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A Note on the Calculation of the Long-Wavelength Limit of the Bosonic Excitation Spectrum

Abstract: An approach is proposed to analyse an interacting bosonic system using two-time temperature Green’s functions on the collective variables. Two systems are studied: liquid helium-4 and the Yukawa Bose liquid being a model of the nuclear matter. The suggested decoupling in the equations of motion for Green’s functions yields a good description of the elementary excitation spectrum in the long-wavelength limit.

Keywords: Bose-System; Excitation Spectrum; Liquid Helium-4; Nuclear Matter; Yukawa Bose Liquid.

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1 Introduction

In this article, I address a rather classical problem of the low-temperature physics and the theory of Bose systems specifically. The excitation spectrum of a Bose liquid was an important element in the formulation of the theory of superfluidity of liquid helium-4. Phenomenologically formulated by Landau [1, 2], the spectrum was microscopically derived by Bijl [3], Bogoliubov [4], Feynman and Cohen [5, 6]. In the following decades, numerous works on this subject appeared [7–16] to mention a few.

Experimental observation of the Bogoliubov excitations in exciton–polariton Bose condensates was reported by Utsunomiya et al. [17]. Such systems [18, 19] constitute another group for probing Bose condensation, alongside dilute alkali gases [20].

Approaches based on the Hamiltonian of an interacting Bose system by Bogoliubov and Zubarev [21] were used by the present author to calculate the effective mass of the ‘He atom and the excitation spectrum of liquid helium-4 [22, 23]. In this work, yet another method is proposed allowing for a proper treatment of the long-wavelength domain of the excitation spectrum. This approach is tested both for helium-4 with a self-consistently derived interatomic potential [24] and for a Bose liquid with the Yukawa potential.

The paper is organised as follows. Section 2 contains all the required definitions of the Hamiltonian and two-temperature Green’s functions, which are further applied in the calculations. Decouplings for Green’s functions are suggested in Section 3, and general expressions for the excitation spectrum are obtained there. Results of calculations for two systems (liquid helium-4 and the Yukawa Bose liquid) are given in Section 4. A short discussion in Section 5 concludes the article.

2 Green’s Functions

Let us consider the Hamiltonian of a Bose system of $N$ particles in the volume $V$ interacting via pairwise $\Phi(r_1-r_2)$ and three-particle $\Phi_3(r_1,r_2,r_3)$ potentials:

$$H = \frac{\hbar^2}{2mN} \sum_{\mathbf{q} \neq 0} \left( \epsilon(\mathbf{q}) - \mathbf{q} \cdot \mathbf{v}_k \right) \rho_{\mathbf{k} \mathbf{q}} + \frac{\hbar^2}{2m} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} \left[ \mathbf{q} \cdot \mathbf{V}_{\mathbf{k} \mathbf{q}} \mathbf{\rho}_{\mathbf{k} \mathbf{q}} \right],$$

where $m$ is the mass of a particle and $\Delta_j$ is the Laplace operator with respect to the $j$th coordinate $\mathbf{r}_j$. In the case of a Bose system, it is possible to pass to the so-called collective variables:

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{k} \cdot \mathbf{r}_j}, \quad \partial_{\mathbf{k}} = \frac{\partial}{\partial \rho_{\mathbf{k}}}, \quad \text{where} \quad \mathbf{k} \neq 0.$$ 

Hamiltonian (1) becomes as follows [21, 25]:

$$H = \sum_{\mathbf{k} \neq 0} \left[ \epsilon(\mathbf{k}) \rho_{\mathbf{k}} - \mathbf{k} \cdot \mathbf{v}_k \rho_{\mathbf{k}} - \frac{\hbar^2}{2m} \mathbf{q} \cdot \mathbf{V}_{\mathbf{k} \mathbf{q}} \mathbf{\rho}_{\mathbf{k} \mathbf{q}} \right] + \frac{\hbar^2}{2m} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} \left[ \mathbf{q} \cdot \mathbf{V}_{\mathbf{k} \mathbf{q}} \mathbf{\rho}_{\mathbf{k} \mathbf{q}} \right],$$

