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Excitation Spectrum of a Many-Boson System

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It is shown within the framework of certain approximations that the excitation spectrum of a many-boson system satisfies the dispersion equation $E_{\mathbf{q}}=|\mathbf{q}|v$, where $\mathbf{q}$ is the momentum of the excitation and v is the macroscopic sound velocity. The approximations which are necessary are described in the text. A method of avoiding the difficulties which arise in discussing a system with attractive forces is suggested, so that it may be possible to perform a calculation of the properties of liquid helium.

I. INTRODUCTION

THE quantum mechanical problem of many bosons interacting through a two-body force has received considerable attention in the past few years. In particular, the structure of the excitation spectrum is of interest since it determines the thermodynamic properties of the system. It has been shown that the spectrum decreases to zero as the momentum of the excitation decreases[1] and it has further been shown in lowest order in the density that the spectrum is linear in the momentum.[2]

We wish to show that within certain approximations the excitation energy at low momenta is that of a sound wave; $E_{\mathbf{q}}=|\mathbf{q}|v$, where $\mathbf{q}$ is the momentum of the excitation and v is the velocity of sound. The nature of the approximations made will be explained in the text. This result clarifies a difficulty which has prevented the application of the methods of Brueckner and others to liquid helium. It may be possible to perform a calculation of the properties of liquid helium similar to the calculation of Brueckner and Gammel[3] for nuclear matter.

In the material to follow, we are considering a system of N particles confined in a volume Ω, where N is a fixed large number but Ω may vary. The density N/Ω is denoted by ρ.

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[1] D. Pines and N. M. Hugenholtz, Phys. Rev. **116**, 489 (1959).
[2] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117 (1957).
[3] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1023 (1958).

II. REVIEW OF THE LOWEST ORDER THEORY

The Hamiltonian for the N particle system is

$$H=\sum_{\mathbf{q}}(q^2/2m)\eta_{\mathbf{q}}^{\dagger}\eta_{\mathbf{q}}+\tfrac{1}{2}\sum v(\mathbf{k},\mathbf{l},\mathbf{m},\mathbf{n})\eta_{\mathbf{k}}^{\dagger}\eta_{\mathbf{l}}^{\dagger}\eta_{\mathbf{m}}\eta_{\mathbf{n}}$$

$$v(\mathbf{k},\mathbf{l},\mathbf{m},\mathbf{n})=\tilde{v}(\mathbf{k}-\mathbf{m})=\frac{(2\pi)^3}{\Omega}\delta(\mathbf{k}+\mathbf{l}-\mathbf{m}-\mathbf{n})\times\int d^3r\,\exp[i(\mathbf{k}-\mathbf{m})\cdot\mathbf{r}]V(|\mathbf{r}|),$$

where $\eta_{\mathbf{q}}$ and $\eta_{\mathbf{q}}^{\dagger}$ are, respectively, annihilation and creation operators for a particle of momentum $\mathbf{q}$. Brueckner and Sawada[2] have discussed the problem in the approximation in which the replacement

$$\eta_0^{\dagger}\eta_0=N-\sum_{\mathbf{q}\neq 0}\eta_{\mathbf{q}}^{\dagger}\eta_{\mathbf{q}}$$

is made and only terms containing one momentum sum are taken into account. The Hamiltonian is then approximately

$$H'=\sum_{\mathbf{q}}[q^2/2m+N(v(0,\mathbf{q},0,\mathbf{q})+v(0,\mathbf{q},\mathbf{q},0)-v(0,0,0,0))]\eta_{\mathbf{q}}^{\dagger}\eta_{\mathbf{q}}+\sum_{\mathbf{q}}Nv(0,0,\mathbf{q},-\mathbf{q})\times[\eta_{\mathbf{q}}^{\dagger}\eta_{-\mathbf{q}}^{\dagger}+\eta_{\mathbf{q}}\eta_{-\mathbf{q}}]+\tfrac{1}{2}N^2v(0,0,0,0).$$

The Hamiltonian H' was diagonalized by Brueckner and Sawada to give the ground-state energy of

$$\tfrac{1}{2}N^2\tilde{v}(0)-\tfrac{1}{2}\sum_{\mathbf{q}}\{\beta(\mathbf{q})-[\beta(\mathbf{q})^2-\Gamma(\mathbf{q})^2]^{1/2}\},$$

where

$$\beta(\mathbf{q})=q^2/2m+N\tilde{v}(\mathbf{q}),$$
$$\Gamma(\mathbf{q})=N\tilde{v}(\mathbf{q}),$$

and an excitation spectrum of

$$E_q=[\beta(q)^2-\Gamma(q)^2]^{1/2}$$
$$=[(q^2/2m)(q^2/2m+2N\tilde{v}(\mathbf{q}))]^{1/2}.$$

