels $E(\nu, \mathfrak{N})$ may be found by selecting from the $E(r, N_0)$ only those which satisfy the condition

$$\mathfrak{N} = \bar{N}'(r, N_0) + N_0. \quad (1.5)$$

Thus,

$$\text{G.P.F.} = \sum'_{r, N_0 \mathfrak{N}} \exp\{-\beta[E(r, N_0) - \mu \mathfrak{N}]\}, \quad (1.6)$$

the prime on the summation symbol indicating that only those terms for which the condition (1.5) is satisfied are to be included. Now let us rearrange the terms in the sum, which we assume to be absolutely convergent, so that we first choose N_0 and r , and then \mathfrak{N} . But when we have chosen N_0 and r , \mathfrak{N} is determined for us by Eq. (1.5). Equation (1.6) thus becomes

$$\begin{aligned} \text{G.P.F.} &= \sum_{r, N_0} \exp[-\beta\{E(r, N_0) \\ &\quad - \mu[\bar{N}'(r, N_0) + N_0]\}], \end{aligned} \quad (1.7)$$

μ must now be chosen in such a way that

$$\begin{aligned} \sum_{r, N_0} [\bar{N}'(r, N_0) + N_0] \exp[-\beta\{E(r, N_0) \\ - \mu[\bar{N}'(r, N_0) + N_0]\}] = N \times \text{G.P.F.} \end{aligned} \quad (1.8)$$

We may rewrite Eq. (1.7) in the form

$$\begin{aligned} \text{G.P.F.} &= \sum_{N_0} e^{\mu N_0 \beta} \sum_r \exp[-\beta\{E(r, N_0) - \mu \bar{N}'(r, N_0)\}] \\ &= \sum_{N_0} e^{\mu N_0 \beta} Z(\mu, N_0, \beta), \end{aligned} \quad (1.9)$$

where

$$Z(\mu, N_0, \beta) = \sum_r \exp[-\beta\{E(r, N_0) - \mu \bar{N}'(r, N_0)\}]. \quad (1.10)$$

We may now follow Glassgold *et al.* and take the largest term in (1.9) as a good approximation to the sum, since the summand is a sharply peaked function of N_0 . If this largest term occurs when $N_0 = N_0'$, we have

$$\frac{\partial}{\partial N_0} [\beta \mu N_0 + \ln Z(\mu, N_0, \beta)]|_{N_0=N_0'} = 0,$$

or

$$\mu = - \frac{\partial}{\partial N_0} [\beta^{-1} \ln Z(\mu, N_0, \beta)]|_{N_0=N_0'}. \quad (1.11)$$

As usual, the statistical average value of N_0 is equal to N_0' . We may now work with Z , which is the grand partition function for a system with a non-particle-conserving Hamiltonian $H(N_0)$. The zero-momentum state has been separated out, just as it was by Hugenholtz and Pines for $T=0$.

2. THEOREM ON THE ELEMENTARY EXCITATION SPECTRUM

We shall next extend the Hugenholtz-Pines theorem on the elementary excitation spectrum to nonzero temperatures. Their proof rests on the use of Green's functions:

$$\mathcal{G}(\mathbf{k}, t-t') = -i \langle \psi_0 | T a_{\mathbf{k}}(t) a_{\mathbf{k}}^\dagger(t') | \psi_0 \rangle, \quad (2.1)$$

where T is the time-ordering symbol, and $|\psi_0\rangle$ is the ground-state wave function. $a_{\mathbf{k}}(t)$ is an operator in the Heisenberg representation, so that:

$$a_{\mathbf{k}}(t) = e^{iH't} a_{\mathbf{k}}(0) e^{-iH't}. \quad (2.2)$$

The Fourier transform $\mathcal{G}(\mathbf{k}, \epsilon)$ of this function can be shown to take the form:

$$\mathcal{G}(\mathbf{k}, \epsilon) = \frac{\epsilon + \frac{1}{2}k^2 - \mu_{\text{H.P.}} + \Sigma_{11}(\mathbf{k}, -\epsilon)}{\{\epsilon - \frac{1}{2}[\Sigma_{11}(\mathbf{k}, \epsilon) - \Sigma_{11}(\mathbf{k}, -\epsilon)]\}^2 - \{\frac{1}{2}k^2 - \mu_{\text{H.P.}} + \frac{1}{2}[\Sigma_{11}(\mathbf{k}, \epsilon) + \Sigma_{11}(\mathbf{k}, -\epsilon)]\}^2 + [\Sigma_{02}(\mathbf{k}, \epsilon)]^2}, \quad (2.3)$$

where $\Sigma_{11}(\mathbf{k}, \epsilon)$ is the proper vertex part for one ingoing and one outgoing line of momentum \mathbf{k} and energy ϵ ,

