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Elementary excitations in superfluid liquid helium based on the Bogoliubov-Zubarev formalism

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The Bogoliubov-Zubarev (BZ) formulation of the superfluid Bose liquid in terms of density as a collective variable leads to a non-Hermitian Hamiltonian (H_{BZ}) for describing the elementary excitations. An appropriate mathematical framework for dealing with non-Hermitian operators is here employed for the first time to develop schemes for studying the elementary excitations of the Bose liquid. The energies of the ground and the first excited states associated with H_{BZ} in "perturbation" theory are derived. A consistent scattering theory appropriate to H_{BZ} is also given from which the two-roton scattering amplitude in the leading order of "perturbation" theory is explicitly deduced. A finite-temperature Green's-function theory is also presented. These results are shown to be equivalent to those based on the Sunakawa Hamiltonian. Results for the energy spectrum are also shown to be equivalent with those evaluated by means of a variation-perturbation procedure based on the method of correlated basis functions in the uniform limit.

I. INTRODUCTION

In 1941, with remarkable insight, Landau[1] proposed the now well-known excitation spectrum of superfluid liquid helium as a microscopic explanation of the two-fluid model.[2] The experimental observations[3] are in qualitative agreement with Landau's conjecture for all momenta up to the roton region, while for larger momenta the spectrum flattens out into a plateau region as was proposed by Pitaevskii,[4] instead of following a free-particle-like spectrum. Also, it was found that there are two branches in the spectrum of excitations.[3] There are several first-principles microscopic theories all of whose aim is to *derive* the Landau spectrum; they may broadly be classified into two types. One, which employs a particle description, was initiated by Bogoliubov[5] in 1947. This theory was based on a weakly interacting system of Bose particles as a model for the liquid and deduced essentially the Landau spectrum by assuming that there is a finite fraction of the atoms in the zero momentum condensate. The second class of theories employs a collective description of the fluid, using density as a variable. Here, we may divide such theories into two subclasses. Feynman and Cohen[6] in 1956 suggested a variational procedure for computing the Landau spectrum, which brought forth important ideas about the structure of the wave function for a strongly correlated system such as liquid helium. This led to the concept of "back flow" as a physical description of the spectrum near the roton region, even though the actual comparison with the experimental result near this region is not satisfactory. The principles of the Feynman-Cohen theory have culminated into a very sophisticated formalism pioneered by Feenberg,[7] known as the "correlated-basis-function" approach. The other subclass of theories is a field theory which employs density as a collective variable to describe a liquid; such a theory was first advanced by Bogoliubov and Zubarev[8] (BZ) in 1955. This theory obtained the same spectrum as was derived by Bogoliubov before,[5] but without the appearance of the number of atoms in the zero momentum condensate in the expression for the Landau spectrum. But the unpalatable feature of this theory (which perhaps also explains why not much development in this direction took place) is that it led to a non-Hermitian Hamiltonian for describing the collective excitations of the system. This work is, however, remarkable in that the associated wave function in this description was shown by these authors to have the same appearance as Feynman-Cohen's variational wave function. Also, they explained how to reconcile the result that the single-particle spectrum[5] and the density-fluctuation spectrum[8] could be the same for long wavelengths. Later, Gavoret and Nozieres[9] proved that the one-particle spectrum and the density-fluctuation spectrum for a superfluid liquid are identical to all orders in perturbation theory, in the long-wavelength limit.

While all these theories are in qualitative agreement with the experimental spectrum up to the roton region,[3] none of them could explain the plateau region and the second branch, until 1970 when Ruvalds and Zawadowski[10] advanced an ingenious explanation involving two-roton bound states. In the Feynman language, for momenta larger than the roton momentum, multiple-roton excitations ought to become an important process; Ruvalds and Zawadowski gave a procedure to deal with such processes, including final-state interactions.

The first attempt at connecting the various different approaches to the theory of a many-boson system was made in particular for a charged Bose gas. Brueckner[11] evaluated the ground-state energy through second order by summing one- and two-ring diagrams in the Bogoliubov occupation-number representation.[5] Lee[12] showed this to be equivalent to that obtained by the method of correlated basis functions (CBF) in the uniform limit.[7] This fact is remarkable in that the CBF result, which relies on a variational description of the ground state in the Bijl-Dingle-Jastrow (BDJ) type wave function, is thus non-field-theoretic in approach while the occupation number representation is field theoretic in nature. While the CBF result is valid in the uniform limit (the radial distribution function at the origin is not far from unity), the other result is valid in the weak-coupling limit. By calculating the leading order corrections to the variational energy by a perturbation theory which takes into account the three phonon contributions absent in the BDJ wave functions,[13] Lee[12] has extended this analysis to other many-boson systems.

Connections with the collective-variable approach of Bogoliubov and Zubarev[8] to the CBF results was first considered by Berdahl and Lee.[14] They explicitly showed the equivalence of the second-order corrections to the ground-state energy obtained by BZ[8] with the results obtained from a variational perturbation formalism in the uniform limit. They also compared the wave functions obtained from these two methods, but since they did not take into account the non-Hermiticity of the BZ Hamiltonian, the connection seems less than satisfying. Lee[15] has also considered the extension of the BZ formalism to the energy spectrum for elementary excitations. He has, by an incorrect formalism, attempted to calculate the second-order corrections to the Bogoliubov excitation spectrum. He does write what seems to be the correct second-order energy shift but its derivation is incorrect as shown here. Using this energy shift, he has shown that the results agree completely with a CBF variational-perturbation theory in the uniform limit. Thus with our demonstration of the connection of the Sunakawa results to those of BZ, we deduce their equivalence to the CBF theories.

It should be noted that all previous attempts to show equivalence between various theories have been concerned with calculating the ground and first excited states through second order in perturbation theory. In view of the recent discussion of the existence of the bound-roton pairs by Ruvalds and Zawadowski,[10] it is important to consider also the equivalence of the two-roton scattering amplitude, calculated by the use of different formalisms. This has in fact been done in this paper for the BZ and Sunakawa Hamiltonians.

Our concern in the present paper is to develop a practical mathematical procedure for dealing with the Bogoliubov-Zubarev Hamiltonian. The reasons for this are best explained by reviewing briefly the theories of superfluid liquid helium, using the collective description. The Bogoliubov and Zubarev[8] paper contains many new concepts, both mathematical and physical. The idea of using density as a variable for describing the superfluid is very physical but this means in mathematical terms the introduction of a "wave functional" of density. Chan and Valatin[16] published an account of how one can deal with such new functionals. The origin of the non-Hermitian nature of the Hamiltonian was explained by Bogoliubov and Zubarev as due to their not employing a variable canonically conjugate to density. This immediately raised the question whether one could introduce such a canonically conjugate variable or whether one should reformulate the collective-variable approach differently. Hiroike[17] reformulated the BZ approach and successfully obtained a Hermitian Hamiltonian which contained an infinite series of interaction terms in contrast to the BZ Hamiltonian and with an arbitrary cutoff wave-vector to ensure conservation of particle density. A more successful approach was proposed by Sunakawa and co-workers[18] who sought a canonical conjugate variable to density. This formulation also led to a Hermitian Hamiltonian but with an infinite series of interaction terms. It turns out that the conjugate variable is the "velocity operator" for the fluid[1] but the mathematical existence of such an operator has been seriously questioned by many. See, for instance, a recent discussion of this aspect by Kobe and Coomer.[19] In the more recent works, Sunakawa uses a projection operator to derive the Hamiltonian in terms of the density and the velocity operators. The success of the Sunakawa theory (S) is that by using a model for the potential of interaction between two helium atoms, the spectrum of the excitations in liquid helium has been numerically computed and seems to be in fair agreement with the experimental results including the multibranch spectrum. Similar numerical agreement with experimental results is obtained also by the Feenberg school. Moreover, the theory of two-roton scattering amplitude based on the S formalism has been developed by Rajagopal, Bagchi, and Ruvalds[20] and they find some evidence for the attractive two-roton interaction postulated by Ruvalds and Zawadowski[10] earlier as a mechanism to explain the spectrum beyond the roton momentum region. Straley[21] has recently reviewed many of these theories and concluded that the BZ approach is perhaps the best collective-variable approach but pointed out that there seems to be no available mathematical method of dealing with the non-Hermitian Hamiltonian. He argued that the BZ theory is similar in some respects to the Dyson theory[22] of spin-wave interactions in the theory of the Heisenberg ferromagnet, where also a non-Hermitian Hamiltonian plays a significant role. We may add here in this connection that a Hermitian Hamiltonian was derived by Holstein and Primakoff[23] which contained an infinite series of interactions. In a sense, the S theory parallels that of Holstein-Primakoff theory while the BZ formalism parallels Dyson's. Dyson developed a mathematical method for dealing with his non-Hermitian Hamiltonian by introducing an indefinite metric. An essentially similar method is employed in the present paper, except that it has a simpler structure because of the nature of the BZ Hamiltonian.

Berdahl[24] has developed another collective-variable theory employing density as a variable but phase as its conjugate. He has shown that in particular there are two equivalent combinations of these, one leading to the non-Hermitian Hamiltonian. The latter, he finds is identical to the S Hamiltonian, since the gradient of the phase operator turns out to be velocity operator of S. We may also point out that the density and phase operators leading to a Hermitian Hamiltonian was developed earlier by Nishiyama.[25] Berdahl related the two Hamiltonians by a canonical, nonunitary transformation, which he finds to be the "weight factor" derived by Chan and Valatin[16] required to make H_{BZ} Hermitian. Using his Hermitian Hamiltonian, which is also an infinite series, Berdahl proved through second order that the ground-state energy of the system is identical to those obtained by BZ, CBF, and Bogoliubov's original formulation.[5] We may remark here that the Hermitian formulation leads to apparent divergences in all orders of perturbation theory whereas no such divergences appear in our approach presented in this paper.