Brueckner and Sawada showed further that the result for the ground-state energy can be obtained using perturbation theory as one would expect, but that it is necessary to sum an infinite number of terms, the so-called pair terms. It can also be shown[4] that the above expression for the excitation energy can be obtained in perturbation theory, but it is again necessary to perform an infinite sum. The diagonal matrix elements give rise to a first-order energy spectrum of $\beta(\mathbf{q})$. This quantity or a generalization of it will be called the single-particle energy. It can be shown that the pair terms contribute an amount

$$-\beta(\mathbf{q})+[\beta(\mathbf{q})^2-\Gamma(\mathbf{q})^2]^{1/2},$$

which cancels the single-particle energy and gives the result for E_q. This argument will be extended to the general situation.

III. THE GROUND-STATE ENERGY

The ground-state energy of the system is, in perturbation theory, a sum of terms each proportional to the volume of the system and each amenable to a graphical description. The graphs in question consist of n ordered vertices each with 4 directed lines attached, 2 incoming and 2 outgoing, such that every vertex can be reached from every other vertex by following a sequence of lines. Certain lines do not begin with the graph; they will be called incoming lines and correspond in the ground-state case to a particle of zero momentum. These lines will be shown as broken lines. Similarly, certain lines, which will be called outgoing lines, do not end in the graph. Furthermore, the number of outgoing lines is equal to the number of incoming lines. Each incoming or outgoing line contributes a statistical factor $N^{1/2}$ to the term in the energy corresponding to the particular graph.

There is a further type of graph which has been discussed by Sawada[5] which arises because of an inexact cancellation of unlinked terms. These graphs can be described by introducing a new type of linkage in which a vertex at which an incoming or outgoing line is attached is connected to an internal *line* which joins a preceding to a following vertex. Such a linkage will be called an S link. Each S link contributes a factor $(-2N)^{-1}$ to the particular term in the energy. The ground-state energy is then the sum of all terms corresponding to linked diagrams, including S linked diagrams. Since the result is to be derived in the approximation in which all S linked diagrams are neglected, it is not necessary to go into greater detail regarding them.

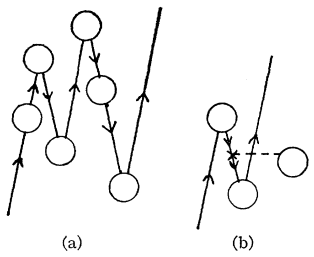

FIG. 1. Examples of graphs whose contributions to the energy have been included in the discussion. An upward arrow denotes a particle of momentum $\mathbf{q}$; a downward arrow a particle of momentum $-\mathbf{q}$.

We note that since the over-all energy is proportional to Ω, and each incoming or outgoing line produces a factor $N^{1/2}$, the contribution to the energy of a graph with p incoming lines is proportional to $N^p\Omega^{(1-p)}$ or is $A\rho^p\Omega$, where A is a number independent of N or Ω which is determined only by the graph.

IV. EXCITED-STATE ENERGIES

To discuss the energy spectrum in perturbation theory the unperturbed state with one zero-momentum particle removed and one particle with momentum $\mathbf{q}$ added is considered. The effect of this on a graph with p incoming lines will be considered in the limit as $\mathbf{q}\rightarrow 0$. If the contribution of a particular graph is $AN^p\Omega^{(1-p)}$, the effect of removing one particle is to change this to $A(N-1)^p\Omega^{(1-p)}$. The quantity of interest is the energy difference which is

$$A(N-1)^p\Omega^{(1-p)}-AN^p\Omega^{(1-p)}\sim -pA\rho^{(p-1)},$$

where terms of lower order in N have been neglected.