$$+ \frac{\hbar^2}{2m} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} \left[ \mathbf{q} \cdot \mathbf{V}_{\mathbf{k} \mathbf{q}} \mathbf{\rho}_{\mathbf{k} \mathbf{q}} \right],$$

$$+ \frac{\hbar^2}{2m} \sum_{\mathbf{k} \neq 0} \sum_{\mathbf{q} \neq 0} \left[ \mathbf{q} \cdot \mathbf{V}_{\mathbf{k} \mathbf{q}} \mathbf{\rho}_{\mathbf{k} \mathbf{q}} \right].$$
where \(\epsilon_k = \hbar^2 k^2 / 2m\) is the free-particle energy, \(n = N/V\) is the particle density, \(v_\rho\) and \(v_\phi(k,q)\) are the Fourier transforms of the pairwise and three-particle potentials, respectively, and

\[
\hat{v}_k = v_k + n v_\phi(k, -k) - \frac{1}{V} \sum_{q>0} v_\phi(k, q).
\]

(5)

With operators \(A\) and \(B\) written in the Heisenberg representation, the two-time temperature Green's functions are defined \([26]\) as

\[
\langle\langle A(t) | B(t') \rangle\rangle = i \theta(t - t') \langle [A(t), B(t')] \rangle,
\]

(6)

where \(\theta(t)\) is the Heaviside step function and \([\cdot, \cdot]\) denotes the commutator.

In the case of \(t=t'\), the equations of motion in the frequency representation are given by

\[
\hbar \omega \langle\langle A | B \rangle\rangle = \frac{1}{2\pi} \langle\langle [A, B] \rangle\rangle + \langle\langle [A, H] | B \rangle\rangle,
\]

(7)

which upon simple transformations with (3) leads to the following set:

\[
\hbar \omega \langle\langle \rho_k | \rho_{-k} \rangle\rangle = -\epsilon_k \langle\langle \rho_k | \rho_{-k} \rangle\rangle + 2\epsilon_k \langle\langle \partial_k | \rho_{-k} \rangle\rangle
- \frac{2}{\sqrt{N}} \sum_{q>0} \frac{\hbar^2}{2m} k q \langle\langle \rho_{k+q} | \partial_{-q} | \rho_{-k} \rangle\rangle,
\]

\[
\hbar \omega \langle\langle \partial_k | \rho_{-k} \rangle\rangle = \frac{1}{2\pi} + \epsilon_k \langle\langle \partial_k | \rho_{-k} \rangle\rangle + n v_\rho \langle\langle \rho_k | \rho_{-k} \rangle\rangle
+ \frac{1}{\sqrt{N}} \sum_{q>0} \frac{\hbar^2}{2m} k q \langle\langle \partial_{k+q} | \partial_{-q} | \rho_{-k} \rangle\rangle
- \frac{n^2}{2} v_\phi(k, q) \langle\langle \rho_{k+q} | \rho_{-q} | \rho_{-k} \rangle\rangle.
\]

(8)

Dropping off three-operator Green's functions, i.e., in the random phase approximation (RPA), one obtains the following expression for one of the solutions of set (8):

\[
\langle\langle \rho_k | \rho_{-k} \rangle\rangle = \frac{\epsilon_k}{\pi} \left( \frac{\hbar \omega}{\epsilon_k} \right)^2 \left( 1 + \epsilon_k / \epsilon_k' \right)^{1/2},
\]

immediately yielding the Bogoliubov spectrum from the poles of Green's functions with respect to \(\hbar \omega\):

\[
E_k = \epsilon_k \alpha_k, \quad \text{where} \quad \alpha_k = (1 + 2 nv_k / \epsilon_k)^{1/2}.
\]

(10)

While it is also possible to derive the equations of motion for three-operator functions as well, no closed-form expression for the excitation spectrum can be obtained with them. So, another option leading to easier calculations of the spectrum is considered in the next section.