The method employed in the present paper exists in the mathematical literature[26] and has been formally employed on two occasions that we know of in many-body physics.[27,28] We give an outline of the formalism in Sec. II and develop "perturbation" theory appropriate to H_{BZ}. We compute the ground-state energy and the spectrum of the one excitation up to "second order." The latter was computed by BZ[8] and more recently again by Berdahl and Lee[14]; the former by Lee.[15] Lee used a trick employed by BZ and we show how this works only for the ground state and not for the excited states. Our results for the ground state agree with the BZ method[14] and disagree with Lee's[15] for the first excited state. In Sec. III we develop an appropriate scattering theory and deduce from it to leading order, the roton-roton scattering amplitude, as this quantity is of importance in any theory of superfluid liquid helium. In Sec. IV, a finite-temperature theory is outlined. Lee in Refs. 14 and 15 tried to relate the BZ results with the correlated-basis-function (CBF) approach, and similar results based on other theories, by comparing only the ground- and excited-state energies. In Sec. V we compare our results with those obtained in the S formalism. Section VI contains explicit proofs of the equivalence of both the energy spectrum and the scattering amplitude. In Sec. VII we discuss the relationship with CBF results. We summarize our results in Sec. VIII. In an Appendix, a formal attempt to relate the S approach and the BZ approach is outlined, which may elucidate some of the features of the two theories.

II. METHOD OF ANALYSIS FOR THE SPECTRUM OF H_{BZ}

Following Berdahl and Lee,[14] we write H_{BZ} in the following form:

$$H_{BZ} = H_0 + H_1 \,. \tag{1}$$

Here

$$H_0 = E_0^B + \sum_k E_B(k)\, b_k^\dagger b_k \,, \tag{2a}$$

$$E_0^B = \tfrac{1}{2}(N-1)\rho V(k=0) - \frac{N}{4\rho}\int E_B(k)\, \frac{(1-\lambda_k)^2}{\lambda_k}\, \frac{d^3k}{(2\pi)^3}\,, \tag{2b}$$

$$E_B(k) = \frac{\hbar^2 k^2}{2m\lambda_k}\,, \quad \lambda_k = \left(1 + \frac{4m\rho V(k)}{\hbar^2 k^2}\right)^{-1/2}\,, \tag{2c}$$

in their notation. $\rho = N/\Omega$, the number density, and $V(k)$ is the Fourier transform of the interatomic (He^4) potential. λ_k is the lowest-order approximation to the experimentally measured structure factor $S(k)$.[13] The b_k, $b_k^\dagger$ are operators obeying the usual boson commutation rules. The interacting part of H_{BZ}, namely, H_1, is written in a more symmetric form than those given elsewhere, and is non-Hermitian:

$$H_1 = \sum_{\substack{k_1, k_2, k_3 \\ (k_i\text{'s} \neq 0)}} \delta_{\vec{k}_1 + \vec{k}_2 + \vec{k}_3, \vec{0}} \left[\gamma_a^{(3)}(k_1 k_2 k_3)\, b_{k_1} b_{k_2} b_{k_3} + \gamma_b^{(3)}(k_1 k_2 k_3)\, b_{k_1}^\dagger b_{k_2}^\dagger b_{k_3}^\dagger + \gamma_c^{(3)}(k_1 k_2 k_3)\, b_{k_1}^\dagger b_{-k_2} b_{-k_3} + \gamma_d^{(3)}(k_1 k_2 k_3)\, b_{-k_3}^\dagger b_{-k_2}^\dagger b_{k_1}\right], \tag{3}$$

with

$$\gamma_a^{(3)}(k_1k_2k_3)=\frac{\hbar^2}{24m}(N\lambda_{k_1}\lambda_{k_2}\lambda_{k_3})^{-1/2}\sum_{P(123)}(\vec{\mathrm{k}}_1\cdot\vec{\mathrm{k}}_2)(\lambda_{k_1}+1)(\lambda_{k_2}+1)\lambda_{k_3}, \tag{3a}$$

$$\gamma_b^{(3)}(k_1k_2k_3)=\frac{\hbar^2}{24m}(N\lambda_{k_1}\lambda_{k_2}\lambda_{k_3})^{-1/2}\sum_{P(123)}(\vec{\mathrm{k}}_1\cdot\vec{\mathrm{k}}_2)(\lambda_{k_1}-1)(\lambda_{k_2}-1)\lambda_{k_3}, \tag{3b}$$

[$P(123)$ here stands for the three cyclic permutation of (k_1, k_2, k_3)]

$$\begin{aligned}\gamma_c^{(3)}(k_1k_2k_3)&=\frac{\hbar^2}{8m}(N\lambda_{k_1}\lambda_{k_2}\lambda_{k_3})^{-1/2}\{(\vec{\mathrm{k}}_2\cdot\vec{\mathrm{k}}_3)(\lambda_{k_2}+1)(\lambda_{k_3}+1)\lambda_{k_1}+[(\vec{\mathrm{k}}_1\cdot\vec{\mathrm{k}}_2)\lambda_{k_3}(\lambda_{k_2}+1)+(\vec{\mathrm{k}}_3\cdot\vec{\mathrm{k}}_1)\lambda_{k_2}(\lambda_{k_3}+1)](\lambda_{k_1}-1)\}\\&=\text{symmetric in }(k_2,k_3),\end{aligned} \tag{3c}$$

and

$$\begin{aligned}\gamma_d^{(3)}(k_1k_2k_3)&=\frac{\hbar^2}{8m}(N\lambda_{k_1}\lambda_{k_2}\lambda_{k_3})^{-1/2}\{(\vec{\mathrm{k}}_2\cdot\vec{\mathrm{k}}_3)(\lambda_{k_2}-1)(\lambda_{k_3}-1)\lambda_{k_1}+[(\vec{\mathrm{k}}_1\cdot\vec{\mathrm{k}}_2)\lambda_{k_3}(\lambda_{k_2}-1)+(\vec{\mathrm{k}}_3\cdot\vec{\mathrm{k}}_1)\lambda_{k_2}(\lambda_{k_3}-1)](\lambda_{k_1}+1)\}\\&=\text{symmetric in }(k_2,k_3).\end{aligned} \tag{3d}$$

Note that this Hamiltonian is complete and does not contain higher-order interaction terms in contrast to the Sunakawa[18] theory.

An outline of the derivation of this Hamiltonian is not given here as they may be found in the recent papers of Straley[21] and Berdahl and Lee.[14] The latter authors calculated the ground-state energy and Lee[15] calculated the energy of the first excited state of H_{BZ} up to second order in H_1, in perturbation theory, by a procedure outlined originally by Bogoliubov and Zubarev.[8] This procedure is questionable in view of the non-Hermitian character of H_1, and so we here give a formulation appropriate to this problem. The basis for this formulation may be found in Ref. 26 (to which the reader is referred to for details), and we quote here only the relevant parts of the formal theory. One may also refer to Schwinger[29] for an application of this to quantum mechanics in general. According to this, if the eigenfunctions of H_{BZ} and $H_{\mathrm{BZ}}^{\dagger}$ are "simple," i.e., obey the equations

$$\begin{aligned}&H_{\mathrm{BZ}}|\Psi\rangle=E|\Psi\rangle,\ \text{or equivalently,}\ \langle\tilde{\Psi}|H_{\mathrm{BZ}}^{\dagger}=\langle\tilde{\Psi}|E^*,\\&\text{and}\\&\langle\tilde{\Phi}|H_{\mathrm{BZ}}=\langle\tilde{\Phi}|\tilde{E}^*,\ \text{or equivalently,}\ H_{\mathrm{BZ}}^{\dagger}|\Phi\rangle=\tilde{E}|\Phi\rangle,\end{aligned} \tag{4}$$

(the star denoting complex conjugate) and if the ranges of $(H_{\mathrm{BZ}}-E)$ and $(H_{\mathrm{BZ}}^{\dagger}-\tilde{E})$ are *closed*, then, the set of eigenvalues $E_1, E_2, \ldots$ of H_{BZ} are also the eigenvalues of $H_{\mathrm{BZ}}^{\dagger}$ and the corresponding eigenfunctions $|\Psi_1\rangle, |\Psi_2\rangle, \ldots$ and $\langle\tilde{\Phi}_1|, \langle\tilde{\Phi}_2|, \ldots$ of H_{BZ} together form a biorthogonal, complete set, i.e., $\langle\tilde{\Phi}_m|\Psi_n\rangle=\delta_{m,n}$, $1=\sum_n|\Psi_n\rangle\langle\tilde{\Phi}_n|$, and $\langle\tilde{\Psi}_n|\Phi_m\rangle=\delta_{m,n}$, $1=\sum_n|\Phi_n\rangle\langle\tilde{\Psi}_n|$. This is a simpler version of the general theory of non-Hermitian operators, which seemed to us to suffice for our purposes. We *assume* that the ranges of $(H_{\mathrm{BZ}}-E)$ and $(H_{\mathrm{BZ}}^{\dagger}-\tilde{E})$ are *closed* and also seek only "simple" eigenfunctions as above. These assumptions seem reasonable to us, as they parallel closely the theory of the Hermitian operators. Moreover, based on these assumptions, we develop a method of computing the eigenvalues of both H_{BZ} and $H_{\mathrm{BZ}}^{\dagger}$ which we will show explicitly to be *equal*, confirming *post facto* the correctness of the assumption. Also, the eigenvalues then admit of the usual interpretation of being "energy eigenvalues."

We thus see that a complete theory can be developed either by using $|\Psi\rangle$ and H_{BZ} in conjunction with $\langle\tilde{\Phi}|$, or by using $|\Phi\rangle$ and $H_{\mathrm{BZ}}^{\dagger}$ in conjunction with $\langle\tilde{\Psi}|$. This aspect also leads to a consistent definition of the Heisenberg representation for operators acting in the appropriate spaces. We shall make use of this in Sec. IV for developing a Green's-function theory based on H_{BZ}.