There is also a contribution to the energy by virtue of the fact that the excited particle may interact with those of zero momentum. Graphically, this means that a line corresponding to the excited particle may enter a particular ground-state energy graph at one of p vertices and may leave it at one of p vertices producing a total contribution of

$$p^2AN^{p-1}\Omega^{(1-p)}.$$

A factor N is removed since one incoming and one outgoing zero-momentum line are removed. The net result for the contribution of a particular graph is

$$p(p-1)A\rho^{p-1},$$

which may be conveniently expressed as

$$\rho(d^2/d\rho^2)(E/\Omega),$$

for fixed N. We will call the quantity

$$q^2/2m+\rho(d^2/d\rho^2)(E/\Omega)$$

the single-particle energy. The single-particle energies have a finite separation from the ground state. As in the lowest order theory, this gap is eliminated by considera-

[4] J. D. Talman, Thesis, Princeton University, 1959 (unpublished).
[5] K. Sawada, Phys. Rev. **116**, 1344 (1959).

tion of the pair states in which one or more pairs of virtual particles of momentum $\mathbf{q}$ and $-\mathbf{q}$ accompany the excited particle. In treating the pair effect, the lowest order vertex $Nv(0, 0, \mathbf{q}, -\mathbf{q})$ must be replaced by a generalized vertex in which a pair of particles is excited from the ground state. This vertex can be evaluated by summing all the graphs in which a pair of particles is produced. The sum may be obtained from the ground-state energy, at least in the limit of small $\mathbf{q}$, in the following way. A graph with p incoming and p outgoing lines of the type previously considered contributes to the ground-state energy a term of the form $AN^p\Omega^{(1-p)}$. The line of momentum $\mathbf{q}$ can leave the graph at any of p outgoing vertices; the line of momentum $-\mathbf{q}$ can leave the graph at any of the $p-1$ remaining vertices. The net contribution of the graph is

$$p(p-1)AN^{p-1}\Omega^{(1-p)},$$

and the generalized vertex can be expressed as before as

$$\rho(d^2/d\rho^2)(E/\Omega).$$

A similar argument applies for the generalized vertex at which a pair is annihilated. Replacing $\beta(q)$ and $\Gamma(q)$ by the generalized single particle energy and the generalized vertex gives the result

$$E_{\mathbf{q}}=\left\{\left[\frac{q^2}{2m}+\rho\frac{d^2}{d\rho^2}\left(\frac{E}{\Omega}\right)\right]^2-\left[\rho\frac{d^2}{d\rho^2}\left(\frac{E}{\Omega}\right)\right]^2\right\}^{1/2}$$

$$\sim|\mathbf{q}|\left[\frac{\rho}{m}\frac{d^2}{d\rho^2}\left(\frac{E}{\Omega}\right)\right]^{1/2}=|\mathbf{q}|\frac{dP}{d\rho_m},$$

where P is the pressure $-(dE/d\Omega)$, and ρ_m is the mass density.

The vertices here considered, either those in which a pair is produced, or the diagonal ones which contribute to the single-particle energy, may occur in the presence of other virtual particles, each of momentum $\mathbf{q}$ or $-\mathbf{q}$. In this case, the energies of the virtual particles modify the energy denominators. This modification has been called by Brueckner[6] the off-the-energy-shell effect. In the limit of small $\mathbf{q}$ the off-the-energy-shell effect will not modify the vertices, since the effect is proportional to q^2. This shows that it is necessary to deal with the unaltered Hamiltonian; if the Hamiltonian were altered by including the single-particle energies in the kinetic energy term the off-the-energy-shell effect would be important. On the other hand, the use of a modified Hamiltonian is known to be the same as summing an infinite class of diagrams. If one assumes that the order of differentiation and summation can be interchanged at will, the theorem applies as well to the modified Hamiltonian.

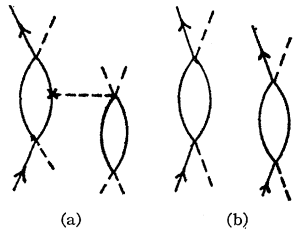

FIG. 2. Graphs which arise because of the inexact cancellation of disconnected diagrams in the linked-cluster theorem. The contributions of these graphs have been neglected.

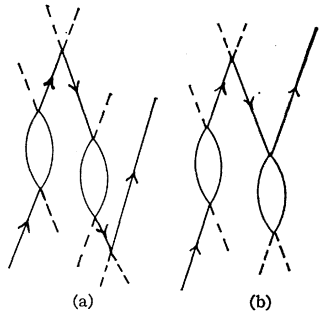

FIG. 3. Examples of graphs in which disconnected ground-state energy contributions overlap. These graphs have been neglected.