### 3 Green's Function Decoupling and Excitation Spectrum

Because Green's functions of the \(\langle\langle AB|C \rangle\rangle\) type are used to calculate averages of triple products \(\langle CAB \rangle\), the following decoupling can be used:

\[
\langle\langle A, B_1 | C_3 \rangle\rangle = \lambda(1,2) \langle\langle A, B_1 | C_3 \rangle\rangle + \mu(1,2) \langle\langle B_1, C | C_3 \rangle\rangle
\]

(11)

with

\[
\lambda(1,2) = (1-\eta) \frac{\langle\langle C, A, B_1 \rangle\rangle}{\langle\langle C, A_{3|1} \rangle\rangle}, \quad \mu(1,2) = \eta \frac{\langle\langle C, A, B_1 \rangle\rangle}{\langle\langle C, B_{1|2} \rangle\rangle},
\]

(12)

where the value of the parameter \(\eta = 0 \div 1\) will be fixed on a later stage.

The following two approximation for averages were tested:

\[
\langle\langle C, A, B_1 \rangle\rangle = \frac{1}{6} \langle\langle CA \rangle\rangle \langle\langle CB \rangle\rangle \langle\langle AB \rangle\rangle + \text{symmetrisation over indices}
\]

(13)

with six items in the parentheses, hence the “s” index, and

\[
\langle\langle C, A, B_1 \rangle\rangle = \frac{1}{4} \left[ \langle\langle AB \rangle\rangle \langle\langle CA \rangle\rangle + \langle\langle AB \rangle\rangle \langle\langle CB \rangle\rangle + \langle\langle A \rangle\rangle \langle\langle CB \rangle\rangle + \langle\langle A \rangle\rangle \langle\langle CB \rangle\rangle \right]
\]

(14)

with four items in the parentheses.

To decouple the functions entering (8) the following averages are required:

\[
\langle\langle \rho_k \rho_{k+q} \partial_{-q} \rangle\rangle_{s,t} = \frac{1}{\sqrt{N}} \langle\langle \rho_k \rho_k \partial_{-k} \rangle\rangle_{s,t} \langle\langle \rho_{k+q} \partial_{-q} \rangle\rangle_{s,t}
\]

(15)

which corresponds to the so-called convolution approximation and is identical for both the suggested decoupling types

\[
\langle\langle \rho_k \rho_{k+q} \partial_{-q} \rangle\rangle_{s,t} = \frac{1}{3\sqrt{N}} \langle\langle \partial_{-q} \partial_{-k} \partial_{k+q} \rangle\rangle_{s,t} \langle\langle \rho_k \partial_{-k} \rangle\rangle_{s,t} + \langle\langle \partial_{-q} \partial_{-k} \partial_{k+q} \rangle\rangle_{s,t} \langle\langle \rho_k \partial_{-k} \rangle\rangle_{s,t}
\]

(16)

and

\[
\langle\langle \rho_k \rho_{k+q} \partial_{-q} \rangle\rangle_{s,t} = \frac{1}{2\sqrt{N}} \langle\langle \partial_{-q} \partial_{-k} \partial_{k+q} \rangle\rangle_{s,t} \langle\langle \rho_k \partial_{-k} \rangle\rangle_{s,t} + \langle\langle \partial_{-q} \partial_{-k} \partial_{k+q} \rangle\rangle_{s,t} \langle\langle \rho_k \partial_{-k} \rangle\rangle_{s,t}
\]

(17)
Expressions for pairwise averages are easily obtained from the solutions of (8) in RPA as follows [22]:

\[
\langle \rho_{-k} \partial_{k} \rangle = \frac{1}{2\sqrt{N}} \left( \langle \rho_{-\text{q}} \partial_{\text{q}} \rangle \right),
\]

\[
\langle \rho_{-k} \partial_{k} \rangle = \frac{1}{2} \left( \frac{1}{\alpha_{k}} - 1 \right),
\]

(20)