⁵ A. E. Glassgold, A. N. Kaufman, and K. M. Watson, Phys. Rev. **120**, 660 (1960).

and $\Sigma_{02}(\mathbf{k}, \epsilon)$ is the proper vertex part for two ingoing and no outgoing lines. The Hamiltonian used in constructing this Green's function is that given in Eq. (1.2).

Hugenholtz and Pines derive an expression for $\mu_{H.P.}$:

$$\mu_{H.P.} = \partial E_0' / \partial N_0, \quad (2.4)$$

where E_0' is the lowest eigenvalues of the Hamiltonian (1.2). Then, by noticing that all diagrams for Σ_{11} and Σ_{02} can be obtained uniquely from diagrams for E_0' by adding two appropriate external lines, they obtain after a little algebra,

$$\mu_{H.P.} = \lim_{k \rightarrow 0} [\Sigma_{11}(k, 0) - \Sigma_{02}(k, 0)] \quad (2.5)$$

We see that, provided that the Σ 's are well behaved for \mathbf{k} and $\epsilon \rightarrow 0$, the poles of $\mathcal{G}(\mathbf{k}, \epsilon)$ for $\mathbf{k} \rightarrow 0$ approach $\epsilon = 0$. Thus, since the poles of $\mathcal{G}(\mathbf{k}, \epsilon)$ give the excitation spectrum for the system, we can have no energy gap in this spectrum.

In the case $T \neq 0$, we first notice that Eq. (2.4) is replaced by Eq. (1.11). Now it is well known⁶ that for $T \neq 0$ the function

$$\Omega = -\beta^{-1} \ln Z(\mu, N_0, \beta) \quad (2.6)$$

can be expanded in a very similar way to the energy expansion for $T=0$. (This is, of course, only possible since we have used a trick to get rid of the difficulties of the zero-momentum state.) Namely, in the "energy" representation, one draws all closed connected graphs and sums over all allowed values of the energy and momentum of the lines of the graph. At zero temperature, the only restrictions imposed on the energies and momenta are the conservation of energy and momentum at each vertex. For $T \neq 0$, an extra condition is imposed: The only allowed values for the "energies" of a line are $\omega_n = 2\pi n/\beta$, where n is an integer.

We may still define proper vertex parts for such graphs, $\Sigma_{11}^\beta(\mathbf{k}, \omega_n)$, $\Sigma_{02}^\beta(\mathbf{k}, \omega_n)$, and we see that we may use exactly the same algebra as Hugenholtz and

Pines to prove that in the case $T \neq 0$:

$$\mu = \lim_{k \rightarrow 0} [\Sigma_{11}^\beta(\mathbf{k}, 0) - \Sigma_{02}^\beta(\mathbf{k}, 0)]. \quad (2.7)$$

In order to study the elementary excitation spectrum, we must consider the Green's functions of the system. We define two such functions,⁷ the temperature-dependent Green's function and the retarded time-temperature-dependent Green's function. The first is defined by

$$\mathcal{G}^\beta(\mathbf{k}, \tau) = \langle T a_{\mathbf{k}}(\tau) a_{\mathbf{k}}^\dagger(0) \rangle, \quad |\tau| < \beta \quad (2.8)$$

where $\langle \cdots \rangle$ denotes a grand canonical average and

$$a_{\mathbf{k}}(\tau) = e^{H'\tau} a_{\mathbf{k}} e^{-H'\tau}, \quad (2.9)$$

where H' is now given by Eq. (1.2) with $\mu_{H.P.}$ replaced by μ .