V. DISCUSSION OF THE APPROXIMATIONS

In proving the theorem, both the ground-state energy and the excitation energy have been approximated. As was mentioned, the S linked graphs were neglected in considering the ground-state energy. In the excited-state energies several types of terms are neglected. These will be described graphically. Figure 1(a) shows a typical term which has been included correctly. The circles denote any ground-state graph with two lines attached. No two circles are allowed to overlap; successive vertices must belong to the same ground-state graph unless they begin or terminate a particular ground-state graph. It is of interest to observe that as $\mathbf{q}\rightarrow 0$ this graph does not reduce to a ground-state graph, so that it is necessary to include it separately from the single-particle energies. Figure 1(b) shows another effect which has been correctly described. The S link shown links an internal line to an incoming or outgoing vertex of a disconnected part. This contribution is part $(-pA\rho^{(p-1)})$ of the single-particle energy of the virtual particle.

Figure 2(a) shows a single-particle energy diagram which includes an S link. Figure 2(b) symbolizes a rather complicated effect which is related to the S linking. In demonstrating the linked cluster expansion there are counter terms which cancel the unlinked terms. If there is no unlinked term to be cancelled, the counter term occurs with a minus sign. In this case Fig. 2(b) cannot occur as an unlinked term, but is present as a counter term, and so gives a contribution (with a minus sign). This effect also produces the S linking. Both Figs. 2(a) and 2(b) have been neglected.

Figures 3(a) and 3(b) depict another omission. In these, ground-state graphs which contribute to the pair contributions overlap. It is conceivable that the overlapping graphs, together with that of Fig. 2(b), compensate for the S link contribution. The situation is, however, very complicated and no way has been found to improve the result.

[6] K. A. Brueckner, Phys. Rev. **100**, 36 (1955).

VI. CONCLUSIONS

It is clear that, even allowing the approximations made, the argument presented is at best a formal one. To justify the differentiations performed the series differentiated must converge uniformly whereas the series in question are known not to converge (or, in fact, exist) at all unless a partial summation of the diagonal matrix elements is first performed. On the other hand, the argument makes the result plausible and shows the arrangement in which terms must be taken to obtain a consistent theory.

The neglect of the S linked terms and the overlapping vertex terms is probably of greater physical interest. It may be possible to take the two effects into consideration simultaneously but if this is the case the correct accounting procedure to be followed is by no means clear. The S linked terms have been shown by Sawada[5] to give rise to the effect termed by other authors[1] the depletion effect. Therefore, neglecting the S linked terms is equivalent to neglecting the depletion effect and is, therefore, perhaps justifiable at low densities only.

The chief interest of this theory may be the fact that it allows a consistent approach to the problem of a bound, but saturated, many-boson system, i.e., liquid helium. The theories of the many-boson system which have been developed all are limited to repulsive forces. The reason is essentially that if the forces are attractive so as to provide a bound state, $\tilde{v}(0)$ is negative. The state in which all particles have zero momentum is then no longer the ground state of the diagonal part (in momentum representation) of the Hamiltonian and so cannot lead to the perturbed ground state. One reflection of this is that the lowest order phonon spectrum becomes imaginary.

It is seen that this difficulty may be avoided in practice for liquid helium by considering densities large enough that the energy versus density curve is concave upwards. The single-particle energies are then positive despite the fact that the ground-state energy is negative and a consistent theory may be obtainable. One need not be overly concerned about neglecting low densities since the system cannot exist stably at a density below the equilibrium density in any event.

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Analytic Properties of the Partition Function near the Normal-to-Superconducting Phase Transition*

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It is shown that the grand partition function for a superconductor has analytic properties near the transition point in the complex temperature plane similar to those described by Lee and Yang in their statistical theory of condensation. The normal and superconducting regions of the complex plane are separated by a line of zeroes which, in the limit of infinite volume, becomes a natural boundary.

THE purpose of this note to point out that an expression for the grand partition function for a superconductor, originally derived by Gaudin,[1] has analytic properties near the transition point in the complex temperature plane similar to those described by Lee and Yang[2] in their statistical theory of condensation.

The Lee-Yang analysis pertains to a classical system of hard-core molecules. Only a finite number of such molecules will fit into a volume Ω; and it follows from this that the grand partition function Z is an entire function of the fugacity y. Z must have a finite number of zeroes distributed symmetrically about the real axis in the complex y plane. None of these zeroes can occur on the real, positive y axis; but as the volume tends to infinity, the zeroes may cluster densely on lines crossing this axis, thus pinching it at some points. Lee and Yang identify such points as phase transitions.

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[1] M. Gaudin, Nucl. Phys. **20**, 513 (1960).

[2] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952); T. D. Lee and C. N. Yang, *ibid.* **87**, 410 (1952).