The scheme is almost suggestive at once because the H_0 part of H_{BZ} is Hermitian with the structure of the Hamiltonian for the uncoupled set of oscillators. Hence, we have a vacuum state $|0\rangle$ with energy E_0^B and such that

$$b_k|0\rangle=0. \tag{5}$$

Its adjoint is of course $\langle 0|\equiv\langle\tilde{0}|$ because H_0 is Hermitian and has the property

$$\langle 0|b_k^{\dagger}=0. \tag{6}$$

Also, the set of states of H_0 form a *complete set* which we shall therefore use to set up a perturbation scheme for H_{BZ}. We have the following well-known facts:

$$\langle 0|b_{k_1}b_{k_1'}^{\dagger}|0\rangle=\delta_{k_1,k_1'}, \tag{7a}$$

$$\langle 0|b_{k_1}b_{k_2}b_{k_1'}^\dagger b_{k_2'}^\dagger|0\rangle = (\delta_{k_1,k_1'}\delta_{k_2,k_2'} + \delta_{k_1,k_2'}\delta_{k_2,k_1'}), \tag{7b}$$

etc.
We note that

$$\langle 0|H_{\rm BZ}|0\rangle = \langle 0|H_{\rm BZ}^\dagger|0\rangle = E_0^B . \tag{8}$$

We first develop perturbation theories of both the Rayleigh-Schrödinger (RS) and the Brillouin-Wigner (BW) types in a general fashion. It is important to note that our result should lead to the same value of E and $\tilde{E}$ in any given order, so that our assumption is borne out.

A. Modified Rayleigh-Schrodinger perturbation method for $H_{\rm BZ}$

Consider the equations

$$\begin{aligned} H_{\rm BZ}|\Psi_n\rangle &= E_n|\Psi_n\rangle , \\ H_{\rm BZ}^\dagger|\Phi_n\rangle &= \tilde{E}_n|\Phi_n\rangle , \end{aligned} \tag{9}$$

Here n stands for the nth excited state. We treat H_1 as a perturbation on H_0 and so we write

$$\begin{aligned} |\Psi_n\rangle &= |\Psi_n^{(0)}\rangle + |\Psi_n^{(1)}\rangle + \cdots , \\ E_n &= E_n^{(0)} + E_n^{(1)} + \cdots ; \end{aligned} \tag{10}$$

$$\begin{aligned} |\Phi_n\rangle &= |\Phi_n^{(0)}\rangle + |\Phi_n^{(1)}\rangle + \cdots , \\ \tilde{E}_n &= \tilde{E}_n^{(0)} + \tilde{E}_n^{(1)} + \cdots ; \end{aligned} \tag{11}$$

and we obtain from (9), (10) and (11) the equations:

$$\begin{aligned} &(H_0 - E_n^{(0)})|\Psi_n^{(0)}\rangle = 0 , \\ &(H_0 - E_n^{(0)})|\Psi_n^{(1)}\rangle + (H_1 - E_n^{(1)})|\Psi_n^{(0)}\rangle = 0 , \\ &(H_0 - E_n^{(0)})|\Psi_n^{(2)}\rangle + (H_1 - E_n^{(1)})|\Psi_n^{(1)}\rangle - E_n^{(2)}|\Psi_n^{(0)}\rangle = 0 , \end{aligned} \tag{12}$$

etc.

$$\begin{aligned} &(H_0 - \tilde{E}_n^{(0)})|\Phi_n^{(0)}\rangle = 0 , \\ &(H_0 - \tilde{E}_n^{(0)})|\Phi_n^{(1)}\rangle + (H_1^\dagger - \tilde{E}_n^{(1)})|\Phi_n^{(0)}\rangle = 0 , \\ &(H_0 - \tilde{E}_n^{(0)})|\Phi_n^{(2)}\rangle + (H_1^\dagger - \tilde{E}_n^{(1)})|\Phi_n^{(1)}\rangle - \tilde{E}_n^{(2)}|\Phi_n^{(0)}\rangle = 0 , \end{aligned} \tag{13}$$

etc.
From the first of Eqs. (12) and (13), since H_0 is Hermitian, $|\Psi_n^{(0)}\rangle$ and $\langle\tilde{\Phi}_n^{(0)}|$ are just n *free-oscillator states* with their energies equal:

$$\begin{aligned} |\Psi_n^{(0)}\rangle &= \prod_{i=1}^{n} b_{k_i}^\dagger|0\rangle[\mathrm{Perm}\{\delta_{k_i,k_j}\}]^{-1/2} = |\Phi_n^{(0)}\rangle , \\ \langle\tilde{\Phi}_n^{(0)}| &= \langle 0| \prod_{i=1}^{n} b_{k_i}[\mathrm{Perm}\{\delta_{k_i,k_j}\}]^{-1/2} = \langle\tilde{\Psi}_n^{(0)}| , \end{aligned} \tag{14}$$

and

$$E_n^{(0)} = \tilde{E}_n^{(0)*} = \sum_{i=1}^{n} E_B(k_i) + E_0^B .$$

Clearly $\langle\tilde{\Phi}_n^{(0)}|$ is the adjoint state of $|\Psi_n^{(0)}\rangle$ and this enables further simplification, as will be seen below. $\mathrm{Perm}\{\delta_{k_i,k_j}\}$ stands for the permanent of the Kronecker delta's δ_{k_i,k_j}. From (12) and (13), we immediately obtain

$$\begin{aligned} E_n^{(1)} &= \langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_n^{(0)}\rangle , \\ \tilde{E}_n^{(1)} &= \langle\tilde{\Psi}_n^{(0)}|H_1^\dagger|\Phi_n^{(0)}\rangle \\ &= E_n^{(1)*} ; \end{aligned} \tag{15}$$

the last statement follows in view of the above observation. Since H_1 (and $H_1^\dagger$) is a cubic polynomial in b and $b^\dagger$, and since the oscillator states of different occupation of levels are mutually orthogonal, we see that

$$E_n^{(1)} = 0 = \tilde{E}_n^{(1)} . \tag{16}$$

Also,

$$|\Psi_n^{(1)}\rangle = \frac{P}{E_n^{(0)} - H_0} H_1|\Psi_n^{(0)}\rangle , \tag{17a}$$

$$\langle\tilde{\Phi}_n^{(1)}| = \langle\tilde{\Phi}_n^{(0)}|H_1 \frac{P}{E_n^{(0)} - H_0} , \tag{17b}$$

where P stands for a projection operator which excludes the $|\Psi_n^{(0)}\rangle$, $\langle\tilde{\Phi}_n^{(0)}|$ states:

$$P = 1 - |\Psi_n^{(0)}\rangle\langle\tilde{\Phi}_n^{(0)}| . \tag{18}$$

The second-order "energy" can now be obtained:

$$E_n^{(2)} = \langle\tilde{\Phi}_n^{(0)}|H_1 \frac{P}{E_n^{(0)} - H_0} H_1|\Psi_n^{(0)}\rangle , \tag{19a}$$

$$\begin{aligned} \tilde{E}_n^{(2)} &= \langle\tilde{\Psi}_n^{(0)}|H_1^\dagger \frac{P}{E_n^{(0)} - H_0} H_1^\dagger|\Phi_n^{(0)}\rangle \\ &= E_n^{(2)*} . \end{aligned} \tag{19b}$$

The last equation follows because of the simple structure of $\langle\tilde{\Phi}_n^{(0)}|$ and $|\Psi_n^{(0)}\rangle$. Since the entire p oscillator states form a complete set, one could write these explicitly:

$$\begin{aligned} E_n^{(2)} = \sum_{\{p\}}{}' &\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_p^{(0)\prime}\rangle\langle\tilde{\Phi}_p^{(0)\prime}|H_1|\Psi_n^{(0)}\rangle \\ &\times (E_n^{(0)} - E_p^{(0)\prime})^{-1} , \end{aligned} \tag{20}$$

where the primes indicate exclusion of the n-particle intermediate states. Two examples should suffice to display these results.

a. Ground-state energy. Here $n=0$, and so

$$E_0^{(2)} = \langle 0|H_1 \frac{P}{E_0^{(0)} - H_0} H_1|0\rangle .$$

From (3) we know that p can only be a three-particle state arising from the $b^\dagger b^\dagger b^\dagger$ and bbb terms in H_1. Since $E_0^{(0)} = E_0^B$ we obtain

$$E_0^{(2)}=\langle 0|\sum_{k_1,k_2,k_3}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}\,b_{k_1}b_{k_2}b_{k_3}\gamma_a^{(3)}(k_1k_2k_3)(E_0^B-H_0)^{-1}\sum_{k_1'k_2'k_3'}\delta_{\vec{k}_1'+\vec{k}_2'+\vec{k}_3',\vec{0}}\,b^\dagger_{k_1'}b^\dagger_{k_2'}b^\dagger_{k_3'}\gamma_b^{(3)}(k_1'k_2'k_3')|0\rangle$$

$$=-6\sum_{k_1,k_2,k_3}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}\,\gamma_a^{(3)}(k_1k_2k_3)\gamma_b^{(3)}(k_1k_2k_3)[E_B(k_1)+E_B(k_2)+E_B(k_3)]^{-1}\,. \tag{21}$$

Explicitly this is seen to be $\tilde{E}_0^{(2)}$, as well as real. This result is in agreement with Berdahl and Lee.[14]

b. First excited state. Here

$$|\Psi_1^{(0)}\rangle=b_k^\dagger|0\rangle,\quad\langle\tilde{\Phi}_1^{(0)}|=\langle 0|b_k,$$

$$E_1^{(0)}=E_0^B+E_B(k),$$

$$E_1^{(2)}=\langle 0|b_kH_1\frac{P}{E_1^{(0)}-H_0}H_1b_k^\dagger|0\rangle\,.$$

Carrying this out explicitly, we observe that $H_1b_k^\dagger|0\rangle$ would involve only the $\gamma_b^{(3)}$ and $\gamma_d^{(3)}$ terms in H_1, whereas $\langle 0|b_kH_1$ would involve only the $\gamma_a^{(3)}$ and $\gamma_c^{(3)}$ terms in H_1. We obtain finally:

$$E_1^{(2)}=-\sum_{k_1',k_2',k_3'}\sum_{k_1,k_2,k_3}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}\,\delta_{\vec{k}_1'+\vec{k}_2'+\vec{k}_3',\vec{0}}\,\gamma_a^{(3)}(k_1'k_2'k_3')\gamma_b^{(3)}(k_1k_2k_3)[E_B(k_1)+E_B(k_2)+E_B(k_3)]^{-1}$$

$$\times\langle 0|b_kb_{k_1'}b_{k_2'}b_{k_3'}b^\dagger_{k_1}b^\dagger_{k_2}b^\dagger_{k_3}b^\dagger_k|0\rangle+P\sum_{k_1',k_2'}\sum_{k_1,k_2}\delta_{\vec{k}_1+\vec{k}_2+\vec{k},\vec{0}}\,\delta_{\vec{k}_1'+\vec{k}_2'+\vec{k},\vec{0}}$$

$$\times\gamma_c^{(3)}(kk_1'k_2')\gamma_d^{(3)}(kk_1k_2)[E_B(k)-E_B(k_1)-E_B(k_2)]^{-1}\langle 0|b_{-k_1'}b_{-k_2'}b^\dagger_{-k_1}b^\dagger_{-k_2}|0\rangle\,.$$