The retarded time temperature-dependent Green's function is defined by

$$G_R^\beta(\mathbf{k}, t) = -i\theta(t) \langle [a_{\mathbf{k}}(t), a_{\mathbf{k}}^\dagger(0)] \rangle, \quad (2.10)$$

where

$$\begin{aligned} \theta(t) &= 1 \quad \text{for } t > 0 \\ &= 0 \quad \text{for } t < 0; \end{aligned} \quad (2.11)$$

$[\ , \]$ denotes a commutator, and $a_{\mathbf{k}}(t)$ is given by Eq. (2.2). $\mathcal{G}^\beta(\mathbf{k}, \tau)$ may be made periodic in τ with period β and may, therefore, be expanded in a Fourier series with Fourier coefficients $\mathcal{G}^\beta(\mathbf{k}, \omega_n)$ ($\omega_n = 2\pi n/\beta$). On the other hand, $G_R^\beta(\mathbf{k}, t)$ may be expressed as a Fourier integral with kernel $G_R^\beta(\mathbf{k}, \omega)$.⁸ It can then be shown⁷ that

$$G_R^\beta(\mathbf{k}, \omega) = -\mathcal{G}^\beta(\mathbf{k}, -i\omega), \quad (2.12)$$

where $\mathcal{G}^\beta(\mathbf{k}, -i\omega)$ is the function obtained formally from $\mathcal{G}^\beta(\mathbf{k}, \omega_n)$ by replacing ω_n by $-i\omega$. The poles of $G_R^\beta(\mathbf{k}, \omega)$ then give the elementary excitation spectrum of the system in the usual way.

A formal expression for $\mathcal{G}^\beta(\mathbf{k}, \omega_n)$ can be found in the same way as that used for $\mathcal{G}(\mathbf{k}, \epsilon)$ at $T=0$. One obtains

$$\mathcal{G}^\beta(\mathbf{k}, \omega_n) = - \frac{i\omega_n + \frac{1}{2}k^2 - \mu + \Sigma_{11}^\beta(\mathbf{k}, -i\omega_n)}{\{i\omega_n - \frac{1}{2}[\Sigma_{11}^\beta(\mathbf{k}, i\omega_n) - \Sigma_{11}^\beta(\mathbf{k}, -i\omega_n)]\}^2 - \{\frac{1}{2}k^2 - \mu + \frac{1}{2}[\Sigma_{11}^\beta(\mathbf{k}, i\omega_n) + \Sigma_{11}^\beta(\mathbf{k}, -i\omega_n)]\}^2 + \{\Sigma_{02}^\beta(\mathbf{k}, i\omega_n)\}^2}, \quad (2.13)$$

where μ is given by Eq. (2.7).

The theorem on the excitation spectrum now follows immediately, provided that the Σ 's are well behaved for $\mathbf{k} \rightarrow 0$ and $\omega \rightarrow 0$.

3. CONCLUSION

It is interesting to consider the charged boson gas in the light of this work, since it has recently been suggested by Foldy⁹ that there possibly exists an energy gap in the elementary excitation spectrum, such that

⁶ C. Bloch and C. de Dominicis, Nuclear Phys. 7, 459 (1958).

the energy $\epsilon_{\mathbf{k}}$ of an elementary excitation of momentum \mathbf{k} does not go to zero as \mathbf{k} goes to zero. If the usual Bogoliubov method can be applied, which in our case is equivalent to putting

$$\Sigma_{11}(\mathbf{k}, \omega) = N_0(V_{\mathbf{k}} + V_0), \quad \Sigma_{02} = N_0 V_{\mathbf{k}}, \quad (3.1)$$

where the $V_{\mathbf{k}}$'s are the usual Fourier components of the

⁷ A. Alekseev, Usp. Fiz. Nauk 73, 41 (1961) [translation: Soviet Phys.—Usp. 3, 320 (1960)].

⁸ D. N. Zubarev, Usp. Fiz. Nauk. 71, 71 (1960) [translation: Soviet Phys.—Usp. 3, 320 (1960)].

⁹ L. L. Foldy, Phys. Rev. 124, 649 (1961).

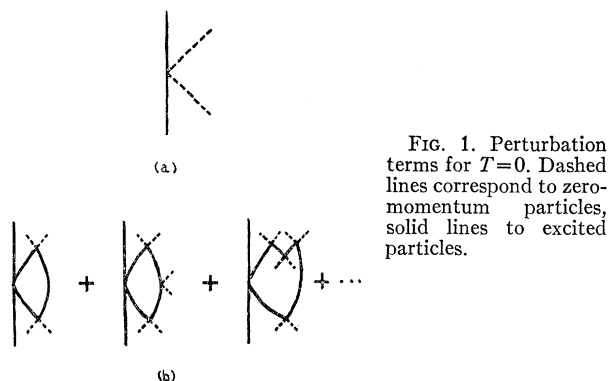


FIG. 1. Perturbation terms for $T=0$. Dashed lines correspond to zero-momentum particles, solid lines to excited particles.