With the decouplings applied, equations of motion (8) become:

\[
\hbar \omega \langle \rho_{-k} | \rho_{-k} \rangle = -\varepsilon_{k}^{(1)} \langle \rho_{-k} | \rho_{-k} \rangle + 2\varepsilon_{k}^{(2)} \langle \partial_{k} | \rho_{-k} \rangle + \varepsilon_{k}^{(3)} \langle \partial_{k} | \rho_{-k} \rangle,
\]

\[
\hbar \omega \langle \partial_{k} | \rho_{-k} \rangle = \frac{1}{2\pi} + \varepsilon_{k}^{(1)} \langle \partial_{k} | \rho_{-k} \rangle + \nu_{k}^{(*)} \langle \rho_{-k} | \rho_{-k} \rangle,
\]

where

\[
\varepsilon_{k}^{(1)} = \frac{2}{\sqrt{N}} \sum_{\text{q} = 0}^{\text{q} = 0} \frac{\hbar^{2}}{2m} \text{q} X(\text{k,q}),
\]

\[
\varepsilon_{k}^{(2)} = \frac{1}{\sqrt{N}} \sum_{\text{q} = 0}^{\text{q} = 0} \frac{\hbar^{2}}{2m} \text{q} Y(\text{k,q}),
\]

\[
\varepsilon_{k}^{(3)} = \frac{2}{\sqrt{N}} \sum_{\text{q} = 0}^{\text{q} = 0} \frac{\hbar^{2}}{2m} \text{q} Z(\text{k,q}),
\]

\[
\nu_{k}^{(*)} = \tilde{\nu}_{k} + \frac{1}{\sqrt{N}} \sum_{\text{q} = 0}^{\text{q} = 0} \nu_{k}(\text{k,q}) T(\text{k,q}).
\]

(21)

The notations used in the aforementioned definitions are as follows:

\[
X(\text{k,q}) = (1-\eta) \frac{\langle \rho_{-k} \partial_{k} \text{q} \rangle}{\langle \rho_{-k} \partial_{k} \rangle},
\]

\[
Y(\text{k,q}) = -\eta \frac{\langle \rho_{-k} \partial_{k} \text{q} \rangle}{\langle \rho_{-k} \partial_{k} \rangle},
\]

\[
Z(\text{k,q}) = \frac{\langle \rho_{-k} \partial_{k} \text{q} \rangle}{\langle \rho_{-k} \partial_{k} \rangle},
\]

\[
T(\text{k,q}) = \frac{\langle \rho_{-k} \partial_{k} \text{q} \rangle}{\langle \rho_{-k} \partial_{k} \rangle}.
\]

(26)

The excitation spectrum is thus given by

\[
E_{k} = \frac{1}{2} \left[ \varepsilon_{k}^{(1)} + \sqrt{\left[ \varepsilon_{k}^{(1)} \right]^{2} + \left[ \varepsilon_{k}^{(2)} \right]^{2} + 2\varepsilon_{k}^{(1)} \varepsilon_{k}^{(2)} + 8\varepsilon_{k}^{(2)} \nu_{k}^{(*)}} \right].
\]

(27)

With the items containing the summations dropped, Bogoliubov’s result (10) immediately follows from this expression.

### 4 Results

The calculations of the excitation spectrum were made for two bosonic systems. The first one is the liquid helium-4 and the second one is the Yukawa Bose liquid with parameters corresponding to the nuclear matter. As data about the details of three-particle interactions in these systems are rather scarce, the contributions of \(\nu_{k}(\text{k,q})\) are neglected.

It was estimated in [23] that in case of helium-4 such an approach does not influence the long-wavelength limit of the excitation spectrum significantly. To facilitate the numerical analysis, summation in (22) through (24) is substituted with integration in the wave-vector space according to such a rule:

\[
\frac{1}{N} \sum_{\text{q} = 0} = \frac{1}{n} \int \text{d} \text{q} .
\]

(28)

Expressions suitable for immediate numerical computations are presented in the Appendix.