In view of the symmetry properties of the γ's and the inner products, we obtain finally,

$$E_1^{(2)}=-6\sum_{\substack{k_1,k_2\\(k_1+k_2\neq 0)}}\gamma_a^{(3)}[k_1k_2-(k_1+k_2)]\,\gamma_b^{(3)}[k_1k_2-(k_1+k_2)][E_B(k_1)+E_B(k_2)+E_B(k_1+k_2)]^{-1}$$

$$+2P\sum_{k_1(\neq -k)}\gamma_c^{(3)}[kk_1-(k+k_1)]\gamma_d^{(3)}[kk_1-(k+k_1)][E_B(k)-E_B(k_1)-E_B(k+k_1)]^{-1}$$

$$-18\sum_{k_1}\gamma_a^{(3)}[kk_1-(k+k_1)]\gamma_b^{(3)}[kk_1-(k+k_1)][E_B(k)+E_B(k_1)+E_B(k+k_1)]^{-1},$$

$$\equiv E_0^{(2)}+\epsilon_2(k)\,. \tag{22}$$

In the above equations, P stands for the principal value.

A similar procedure leads to the result that $\tilde{E}_1^{(2)}=E_1^{(2)}$. It should be pointed out that in view of the structures of $\gamma^{(3)}$'s, these expressions are convergent because $\lambda_k\to 1$ for $k\to\infty$.

Lee[12] missed the last term because the BZ scheme[8] cannot be applied in a straightforward manner to $|\Psi_1\rangle$. This is because he substituted $|\Psi_1^{(1)}\rangle$ from the second equation in (12), into the third equation and then equated coefficients of $|k\rangle$ instead of taking its inner product with $\langle k|$; but then he incorrectly supplied the last term from the first double sum by extracting the terms for which k_1, k_2, $-(k_1+k_2)$ equal k. A comparison of (21) and (22) shows that the first term here is just $E_0^{(2)}$.

B. Modified Brillouin-Wigner perturbation method for H_{BZ}

For the sake of future development we will here outline a Brillouin-Wigner type of perturbation method for H_{BZ}. We first write Eq. (9) in the form

$$(H_0-E_n)|\Psi_n\rangle=-H_1|\Psi_n\rangle,$$

$$(H_0-\tilde{E}_n)|\Phi_n\rangle=-H_1^\dagger|\Phi_n\rangle\,. \tag{9'}$$

Let us take the inner product of these equations with the appropriate p-particle states of the "non-interacting" bosons governed by H_0:

$$(E_p^{(0)\prime}-E_n)\langle\tilde{\Phi}_p^{(0)\prime}|\Psi_n\rangle=-\langle\tilde{\Phi}_p^{(0)\prime}|H_1|\Psi_n\rangle$$

and

$$(E_p^{(0)\prime}-\tilde{E}_n)\langle\tilde{\Psi}_p^{(0)\prime}|\Phi_n\rangle=-\langle\tilde{\Psi}_p^{(0)\prime}|H_1^\dagger|\Phi_n\rangle\,. \tag{23}$$

Here $\langle\tilde{\Phi}_p^{(0)\prime}|$ and $\langle\tilde{\Psi}_p^{(0)\prime}|$ are p-particle states with different momenta k labels than those in $|\Psi_n\rangle$ and $|\Phi_n\rangle$, respectively. If the *k labels are the same, we denote them by corresponding symbols without the prime.* Let us choose the normalization

$$\langle\tilde{\Phi}_n^{(0)}|\Psi_n\rangle=1=\langle\tilde{\Psi}_n^{(0)}|\Phi_n\rangle\,. \tag{24}$$

Then we obtain, from (23),

$$\begin{aligned}E_n&=E_n^{(0)}+\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_n\rangle\,,\\ \tilde{E}_n&=E_n^{(0)}+\langle\tilde{\Psi}_n^{(0)}|H_1^\dagger|\Phi_n\rangle\;.\end{aligned} \tag{25}$$

Now, we use the completeness of $\{p\}$-oscillator states to write $|\Psi_n\rangle$ in the following form:

$$\begin{aligned}|\Psi_n\rangle&=\sum_{\{p\}}|\Psi_p^{(0)\prime}\rangle\langle\tilde{\Phi}_p^{(0)\prime}|\Psi_n\rangle\\ &=|\Psi_n^{(0)}\rangle+\sum_{\{p\}\neq n}|\Psi_p^{(0)\prime}\rangle\langle\tilde{\Phi}_p^{(0)\prime}|\Psi_n\rangle\,,\end{aligned}$$

and from (23), we obtain

$$|\Psi_n\rangle=|\Psi_n^{(0)}\rangle+\sum_{\{p\}\neq n}|\Psi_p^{(0)\prime}\rangle\times\langle\tilde{\Phi}_p^{(0)\prime}|H_1|\Psi_n\rangle\,(E_n-E_p^{(0)\prime})^{-1}\,, \tag{26a}$$

$$E_n=E_n^{(0)}+\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_n^{(0)}\rangle+\sum_{\{p\}\neq n}\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_p^{(0)\prime}\rangle\langle\Phi_p^{(0)\prime}|H_1|\Psi_n\rangle\,(E_n-E_p^{(0)\prime})^{-1}\,. \tag{26b}$$

The sum here on $\{p\}$ indicates integration over the corresponding momenta variables also. One may iterate (26a) to obtain the usual type BW series in H_1. Exactly similar analysis leads to an equation for $|\Phi_n\rangle$ involving $H_1^\dagger$. To second order, for example, one has the BW equation for the eigenvalues:

$$E_n=E_n^{(0)}+\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_n^{(0)}\rangle+\sum_{\{p\}\neq n}\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_p^{(0)\prime}\rangle\times\langle\tilde{\Phi}_p^{(0)\prime}|H_1|\Psi_n^{(0)}\rangle(E_n-E_p^{(0)\prime})^{-1}\,, \tag{27}$$

$$\tilde{E}_n=E_n^{(0)}+\langle\tilde{\Psi}_n^{(0)}|H_1^\dagger|\Phi_n^{(0)}\rangle+\sum_{\{p\}\neq n}\langle\tilde{\Psi}_n^{(0)}|H_1^\dagger|\Phi_p^{(0)\prime}\rangle\times\langle\tilde{\Psi}_p^{(0)\prime}|H_1^\dagger|\Phi_n^{(0)}\rangle\,(\tilde{E}_n-E_p^{(0)\prime})^{-1}\,. \tag{28}$$

As shown in the previous discussion, $\langle\tilde{\Phi}_n^{(0)}|H_1|\Psi_n^{(0)}\rangle=0=\langle\tilde{\Psi}_n^{(0)}|H_1^\dagger|\Phi_n^{(0)}\rangle$, and because of the other properties, noted earlier, one can only deduce that $\tilde{E}_n^*$ and E_n obey the *same* transcendental equation. To second order in H_1, using the properties of the matrix elements, one can write down the equations for the ground- and excited-state energies E_0 and E_1 as before, and because of the structure of $\gamma^{(3)}$'s we may note that E_0 and E_1 may indeed be the same as $\tilde{E}_0$ and $\tilde{E}_1$. We shall not discuss this formulation any further.

III. SCATTERING THEORY BASED ON $H_{\rm BZ}$

An elegant formulation of scattering theory in a general fashion may be given via the Lippmann-Schwinger (LS) equation for the T matrix.[30] A suitable modification of this theory is given here for our purposes. The fact that one has a "biorthogonal expansion" in terms of $\{|\Psi\rangle,\langle\tilde{\Phi}|\}$ or $\{|\Phi\rangle,\langle\tilde{\Psi}|\}$ for a simple operator (with closed ranges) enables us to express the resolvent operator associated with $H_{\rm BZ}$ or $H_{\rm BZ}^\dagger$ in the form

$$\begin{aligned}G(z)&=\sum_\alpha|\Psi_\alpha\rangle\,(E_\alpha-z)^{-1}\langle\tilde{\Phi}_\alpha|\,,\\ \tilde{G}(z)&=\sum_\alpha|\Phi_\alpha\rangle\,(\tilde{E}_\alpha-z)^{-1}\langle\tilde{\Psi}_\alpha|\,,\end{aligned} \tag{29}$$

where z is a complex number, and α stands for a set of labels characterizing the "eigenstates" of $H_{\rm BZ}$ or $H_{\rm BZ}^\dagger$. Equivalently, we have,

$$\begin{aligned}(H_{\rm BZ}-z)\,G(z)&=1=G(z)(H_{\rm BZ}-z)\,,\\ (H_{\rm BZ}^\dagger-z)\tilde{G}(z)&=1=\tilde{G}(z)(H_{\rm BZ}^\dagger-z)\,.\end{aligned} \tag{30}$$

Let us introduce the resolvent operator associated with the Hermitian-part H_0:

$$(H_0-z)\,G_0(z)=1=G_0(z)(H_0-z)\,. \tag{31}$$

Rewriting $H_{\rm BZ}=H_0+H_1$, we have an equation for G:

$$G(z)=G_0(z)+G_0(z)H_1G(z)\,. \tag{32}$$

Introduce a T operator in the usual way,

$$G(z)=G_0(z)+G_0(z)\,T(z)\,G_0(z)\,, \tag{33}$$

so that if $|\Psi_i\rangle$ is an initial state and $\langle\tilde{\Phi}_f|$ is a final state, the scattering amplitude is $\langle\tilde{\Phi}_f|T|\Psi_i\rangle$ with z taken to be the energy of the initial (or the final) state. From (33) and (32) one has a LS equation:

$$T(z)=H_1+H_1\,G_0(z)\,T(z)\,. \tag{34}$$

Had we used the right-hand side of the Eq. (30) we would have an equivalent T operator, denoted for the sake of clarity $\tilde{T}$, which would obey the equation

$$\tilde{T}(z)=H_1^\dagger+\tilde{T}(z)\,G_0(z)H_1^\dagger\,, \tag{34$'$}$$

corresponding to

$$\tilde{G}(z)=G_0(z)+\tilde{G}(z)H_1^\dagger\,G_0(z) \tag{32$'$}$$

and

$$\tilde{G}(z)=G_0(z)+G_0(z)\,\tilde{T}(z)\,G_0(z)\,. \tag{33$'$}$$

These two formulations should yield the same physical scattering amplitude for this theory to be of any physical significance for our problem, when one calculates $\langle \tilde{\Psi}_f | \tilde{T} | \Phi_i \rangle$. As in our perturbation scheme, this can be verified term by term for the Born-type series for T and $\tilde{T}$.[31]