two-body potential, we obtain for ϵ_k

$$\epsilon_k^2 = (k^2/2m)^2 + N_0 V_k k^2/m. \quad (3.2)$$

For the charged boson gas with a uniform positive background,

$$V_k = 4\pi e^2/k^2 v, \quad k \neq 0, \\ = 0, \quad k = 0, \quad (3.3)$$

where v is the volume of the system, and it appears that we obtain an energy gap for $k \rightarrow 0$. This results from taking Σ 's which are not well behaved at the origin, namely,

$$\lim_{k \rightarrow 0} V_k \neq V_0.$$

Thus, the energy gap is probably a result of the approximations. The uniform positive background model leads directly to this discontinuity and the replacement of this by discrete positive charges will remove it. Further, higher approximations to the Σ 's may not have the $1/k^2$ dependence for low k .

Lastly, we notice that the importance of using factors N_0 rather than N in Eq. (3.1) has often been stressed. It is, however, easy to see that the sum of all diagrams like those in Fig. 1(b) contributing to $\Sigma_{11}(\mathbf{k}, \omega)$ give us $2N'V_0$ for low values of \mathbf{k} and ω approximately, whereas the diagram in Fig. 1(a) gives us $N_0(V_0 + V_k)$, the contribution we have already included in Eq. (3.1), giving a total contribution of $2NV_0$. A similar argument can be applied for $\Sigma_{11}^\beta(\mathbf{k}, \omega)$ at nonzero temperatures. For slowly varying potentials it may, therefore, be a better approximation to put

$$\Sigma_{11}^\beta(\mathbf{k}, \omega) = N(V_0 + V_k).$$

Similar considerations could apply if we replaced V_k by a reaction matrix element. There is no analogous argument for Σ_{02} . A reasonable model for discussing the condensed boson gas at temperatures different from zero might be to assume that Σ_{11} was independent of temperature and that Σ_{02} depended on the temperature solely through its factor of N_0 .

Static Approximation and Bounds on Single-Channel Phase Shifts*†

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A single-channel scattering process with the set of quantum numbers C is completely characterized by a phase shift, η_C . A common approximation in the determination of η_C for the scattering of a particle by a compound system is to assume that, apart from the possibility of an exchange of the incident particle with an identical target particle, the target is unaffected by the incident particle. The incident particle is then scattered by the static potential generated by the target in its ground state. The phase shift determined in this approximation, to be called η_C^P , can be calculated for a number of scattering processes. Let H represent the Hamiltonian of the entire system, incident particle plus target, let E_{T0} be the ground-state energy of the target, and let $E'_C{}^Q$ be the smallest energy for which $E'_C{}^Q + E_{T0} - H$ is a negative definite operator in the space in which the given quantum numbers are C

and in which the ground state of the target is projected out. Utilizing the generalized optical potential formalism due to Feshbach and others, it can then be shown that $\eta_C > \eta_C^P$ if the incident energy is less than $E'_C{}^Q$. (The bound is probably valid for higher energies, perhaps for all energies for which the process remains a single-channel process. If so, however, the difference between η_C and η_C^P for these higher energies will generally be large, of the order of a multiple of π , and the bound will not be immediately useful. We will, therefore, be concerned primarily with incident energies E' less than $E'_C{}^Q$.) Furthermore, as one allows for more and more virtual excitation of the target system, the approximate phase shift is guaranteed to improve if E' is less than $E'_C{}^Q$, and $E'_C{}^Q$ will itself increase. Applications are given to the scattering of electrons and of positrons by hydrogen atoms.

1. INTRODUCTION

THE minimum principle formulation for the determination of the scattering length in single-channel scattering^{1,2} has most of the properties that one

would want to have. At nonzero incident energies, however, the minimum principle formulation for the

† A preliminary report of this work was given at the New York Meeting of the American Physical Society [Bull. Am. Phys. Soc. 7, 41 (1962)].

¹ L. Spruch and L. Rosenberg, Phys. Rev. 116, 1034 (1959); 117, 1095 (1960).

² L. Rosenberg, L. Spruch, and T. F. O'Malley, Phys. Rev. 118, 184 (1960).

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