The following set of parameters is used for the calculations of the helium-4 excitation spectrum:

\[
m = 4.0026 \text{ a.u.}, \quad n = 0.02185 \text{ Å}^{-3}.
\]

The data for the interatomic potential \(\nu_{k}\) are taken from [24]. Note that accurate pairwise potentials based on semi-phenomenological and quantum-mechanical computations [27–29] are not very suitable for such calculations. The potential from [24] was obtained in a self-consistent manner within the approach of collective variables and is in a certain sense an effective pairwise potential incorporating contributions from many-body interactions. This makes it similar to the Yukawa potential, analysed following, thought as a screened Coulomb potential.

Results for the excitation spectrum of helium-4 according to (27) are shown in Figure 1 and Table 1 compared to the RPA approximation (Bogoliubov’s spectrum) and experimental data. The parameter \(\eta\) is set equal to 1 as for smaller values the correction to the RPA result appear insufficient to produce the correct slope of the phonon (linear at \(k \to 0\)) branch. It means that the term \(\langle \rho_{-k} \partial_{k} \text{q} \rangle\) thus leads to an undesired mutual compensation of corrections.

Both of the suggested \(s\) and \(f\) decoupling types are found suitable to describe the long-wavelength behaviour of the helium-4 spectrum without introduction of the effective mass, which is required in the RPA, cf. [22]. Conversely, the proposed method still fails at higher values of the wave vector and further modifications should be
sought for to reproduce the maxon and roton domains successfully in this approach.

Another interesting problem for analysis is the nuclear matter, where different types of Bose condensation are predicted [31, 32]. It is possible to model the nuclear matter as a Bose liquid interacting via the Yukawa potential
\[
\Phi(r) = \frac{\epsilon \sigma}{\sigma + \frac{r}{\pi \Lambda}}.
\]

The Fourier transform of this potential [34] reads
\[
\nu_k = \frac{4\pi \epsilon \sigma^3}{1 + \sigma^2 k^2},
\]
with the following values of the parameters [33]:
\[
\epsilon = 5725 \text{ MeV}, \quad \sigma = 0.244 \text{ fm}^{-1}.
\]

Table 1  Excitation spectrum of the liquid helium-4.

| $k$, Å⁻¹ | $E_s^0$ | $E_{\text{type}}$ | $E_{\text{type}}$ | $E_{\text{exp}}$ | $\Delta E$ |
|----------|---------|-----------------|-----------------|----------------|---------|
| 0.2      | 4.21    | 3.79            | 3.69            | 3.70 ± 0.5     |         |
| 0.3      | 6.31    | 5.60            | 5.44            | 5.65 ± 0.2     |         |
| 0.4      | 8.53    | 7.48            | 7.21            | 7.40 ± 0.2     |         |
| 0.5      | 10.84   | 9.37            | 8.97            | 9.15 ± 0.2     |         |
| 0.6      | 13.27   | 11.32           | 10.75           | 10.75 ± 0.2    |         |
| 0.7      | 15.80   | 13.31           | 12.52           | 11.75 ± 0.2    |         |
| 0.8      | 18.26   | 15.22           | 14.17           | 12.65 ± 0.2    |         |
| 0.9      | 20.47   | 16.90           | 15.60           | 13.15 ± 0.2    |         |
| 1.0      | 22.14   | 18.13           | 16.59           | 13.55 ± 0.2    |         |
| 1.2      | 23.55   | 19.09           | 17.29           | 13.75 ± 0.25   |         |
| 1.4      | 22.83   | 18.78           | 17.17           | 12.95 ± 0.2    |         |
| 1.6      | 20.45   | 17.89           | 17.05           | 11.20 ± 0.2    |         |
| 1.8      | 18.23   | 18.12           | 18.43           | 9.25 ± 0.2     |         |
| 2.0      | 19.57   | 21.23           | 22.20           | 8.95 ± 0.2     |         |

Calculated values in the Bogoliubov approximation $E_s^0$ and two decoupling types (s and f) are compared to the experimental data [30]. Energies are in Kelvin.

Results for the excitation spectrum are given in Figure 2. The obtained correction to the RPA changes the shape of the $E_k$ curve leading to a good qualitative agreement with other data [34, 35]. It should be mentioned that the values of the $\eta$ parameter are close to zero in this case as for $\eta \approx 0.2$ unphysical divergences in the domain of the minimum ($k=4\div6$ fm⁻¹) appear.