As an example, we compute the two-roton scattering amplitude[20] from $T(z)$. The initial state is

$$|\Psi_i\rangle = b_k^\dagger b_{k'}^\dagger |0\rangle , \tag{35a}$$

and the final state is

$$\langle \tilde{\Phi}_f | = \langle 0 | b_{k+q} b_{k'-q} , \quad q \neq 0, (k'-k) \text{ and } k \neq k' . \tag{35b}$$

Since H_1 is cubic in $b, b^\dagger$ operators, the first term in (34) would yield zero. So, we iterate (34) once and consider the new equation as our starting point:

$$T = (H_1 + H_1 G_0 + H_1) + (H_1 G_0 H_1) G_0 T . \tag{35c}$$

In Ref. 20, $\langle \tilde{\Phi}_f | H_1 G_0 H_1 | \Psi_i \rangle$ was calculated based on a Hamiltonian due to Sunakawa *et al.*[18] This effort is motivated by recent conjectures on the nature of the roton-roton coupling, especially since it has been demonstrated[10] that an arbitrarily weak attractive coupling gives a bound state of two rotons.

In Sec. V, this expression will be shown to be identical to that derived in Ref. 20. We give here the expression for $\langle \tilde{\Phi}_f | H_1 G_0 H_1 | \Psi_i \rangle$ whose derivation is straightforward:

$$\langle \tilde{\Phi}_f | H_1 G_0 H_1 | \Psi_i \rangle = \sum_{i=1}^{6} A_i^{(\mathrm{BZ})} , \tag{36a}$$

$$A_1^{(\mathrm{BZ})} = 4\gamma_c^{(3)}(k+k', -k, -k')\gamma_d^{(3)}(k+k', -k-q, -k'+q)[E_B(k) + E_B(k') - E_B(k+k')]^{-1} , \tag{36b}$$

$$A_2^{(\mathrm{BZ})} = 4\gamma_c^{(3)}(k'-q, q, -k')\gamma_d^{(3)}(k, q, -k-q)[E_B(k) - E_B(k+q) - E_B(q)]^{-1} , \tag{36c}$$

$$A_3^{(\mathrm{BZ})} = 4\gamma_d^{(3)}(k', -q, -k'+q)\gamma_c^{(3)}(k+q, -q, -k)[E_B(k') - E_B(k'-q) - E_B(q)]^{-1} , \tag{36d}$$

$$A_4^{(\mathrm{BZ})} = 4\gamma_d^{(3)}(k_1' - k - q, -k' + k + q)\gamma_c^{(3)}(k'-q, -k, -k'+q+k)[E_B(k') - E_B(k+q) - E_B(k-k'+q)]^{-1} , \tag{36e}$$

$$A_5^{(\mathrm{BZ})} = 4\gamma_d^{(3)}(k, q-k', -k+k'-q)\gamma_c^{(3)}(k+q, -k', -k-q+k')[E_B(k) - E_B(k'-q) - E_B(k-k'+q)]^{-1} , \tag{36f}$$

and

$$A_6^{(\mathrm{BZ})} = -36\gamma_b^{(3)}(k'-q, k+q, -k-k')\gamma_a^{(3)}(k, k', -k-k')[E_B(k+k') + E_B(k+q) + E_B(k'-q)]^{-1} . \tag{36g}$$

Here we have made use of the permutation symmetries of $\gamma^{(3)}$'s.

IV. FINITE-TEMPERATURE THEORY BASED ON H_{BZ}

In order to develop a finite-temperature theory, we must define the statistical operator P_{op}, associated with H_{BZ}. Formally this can be done because we have assumed that the ranges of $(H_{\mathrm{BZ}} - E)$ and $(H_{\mathrm{BZ}}^\dagger - E)$ are closed, so that we have the eigenvalues of H_{BZ} and $H_{\mathrm{BZ}}^\dagger$ the same. Thus,

$$P_{\mathrm{op}} = \sum_n |\Psi_n\rangle e^{-\beta E_n} \langle \tilde{\Phi}_n | , \quad \beta = 1/kT . \tag{37}$$

With respect to this P_{op}, the thermodynamic averages of physical quantities may be defined:

$$\langle X \rangle = \mathrm{Tr} P_{\mathrm{op}} X / \mathrm{Tr} P_{\mathrm{op}} , \tag{38a}$$

where

$$\mathrm{Tr} A = \sum_n \langle \tilde{\Phi}_n | A | \Psi_n \rangle . \tag{38b}$$

It should again be stressed that the biorthogonal set of states must be used consistently, as in the definition (38b) of the trace. Henceforth we shall use the set $\{|\Psi_n\rangle, \langle \tilde{\Phi}_n|\}$; we could of course use the equivalent set $\{|\Phi_n\rangle, \langle \tilde{\Psi}_n|\}$.

The finite-temperature theory is best developed via the introduction of the temperature-dependent Green's function. We will first define the "Heisenberg representation" of b_k and $b_k^\dagger$ introduced in Sec. II by observing that in the Schrödinger representation, the equations of motion of a one-particle state are

$$i\hbar \frac{d}{dt} |\Psi_n(t)\rangle = H_{\mathrm{BZ}} |\Psi_n(t)\rangle , \qquad -i\hbar \frac{d}{dt} \langle \tilde{\Phi}_n(t) | = \langle \tilde{\Phi}_n(t) | H_{\mathrm{BZ}} . \tag{39a}$$

Equivalently,

$$|\Psi_n(t)\rangle = e^{-iH_{\mathrm{BZ}}t/\hbar} |\Psi_n^{(0)}\rangle ; \quad \langle \tilde{\Phi}_n(t) | = \langle \tilde{\Phi}_n(0) | e^{iH_{\mathrm{BZ}}t/\hbar} . \tag{39b}$$

Proceeding in the usual way to construct operators in the Heisenberg representation, we obtain the time dependence of an arbitrary operator in the $\{|\Psi\rangle, \langle\tilde{\Phi}|\}$ space:

$$i\hbar \frac{d}{dt} O_H(t) = i\hbar \frac{\partial}{\partial t} O_H(t) + [O_H(t), H_{\mathrm{BZ}}]_- , \tag{40}$$

where

$$O_H(t) = e^{iH_{\mathrm{BZ}} t/\hbar} O_s(t) e^{-iH_{\mathrm{BZ}} t/\hbar} , \tag{41}$$

with $O_s(t)$, the operator in the Schrödinger representation. $[A, B]_-$ in (40) represents the commutator, $(AB - BA)$. Had we chosen to employ the operator defined in the complementary space, $\{|\Phi\rangle, \langle\tilde{\Psi}|\}$, the equations (40) and (41) would contain $H_{\mathrm{BZ}}^\dagger$ instead of H_{BZ}. As stated in Sec. II, the final results in either development should be equivalent. We can now define the Green's functions in a consistent fashion, for example, the one-boson Green's function may be defined as

$$i\hbar \mathcal{G}(kt; k't') = \frac{\mathrm{Tr}\{P_{\mathrm{op}}[b_k(t) b_{k'}^\dagger(t')]_+\}}{\mathrm{Tr}\{P_{\mathrm{op}}\}} , \tag{42}$$

where $[\ ]_+$ indicates the time-ordering symbol. In a fairly straightforward way, we can show [by working in terms of the states of H_{BZ}, $\{|\Phi\rangle, \langle\tilde{\Psi}|\}$ or $H_{\mathrm{BZ}}^\dagger$, $\{|\Psi\rangle, \langle\tilde{\Phi}|\}$ if one employed the operators acting on the appropriate space], the usual properties of $\mathcal{G}(kt; k't')$ indicate that it is a function of $(t - t')$ and that it obeys the periodicity condition in the complex time domain. One can then proceed to develop the Fourier-series representation, etc., as for the usual temperature-dependent Green's function.[32] The Dyson equations obeyed by $\mathcal{G}$ follows by using (40). We must bear in mind the statements made in Sec. II concerning the properties of $|\Psi_n\rangle$ and $\langle\tilde{\Phi}_n|$. As an illustration we shall write down here, without derivation, the expression for the excitation energy for the uniform system in second order in $(N)^{-1/2}$:

$$\begin{aligned}\Sigma^{(2)}(k; E_B(k)) = &-18 \sum_{k_2} \frac{\gamma_a^{(3)}(k, k_2, -k-k_2)\gamma_b^{(3)}(k, k_2, -k-k_2)}{E_B(k) + E_B(k_2) + E_B(k+k_2)} [1 + n_B(k_2) + n_B(k+k_2)] \\ &+ 2P \sum_{k_2} \frac{\gamma_c^{(3)}(k, k_2, -k-k_2)\gamma_d^{(3)}(k, k_2, -k-k_2)}{E_B(k) - E_B(k_2) - E_B(k+k_2)} [1 + n_B(k_2) + n_B(k+k_2)] \\ &- 4P \sum_{k_2} \frac{\gamma_c^{(3)}(k_2, k, -k-k_2)\gamma_d^{(3)}(k_2, k, -k-k_2)}{E_B(k) + E_B(k+k_2) - E_B(k_2)} [n_B(k_2) - n_B(k+k_2)] .\end{aligned} \tag{43}$$

This is the finite-temperature version of Eq. (22). Here $n_B(k) = [\exp\beta E_B(k) - 1]^{-1}$. Straley[21] has written down "formally" a Green's-function theory of H_{BZ} for $T = 0$ °K. The analysis given above is not only a derivation of it but also an extension for $T \neq 0$ °K. As the Hamiltonian describes only irrotational flow, the finite-temperature extension given here is only valid when the superfluid density is much greater than the normal fluid density, i.e., $T < 0.5$ °K.[1, 32]

V. THE SUNAKAWA HAMILTONIAN

In the BZ formalism, one introduced the collective coordinate

$$\rho_k = N^{-1/2} \sum_{i=1}^{N} e^{i\vec{k}\cdot\vec{r}_i} \quad (\vec{k} \neq 0) , \tag{44}$$

and expressed the Hamiltonian in terms of ρ_k. Finally, creation and destruction operators are defined and the Hamiltonian is expressed in the form of Eqs. (1)-(3). Because of the problems that arise due to the non-Hermiticity of the Hamiltonian, several authors have considered alternate derivations of the Hamiltonian.

Sunakawa *et al.*[18] have obtained a completely Hermitian, but an infinite-series Hamiltonian by introducing a "velocity operator" $\vec{v}_k$ which is canonically conjugate to ρ_k. By introducing a projection operator, Sunakawa was able to write the Hamiltonian in terms of these canonically conjugate pair of operators. One then introduces the boson creation and annihilation operators, B_k and B_k^*, for the "excitations" of the He^4 liquid, when the fluid is assumed to be irrotational,

$$\begin{aligned}\rho_k &= (\lambda_k)^{1/2}(B_k + B_{-k}^*) , \\ \vec{v}_k &= \tfrac{1}{2}\hbar\vec{k}(\lambda_k)^{-1/2}(B_{-k} - B_k^*) .\end{aligned} \tag{45}$$

The Hamiltonian can then be written as (following notation introduced in Ref. 20):

$$H = H_0 + H_{\mathrm{I}} , \tag{46}$$

$$H_0 = E_0^B + \sum_k E_B(k) B_k^* B_k . \tag{47}$$

From the manner in which b_k and $b_k^\dagger$ were introduced in the BZ formalism, it is evident that the BZ Hamiltonian also describes an irrotational Bose fluid.

The interaction Hamiltonian H_{I} is an infinite series in powers of $N^{-1/2}$ in this formalism. The first two terms are of importance here and are given by

$$H_{\mathrm{I}}^{(3)}=\sum_{\substack{k_1,k_2\,(\neq 0)\\(\vec{k}_1+\vec{k}_2\neq 0)}}[g_a^{(3)}(k_1k_2)B_{k_1}^*B_{k_2}^*B_{-k_1-k_2}^*+g_b^{(3)}(k_1k_2)B_{-k_2}^*B_{k_1+k_2}^*B_{k_1}]+[\mathrm{H.c.}],\tag{48}$$

where we observe that the $g_{a,b}^{(3)}$ are related to the $\gamma^{(3)}$'s of H_{BZ}:

$$g_a^{(3)}(k_1k_2)=\tfrac{1}{2}[\gamma_a^{(3)}(k_1k_2k_3)+\gamma_b^{(3)}(k_1k_2k_3)],\tag{49a}$$

$$g_b^{(3)}(k_1k_2)=\tfrac{1}{2}[\gamma_c^{(3)}(k_1k_2k_3)+\gamma_d^{(3)}(k_1k_2k_3)],\tag{49b}$$

with

$$k_3=-k_1-k_2\,.\tag{49c}$$

The biquadratic interaction can be written as

$$H_{\mathrm{I}}^{(4)}=\sum_{\substack{k_1,k_2,q\\(\neq 0)}}\{[g_a^{(4)}(k_1k_2q)(B_{k_1+q}^*B_{k_2-q}^*B_{-k_2}^*B_{-k_1}^*+4B_{k_1+q}^*B_{-k_2+q}B_{k_2}B_{k_1})]+[\mathrm{H.c.}]+6g_a^{(4)}(k_1k_2q)B_{k_1+q}^*B_{k_2-q}^*B_{k_2}B_{k_1}\}$$
$$+\sum_{k_1,k_2}\left[\left(\frac{\hbar^2}{8mN}\lambda_{k_1}\lambda_{k_2}(k_1^2+k_2^2)(B_{k_2}B_{-k_2}+B_{k_2}^*B_{k_2}+\tfrac{1}{4})\right)+[\mathrm{H.c.}]\right],\tag{50}$$

where

$$g_a^{(4)}(k_1k_2q)=\frac{\hbar^2}{48mN}(\lambda_{k_1+q}\lambda_{k_2-q}\lambda_{k_2}\lambda_{k_1})^{1/2}[k_1^2+k_2^2+q^2+\vec{q}\cdot(\vec{k}_1-\vec{k}_2)].\tag{51}$$

One property of this Hamiltonian is worth noting here. $H_{\mathrm{I}}^{(3)}$ has the interesting property that, formally,

$$H_{\mathrm{I}}^{(3)}=\tfrac{1}{2}(H_1+H_1^\dagger),\tag{52}$$

where H_1 is the interaction part of H_{BZ}, and $H_1^\dagger$ is the Hermitian conjugate of H_1. This property will be very useful in proving equivalences in Sec. VI. In Eq. (50) the terms BB, B^*B^*, B^*B arise from normal ordering of operators, and their coefficients are seen to be divergent. In actual calculations of physical quantities, we will later show that these are *canceled* by similar divergences arising from terms elsewhere. The zeroth-order eigenfunctions and eigenvalues for the low-lying excited state with a single elementary excitation are given by

$$|\Psi_{1s}^{(0)}\rangle=|k\rangle=B_k^*|0\rangle,\tag{53}$$

$$E_{1s}^{(0)}=E_0^B+E_B(k)\,.\tag{54}$$

Using standard Rayleigh-Schrödinger perturbation theory, the first-order shift in the energy is zero but the second-order shift is

$$E_{1s}^{(2)}=-6\sum_{p_1,p_2}\frac{[g_a^{(3)}(p_1p_2)]^2}{E_B(p_1)+E_B(p_2)+E_B(p_1+p_2)}-18\sum_{k_2}\frac{[g_a^{(3)}(kk_2)]^2}{E_B(k)+E_B(k_2)+E_B(k+k_2)}$$
$$+2P\sum_{k_2}\frac{[g_b^{(3)}(kk_2)]^2}{E_B(k)-E_B(k_2)-E_B(k+k_2)}+\langle k|H_{\mathrm{I}}^{(4)}|k\rangle,\tag{55a}$$

where

$$\langle k|H_{\mathrm{I}}^{(4)}|k\rangle=\frac{\hbar^2}{48mN}\sum_{p_1,p_2}(\lambda_{p_2}\lambda_{p_3}p_1^2+\lambda_{p_3}\lambda_{p_1}p_2^2+\lambda_{p_1}\lambda_{p_2}p_3^2)+\frac{\hbar^2\lambda_k}{8mN}\sum_{k_2}[\lambda_{k_2}(\vec{k}+\vec{k}_2)^2+\lambda_{k+k_2}k_2^2]\quad(p_3=-p_1-p_2)\,.\tag{55b}$$

Eq. (55b) has been written in a completely symmetric form which will be more convenient for later calculations. Separating out the second-order shift to the ground-state energy, $E_{\mathrm{os}}^{(2)}$, one can write down the k-dependent second-order shift to the Bogoliubov excitation spectrum,

$$E_{1s}^{(2)}=E_{\mathrm{os}}^{(2)}+\epsilon_{2s}(k)\,.\tag{56}$$

$$E_{\mathrm{os}}^{(2)}=-6\sum_{p_1,p_2}\frac{[g_a^{(3)}(p_1p_2)]^2}{E_B(p_1)+E_B(p_2)+E_B(p_1+p_2)}$$
$$+\frac{\hbar^2}{48mN}\sum_{p_1,p_2}(\lambda_{p_1}\lambda_{p_2}p_3^2+\lambda_{p_2}\lambda_{p_3}p_1^2+\lambda_{p_3}\lambda_{p_1}p_2^2),\tag{57a}$$

$$\epsilon_{2s}(k) = -18 \sum_{k_2} \frac{[g_a^{(3)}(kk_2)]^2}{E_B(k) + E_B(k_2) + E_B(k+k_2)} + 2P \sum_{k_2} \frac{[g_b^{(3)}(kk_2)]^2}{E_B(k) - E_B(k_2) - E_B(k+k_2)} + \frac{\hbar^2}{8mN}\lambda_k \sum_{k_2} [\lambda_{k_2}(\vec{k}+\vec{k}_2)^2 + \lambda_{k+k_2}k_2^2]. \quad (57b)$$

It should be noted that Kebukawa[18] has recently obtained the second-order correction to the elementary excitation energy using RS perturbation theory involving $H_{\text{I}}^{(3)}$ only and obtained a divergent result. The last term in (57b) arises from the normal-ordering terms in $H_{\text{I}}^{(4)}$, and as will be soon evident, these are necessary to cancel the divergence found by Kebukawa.

By similar means, it is possible to calculate the scattering amplitude for two rotons which have initial momenta k and k' going into a final state with momenta $k+q$ and $k'-q$. $H_{\text{I}}^{(4)}$ is treated in first order while $H_{\text{I}}^{(3)}$, in second order, and one thus keeps track of the equivalent processes completely. The initial state is

$$|\Psi_i\rangle = B_k^* B_{k'}^* |0\rangle \equiv |k, k'\rangle \quad (58a)$$

and final state is

$$|\Psi_f\rangle = B_{k+q}^* B_{k'-q}^* |0\rangle \equiv |k+q, k'-q\rangle , \quad (58b)$$

where $\vec{q} \neq (0, \vec{k} - \vec{k}')$, and $k \neq k'$. To lowest order, the scattering amplitude for the two-roton scattering is given by

$$\langle k+q, k'-q | T | k, k'\rangle = \langle \Psi_f | H_{\text{I}}^{(4)} + H_{\text{I}}^{(3)}(E - H_0)^{-1} H_{\text{I}}^{(3)} | \Psi_i\rangle \equiv \langle \Psi_f | T_4 | \Psi_i\rangle + \langle \Psi_f | T_3 | \Psi_i\rangle . \quad (59)$$

Here, $E = E_B(k) + E_B(k') = E_B(k+q) + E_B(k'-q)$. The calculation was done in Ref. 20, and one may refer to this paper for the final expression.