Other quantities used to model the nuclear matter are as follows:
\[
\Lambda = \frac{2\pi \hbar}{\sigma \sqrt{m}} = 1.08, \quad n = 0.16 \text{ fm}^{-3}.
\]

Figure 1 (Colour online.) Excitation spectrum of the liquid helium-4. The right graph is the enlarged view of the marked rectangular area of the left graph. Red solid line – RPA result (Bogoliubov’s spectrum); green dashed line – spectrum (27) with the $s$-type decoupling, $\eta=1$; magenta dotted line – spectrum (27) with the $f$-type decoupling, $\eta=1$. Circles (errorbars) are the experimental data from [30].

Figure 2 (Colour online.) Excitation spectrum of the Yukawa Bose liquid with parameters corresponding to the nuclear matter. Red solid line – RPA result (Bogoliubov’s spectrum); green dashed line – spectrum (27) with the $s$-type decoupling, $\eta=0$; magenta dotted line – spectrum (27) with the $f$-type decoupling, $\eta=0$; blue dashed-dotted line – spectrum (27) with the $s$-type decoupling, $\eta=0.1$. 

5 Discussion

In summary, an approach was proposed to treat an interacting bosonic system using two-time temperature Green’s functions on the collective variables leading to a good description of the elementary excitation spectrum in the long-wavelength limit. It appears that a correct description of the phonon branch for liquid helium-4 is obtained here without applying the notion of an effective mass. For two models considered in the work different values of the Green’s function decoupling parameter \( \eta \) should be taken: \( \eta = 1 \) for the liquid helium-4 and \( \eta = 0 \) for the Yukawa Bose liquid. The choice of this parameter thus seems to be governed by the nature of interactions. For an essentially short-range potential in liquid helium, an effective change of the interaction term \( \epsilon^{(2)}_k \nu_k \) in expression (27) for the spectrum occurs. Conversely, for a long-range Yukawa potential “kinetic” terms \( \epsilon^{(2)}_k \) should be affected instead.

To obtain a better description of liquid helium spectrum beyond the long-wavelength domain, some modifications of the applied method are required. In particular, inclusion of three-body interactions, as well as search for other approximations of three-operator, Green’s functions on the collective variables leading to a good description of the elementary excitation spectrum in the acting bosonic system using two-time temperature Green’s functions.

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It is convenient to make the integration in these formulas using spherical coordinates.

For the \( f \)-type decoupling:

\[
\epsilon^{(1)}_k = \epsilon_k + \frac{(1 - \eta) \hbar^2}{(2 \pi)^3} \int dq (kq) \left( \frac{S_{L_k} L_{k_1} + L_{S_k} S_{k_1} + L_{L_k} S_{k_1}}{3 S} \right), \]
\[
\epsilon^{(2)}_k = \epsilon_k - \frac{\eta \hbar^2}{(2 \pi)^3} \int dq (kq) \left( \frac{S_{L_k} L_{k_1} + L_{S_k} S_{k_1} + L_{L_k} S_{k_1}}{3 S} \right), \]
\[
\epsilon^{(3)}_k = \epsilon_k + \frac{1}{(2 \pi)^3} \int dq (kq) \left( \frac{S_{L_k} L_{k_1} + L_{S_k} S_{k_1} + L_{L_k} S_{k_1}}{3 S} \right). \]  

(34)

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\[
\epsilon^{(2)}_k = \epsilon_k - \frac{\eta \hbar^2}{(2 \pi)^3} \int dq (kq) \left( \frac{S_{L_k} L_{k_1} + L_{S_k} S_{k_1}}{2} \right), \]
\[
\epsilon^{(3)}_k = \epsilon_k + \frac{1}{(2 \pi)^3} \int dq (kq) \left( \frac{S_{L_k} L_{k_1} + L_{S_k} S_{k_1}}{2} \right). \] 

(35)

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