As an interesting example of the usefulness of this last formulation, consider the special case of two-roton scattering into two rotons. In center-of-mass frame where $\vec{k} + \vec{k}' = 0$ and q is such that $|\vec{k} + \vec{q}| = |\vec{k}' - \vec{q}| = k_0$, where k_0 is the momentum at the roton minimum, we have $A_1 = 0 = A_6$ and

$$\langle k+q, k'-q | T_4 | k, k'\rangle = \lambda_{k_0}^2 \hbar^2 k_0^2 / mN , \quad (60)$$

where $|\vec{k} + \vec{q}| = k_0$ implies $2\vec{k} \cdot \vec{q} + q^2 = 0$. After some algebra, it can be shown that the total scattering amplitude is

$$T = \left(\frac{\lambda_{k_0}^2 \hbar^2 k_0^2}{mN}\right)\left[1 - \frac{\hbar^2 \lambda_q}{8mk_0^2 E_B(q)}\left(k_0^2 + \tfrac{1}{2}q^2 - \frac{(k_0^2 - \frac{1}{2}q^2)}{\lambda_{k_0}^2}\right)^2 - \frac{\hbar^2 \lambda_{2k+q}}{8mk_0^2 E_B(2k+q)}\left(3k_0^2 - \tfrac{1}{2}q^2 + \frac{(k_0^2 - \frac{1}{2}q^2)}{\lambda_{k_0}^2}\right)^2\right]. \quad (61)$$

If one now follows Ref. 20, and uses the experimental excitation energy and structure factor, T is in fact less than zero for all values of q and therefore this process has an attractive component. This is quite suggestive of a bound state for the process as was first surmised by Ruvalds and Zawadowski.[10] The actual strength of the interaction is in fact too strong and renormalization of vertices and roton propagators become important. For a complete discussion of this point see Ref. 20.

VI. PROOF OF EQUIVALENCE

A. Energy spectrum

In this section, we compare the results for the energy spectrum of elementary excitations derived from the BZ Hamiltonian in Sec. II with those derived in Sec. V for the Sunakawa Hamiltonian. The second-order shift to the ground-state energy, Eq. (57a) can be shown to be equal to the BZ result, Eq. (21), but this proof is similar to the proof of equivalence of the shift in the Bogoliubov excitation spectrum and therefore will not be shown. Substituting Eq. (49a) and (49b) into (57b) and identifying $\epsilon_{2\text{BZ}}(k)$ of Eq. (22), we have

$$\epsilon_{2s}(k) = \tfrac{1}{2}\epsilon_{2\text{BZ}}(k) - \frac{9}{2}\sum_{k_2} \frac{[\gamma_a^{(3)}(k, k_2, k_3)]^2 + [\gamma_b^{(3)}(k, k_2, k_3)]^2}{E_B(k) + E_B(k_2) + E_B(k_3)} + \tfrac{1}{2}P \sum_{k_2} \frac{[\gamma_c^{(3)}(k, k_2, k_3)]^2 + \gamma_d^{(3)}(k, k_2, k_3)]^2}{E_B(k) - E_B(k_2) - E_B(k_3)} + \frac{\hbar^2 \lambda_k}{8mN}\sum_{k_2} (\lambda_{k_2} k_3^2 + \lambda_{k_3} k_2^2), \quad \text{with } k_3 = -k_2 - k . \quad (62)$$

This result can be simplified using the following identities which can be proved after some straightforward algebra:

$$[\gamma_a^{(3)}(k, k_2, k_3)]^2 + [\gamma_b^{(3)}(k, k_2, k_3)]^2 = 2\gamma_a^{(3)}(k, k_2, k_3)\gamma_b^{(3)}(k, k_2, k_3) + \frac{\hbar^2}{72mN}[E_B(k) + E_B(k_2) + E_B(k_3)](\lambda_k \lambda_{k_2} k_3^2 + \lambda_k \lambda_{k_3} k_2^2 + \lambda_{k_2} \lambda_{k_3} k^2) , \quad (63a)$$

$$[\gamma_c^{(3)}(k,k_2,k_3)]^2+[\gamma_d^{(3)}(k,k_2,k_3)]^2=2\gamma_c^{(3)}(k,k_2,k_3)\gamma_d^{(3)}(k,k_2,k_3)$$
$$+\frac{\hbar^2}{8mN}[E_B(k)-E_B(k_2)-E_B(k_3)](\lambda_{k_2}\lambda_{k_3}k^2-\lambda_k\lambda_{k_2}k_3^2-\lambda_k\lambda_{k_3}k_2^2)\,. \tag{63b}$$

Substituting (63a) and (63b) into (62), we obtain

$$\epsilon_{2s}(k)=\epsilon_{2\mathrm{BZ}}(k)-\frac{\hbar^2}{16mN}\sum_{k_2}(\lambda_k\lambda_{k_2}k_3^2+\lambda_{k_2}\lambda_{k_3}k^2+\lambda_k\lambda_{k_3}k_2^2)+\frac{\hbar^2}{16mN}\sum_{k_2}(\lambda_{k_2}\lambda_{k_3}k^2-\lambda_k\lambda_{k_2}k_3^2-\lambda_k\lambda_{k_3}k_2^2)$$
$$+\frac{\hbar^2}{8mN}\sum_{k_2}(\lambda_k\lambda_{k_2}k_3^2+\lambda_k\lambda_{k_3}k_2^2)\,, \tag{64}$$

and thus we clearly obtain

$$\epsilon_{2s}(k)=\epsilon_{2\mathrm{BZ}}(k)\,. \tag{65}$$

This demonstrates the explicit equivalence of the second-order corrections to the Bogoliubov excitation energy. Since H_{BZ} is non-Hermitian, it is worth noting that no such equivalence for the wave functions is expected. Moreover, in view of the remarks made earlier, $\epsilon_{2s}(k)$ is convergent.[33] By a similar analysis, it can be shown that the self-energy calculated to second order for finite temperatures in both the BZ and S theories are equivalent.

B. Scattering amplitude

As shown in Sec. III, if the BZ Hamiltonian is to describe a real system, then the scattering amplitude must satisfy the property that

$$\langle k+q,k'-q|H_1^{\mathrm{BZ}}G_0H_1^{\mathrm{BZ}}|k,k'\rangle$$
$$=\langle k+q,k'-q|H_1^{\mathrm{BZ}\dagger}G_0H_1^{\mathrm{BZ}\dagger}|k,k'\rangle\,. \tag{66}$$

It is the intent of this subsection to not only prove Eq. (66) but also show its equivalence with the corresponding result obtained in Ref. 20 for the Sunakawa Hamiltonian. We will in fact show that Eqs. (36a)–(36g) and this expression are equivalent and the proof of (66) will then become self-evident. Two identities are needed:

$$\gamma^{(3)}_{\substack{c\\d}}(k,k_2,k_3)=g_b^{(3)}(k,k_2)\pm\tfrac{1}{4}(N^{-1}\lambda_k\lambda_{k_2}\lambda_{k_3})^{1/2}$$
$$\times[E_B(k)-E_B(k_2)-E_B(k_3)]\,, \tag{67a}$$

$$\gamma^{(3)}_{\substack{a\\b}}(k,k_2,k_3)=g_a^{(3)}(k,k_2)\mp\tfrac{1}{12}(N^{-1}\lambda_k\lambda_{k_2}\lambda_{k_3})^{1/2}$$
$$\times[E_B(k)+E_B(k_2)+E_B(k_3)]\,. \tag{67b}$$

When these two expressions are substituted into Eq. (36) and use is made of energy conservation it is found that after a great deal of algebra, that each $A_i^{(\mathrm{BZ})}$ can be written in terms of A_i given in Ref. 20 plus other terms. When the sum over all the six $A_i^{(\mathrm{BZ})}$ is performed, many terms cancel and one is left with the following result:

$$\sum_{i=1}^{6}A_i^{(\mathrm{BZ})}=\sum_{i=1}^{6}A_i+\frac{1}{2N}(\lambda_k\lambda_{k'}\lambda_{k+q}\lambda_{k'-q})^{1/2}[\lambda_qE_B(q)+\lambda_{k-k'+q}E_B(k-k'+q)+\lambda_{k+k'}E_B(k+k')]$$
$$=\sum_{i=1}^{6}A_i+\frac{\hbar^2}{2mN}(\lambda_k\lambda_{k'}\lambda_{k+q}\lambda_{k'-q})^{1/2}[k^2+k'^2+q^2+\vec{\mathrm{q}}\cdot(\vec{\mathrm{k}}-\vec{\mathrm{k}}')]$$
$$=\sum_{i=1}^{6}A_i+24g_a^{(4)}(k,k',q); \tag{68}$$

therefore the scattering amplitude for two-roton scattering through second order computed from the two Hamiltonians is equivalent. Equation (66) can be proved by a similar process and will not be shown here.

VII. COMPARISON WITH CBF RESULTS

The present analysis of the two collective-variable approaches to the theory of many-boson systems is of particular interest in that further connections to other theories are also possible. The other major technique for many-boson systems is the theory of correlated basis functions. When perturbative corrections are added to the BDJ wave functions to take into account the second-order energy generated by the three-phonon components, Lee[15] has shown that the excitation energy is given by

$$E_1^{(2)}(k) = E_B(k) + \epsilon_{1v}(k) + \epsilon_{1p}(k)\,, \tag{69a}$$

$$\epsilon_{1v}(k) = -\frac{\lambda_k^2 E_B(k)}{4(2\pi)^3\rho}\int d^3k_2\left(1+\frac{2k_2^2}{k^2}\right)(1-\lambda_{k_2})(1-\lambda_{k_3})\,, \tag{69b}$$

$$\epsilon_{1p}(k) = \frac{N}{2(2\pi)^3\rho}\,P\int\frac{d^3k_2\,|\langle -k_2, -k_3\,|\,\delta H\,|\,k\rangle|^2}{E_B(k) - E_B(k_2) - E_B(k_3)} - \frac{N}{2(2\pi)^3\rho}\int\frac{d^3k_2\,|\langle k, k_2, k_3\,|\,\delta H\,|0\rangle|^2}{E_B(k) + E_B(k_2) + E_B(k_3)}\,, \tag{69c}$$

and Lee made the observation

$$\langle -k_2, -k_3\,|\,\delta H\,|\,k\rangle = 2\gamma_d^{(3)}(k, k_2, k_3)\,, \tag{70a}$$

$$\langle k, k_2, k_3\,|\,\delta H\,|0\rangle = 6\gamma_b^{(3)}(k, k_2, k_3)\,, \tag{70b}$$

where the matrix elements have been evaluated with use of the convolution approximation for the three-particle distribution function. Lee[15] has shown that (69a)–(69c) and the k-dependent part of (22) are equivalent.

VIII. SUMMARY AND CONCLUDING REMARKS

The main objective of this paper was to set up a mathematical procedure for calculating physical quantities of interest from the non-Hermitian Hamiltonian derived by Bogoliubov and Zubarev.[8] We have set up a perturbation scheme for calculating both the energies and scattering amplitudes using the complete, orthonormal states of the Hermitian part of H_{BZ}, treating the non-Hermitian part as a perturbation. We have also set up a finite-temperature Green's-function theory by suitably defining the statistical operator and the Heisenberg equations of motion. With this, we hope to have answered the queries of Hiroike[17] and Straley.[21]

We show that the energies for the ground-, and first excited states, the temperature-dependent self-energy of a boson, and two-roton scattering amplitudes obtained in Rayleigh-Schrödinger perturbation theory are completely equivalent to the corresponding results computed in the second order from the Sunakawa formalism. In the Sunakawa formalism, one develops the Hamiltonian operator to a given order in $N^{-1/2}$ and then carries out the usual perturbation calculation to an appropriate order in $N^{-1/2}$. It thus appears that our scheme involving H_{BZ} is simpler in its structure because it is not an infinite series. Also the coefficients appearing in the interaction part of the Hamiltonian are not divergent as in the S theory.

A major problem in these field theoretic approaches is the appearance of λ_k, since this depends on the poorly known interaction potential, $V(k)$. A numerical evaluation of physical quantities of interest therefore becomes difficult. The only hope is that λ_k is the lowest-order approximation to the experimentally measurable structure factor, $S(k)$, and this must somehow be exploited in the actual numerical computations. $S(k)$ is defined by

$$S(k) = \langle\tilde{G}\,|\rho_k\rho_k^*|\,G\rangle/\langle\tilde{G}\,|\,G\rangle\,, \tag{71}$$

Where $|G\rangle$ is exact ground state of H_{BZ} and $\langle\tilde{G}|$ its counterpart. Expanding $|G\rangle$, $\langle\tilde{G}|$ to order $(1/N)$, we have

$$\begin{aligned} S(k) &= \lambda_k + 4\lambda_k\sum_p\frac{9\gamma_a^{(3)}(k, p, -k-p)\gamma_b^{(3)}(k, p, -k-p)}{[E_B(k)+E_B(p)+E_B(p+k)]^2} \\ &\quad + 6\lambda_k\sum_P\frac{\gamma_a^{(3)}(k, p, -k-p)\gamma_d^{(3)}(k, p, -k-p)+\gamma_b^{(3)}(k, p, -k-p)\gamma_c^{(3)}(k, p, -k-p)}{[E_B(k)+E_B(p)+E_B(p+k)]E_B(k)} + O\left(\frac{1}{N^2}\right) \\ &\equiv \lambda_k + S_1(k)\,. \end{aligned} \tag{72}$$

This expression does not agree with the result derived by Lee.[12]

Since it is well known that $E_F(k) = \hbar^2k^2/2mS(k)$ gives the correct sound velocity for liquid helium,[6] it is interesting to examine if the corrections to $E_B(k)$ using our formalism agree with this result. From Eq. (22),

$$\begin{aligned} E(k) &= E_B(k) + \epsilon_2(k) + O(1/N^2) \\ &= E_F(k) + \frac{\hbar^2k^2}{2m}\left(\frac{1}{\lambda_k} - \frac{1}{S(k)}\right) + \epsilon_2(k) \\ &= E_F(k) + E_B(k)\frac{S_1(k)}{\lambda_k} + \epsilon_2(k)\,. \end{aligned} \tag{73}$$

In the long-wavelength limit, the last two terms can be reduced further using the expressions given above, and we find

$$E(k) \simeq E_F(k) + (1/N)O(k^3)\,. \tag{74}$$

Thus $E(k)$ derived from the BZ or S formalism approaches the Feynman expression, $E_F(k)$, for $k\to 0$, as it should. It should be noted from (72) that λ_k *does not* have the same slope as $S(k)$ for $k\to 0$, as has been assumed by Sunakawa *et al.*[18] The problem now reduces to finding a good model for the helium-helium potential, or equivalently λ_k so that both $S(k)$ and $E(k)$ can be calculated theoretically and compared with their experimental values in detail.

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APPENDIX

In this Appendix, we outline a transformation method which to a desired order in $(N^{-1/2})$ can make the Hamiltonian H_{BZ} Hermitian, by introducing a canonical but nonunitary transformation of the operators b_k, $b_k^\dagger$ into a new set of boson operators B_k, B_k^*. $b_k^\dagger$ may be considered as the *formal* adjoint of b_k, whereas B_k^* is the Hermitian conjugate of B_k. With this distinction, we seek a polynomial transformation between b_k, $b_k^\dagger$, and B_k, B_k^*:

$$b_{k_1} = B_{k_1} + N^{-1/2} \sum_{k_2, k_3} \frac{\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}}{E_B(k_1)} [P_2^{(a1)}(k_1k_2k_3)B_{-k_2}B_{-k_3} + P_2^{(a2)}(k_1k_2k_3)B^*_{k_2}B^*_{k_3} + P_2^{(a3)}(k_1k_2k_3)B^*_{k_2}B_{-k_3} + P_2^{(a4)}(k_1k_2k_3)B^*_{k_3}B_{-k_2}] + \cdots , \tag{A1}$$

$$b^\dagger_{k_1} = B^*_{k_1} + N^{-1/2} \sum_{k_2, k_3} \frac{\delta_{-\vec{k}_1+\vec{k}_2+\vec{k}_3,\vec{0}}}{E_B(k_1)} [\tilde{P}_2^{(b1)}(k_1k_2k_3)B_{-k_2}B_{-k_3} + \tilde{P}_2^{(b2)}(k_1k_2k_3)B^*_{k_2}B^*_{k_3} + \tilde{P}_2^{(b3)}(k_1k_2k_3)B^*_{k_2}B_{-k_3} + \tilde{P}_2^{(b4)}(k_1k_2k_3)B^*_{k_3}B_{-k_2}] + \cdots . \tag{A2}$$

B_k, B_k^* are assumed to obey also the Bose commutation rules as do $b_k, b_k^\dagger$. It is obvious that this connection must be an *infinite-series* relationship. Writing

$$\begin{aligned} H_{\mathrm{BZ}} &= \tfrac{1}{2}(H_{\mathrm{BZ}} + H^\dagger_{\mathrm{BZ}}) + \tfrac{1}{2}(H_{\mathrm{BZ}} - H^\dagger_{\mathrm{BZ}}) \\ &\equiv H_H + H_{NH} , \end{aligned} \tag{A3}$$

we seek the undetermined coefficients in (A1) and (A2) to be such that to each order in $(N^{-1/2})$, the non-Hermitian part is canceled out, leaving it to be one order higher in $(N^{-1/2})$ only. For instance, carrying this out to first order in $(N^{-1/2})$ is at once easily accomplished and this leads us to the Sunakawa Hamiltonian to order $(N^{-1/2})$ in B_k, B_k^* with the non-Hermitian residue of order $(N^{-1/2})^2$. The choice of $P_2^{(ai)}, \tilde{P}_2^{(bi)}$ in (A1), (A2) that accomplishes this is

$$\begin{aligned} P_2^{(a2)}(k_1k_2k_3) &= -\tilde{P}_2^{(b1)}(k_1k_2k_3) \\ &= \gamma_a^{(3)}(k_1k_2k_3) - \gamma_b^{(3)}(k_1k_2k_3) , \\ -P_2^{(a4)}(k_1k_2k_3) &= \tilde{P}_2^{(b3)}(k_1k_2k_3) \\ &= \gamma_c^{(3)}(k_3k_1k_2) - \gamma_d^{(3)}(k_3k_1k_2) , \\ -P_2^{(a3)}(k_1k_2k_3) &= \tilde{P}_2^{(b4)}(k_1k_2k_3) \\ &= \gamma_c^{(3)}(k_2k_3k_1) - \gamma_d^{(3)}(k_2k_3k_1) , \end{aligned}$$

and

$$\begin{aligned} P_2^{(a1)}(k_1k_2k_3) &= -\tilde{P}_2^{(b2)}(k_1k_2k_3) \\ &= \gamma_c^{(3)}(k_1k_2k_3) - \gamma_d^{(3)}(k_1k_2k_3) . \end{aligned} \tag{A4}$$

From (A1), (A2) and (A4) we observe that the adjoint of (A1) differs from (A2) by terms of order $(N^{-1/2})$ and higher. Proceeding in this way we can, in principle, obtain a Hermitian Hamiltonian from H_{BZ}. This has the following consequence. The commutation rules between $b_k, b_k^\dagger$ will have operator corrections of order $(N^{-1/2})$ and higher, contrary to the originally proposed commutation relations, but which will cancel out when higher-order terms are included. This establishes a point about H_{BZ} and the other Hermitian formulations, namely, that the Hermitian versions will all be an infinite series and H_{BZ} perhaps involves really a set of more complicated operators $b_k, b_k^\dagger$ than was originally intended. Noting that the non-Hermiticity in the BZ formalism arises from introduction[7] of $\partial/\partial\rho_k$, we choose to associate $b_k^\dagger$ as being the formal adjoint of b_k, to differentiate it from the Hermitian adjoint operator. Hiroike[11] essentially tried to set up a "Hermitian" counterpart of $\partial/\partial\rho_k$ by introducing the Jacobian of transformation from the coordinates to the ρ_k variables, and this turned out to be a series in $(N^{-1/2})$. Our demonstration here indicates a basic formal reason for Hermitian, infinite-series Hamiltonians as compared to the simple, non-Hermitian Hamiltonian of BZ.

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