## SOFT MATTER

### DEFORMED HEISENBERG ALGEBRA IN THE THEORY OF LIQUID <sup>4</sup>He

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We propose a method to consider anharmonic oscillations of the density of a Bose fluid using a deformed Heisenberg algebra. The Hamiltonian of a Bose fluid consists of a main harmonic part and an anharmonic part which is usually treated perturbatively. We assume that only the former should be taken into account, whereas the anharmonic terms can be treated indirectly via a deformation of the commutation relations. For a deformation quadratic in the momentum, exact analytic expressions are found for the wave functions and the energy levels. The ground-state energy, elementary excitation spectrum, and the structure at zero temperature are calculated. A 'physical' value of the wave-vector-dependent deformation parameter is found by comparison of our results with 'observable' quantities. An 'effective' pair interaction energy of particles in a fluid is calculated.

#### 1. Introduction

The so-called quantum spaces have been introduced in [1] by deforming the Poisson brackets. Of a special interest are quantum spaces which possess a 'minimal length'. For instance, in the one-dimensional case, one considers a deformation of the quantum Poisson brackets for the coordinate and momentum operators,  $\hat{Q}$  and  $\hat{P}$ , which is quadratic in  $\hat{P}$  [2, 3]:

$$\widehat{Q}\widehat{P} - \widehat{P}\widehat{Q} = i\hbar(1+\beta\widehat{P}^2), \qquad (1.1)$$

where  $\beta$  is the deformation parameter. In this case, the minimal value of the variance is  $\langle (\Delta \hat{Q})^2 \rangle = \hbar^2 \beta$ , and the 'minimal length' is  $\sqrt{\langle (\Delta \hat{Q})^2 \rangle_{\min}} = \hbar \sqrt{\beta} \ (\beta \ge 0)$  provided  $\langle \hat{P} \rangle = 0, \ \langle \hat{Q} \rangle = 0.$ 

The generalizations to an arbitrary space dimension, as well as different types of deformations, have been investigated in numerous works, whose review would require a separate paper. Partially, such a review has been done in Refs. [4–7].

The electromagnetic field with deformation (1.1) has been investigated in Refs. [8–10]. After the standard decomposition of the field into a set of oscillators, the generalized coordinates and momentum are set to satisfy the deformed commutation relations (1.1) for each mode. The Casimir energy of such deformed fields has been studied in Ref. [9], and the intensity of the radiation and absorption of an electromagnetic field as a function of the deformation parameter  $\beta$  has been calculated in Ref. [10]. In these studies, it was assumed that  $\beta > 0$ . In fact,  $\beta$  can also be negative. Indeed, the Heisenberg inequality

$$\langle (\Delta \widehat{Q})^2 \rangle \geqslant \frac{\hbar^2}{4} \, \frac{[1 + \beta \langle (\Delta \widehat{P})^2 \rangle]^2}{\langle (\Delta \widehat{P})^2 \rangle}$$

minimizes its right-hand side when

$$\frac{1}{\langle (\Delta \widehat{P})^2 \rangle} \left( [\beta \langle (\Delta \widehat{P})^2 \rangle]^2 - 1 \right) = 0.$$

Now, excluding non-physical values  $\langle (\Delta \hat{P})^2 \rangle \to \infty$ ,  $\langle (\Delta \hat{Q})^2 \rangle \to \infty$  for  $\beta \neq 0$ , we have two roots: (i)  $\langle (\Delta \hat{P})^2 \rangle = 1/\beta$ , which has the minimal length  $\sqrt{\langle (\Delta \hat{Q})^2 \rangle_{\min}} = \hbar \sqrt{\beta}$ , and (ii)  $\langle (\Delta \hat{P})^2 \rangle = -1/\beta$  which gives (as in the undeformed case)  $\langle (\Delta \hat{Q})^2 \rangle \ge 0$  and the minimal length  $\langle (\Delta \hat{Q})^2 \rangle_{\min} = 0$ . Evidently,  $\beta \leq 0$  in this case. Therefore, negative deformation parameters do not lead to contradictory results, although they also do not lead to the Q space quantization.

The idea of the present work is the following. We consider only the main harmonic part of the Hamiltonian of

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a Bose fluid represented in terms of the collective variables which are the Fourier amplitudes of the density fluctuations. The 'anharmonism' of the Hamiltonian is taken into account by deforming the commutation relations for each fluctuation mode, as in Eq. (1.1).

Application of the Heisenberg algebra to many-body bosonic system has its own history. In particular, to study the low-temperature behavior of the <sup>4</sup>He specific heat, the so-called bosonic q-oscillators (q is the deformation parameter of the commutation relation of the creation and annihilation operators) have been used in Refs. [11, 12] to represent the phonon part of the spectrum cut at the third order in momentum. By fitting a few three parameters which characterize the deformation, a good agreement with experimental results for the heat capacity has been obtained. In Ref. [13], the qdeformation of thermodynamic properties of a q-boson gas has been studied, and it has been shown that, depending on q, one can have either a blurred  $\lambda$ -transition or a typical behavior for an ordinary Bose-gas. In Ref. [14], the virial expansion for the q-bosonic gas has been found; the coefficients of the virial expansion are presented as a power series in the deviation of the qparameter from q = 1, the value of the standard Heisenberg algebra.

#### 2. Hamiltonian of a Bose-Fluids in the Collective Variables Representation

Let us consider a system of spinless Bose particles of mass m described by the Cartesian coordinates  $\mathbf{r}_1, \ldots, \mathbf{r}_N$  which move in the D-dimensional space and occupy a volume V. The Hamiltonian of the system is

$$\widehat{H} = \sum_{j=1}^{N} \frac{\widehat{\mathbf{p}}_{j}^{2}}{2m} + \sum_{1 \leq i < j \leq N} \Phi(|\mathbf{r}_{i} - \mathbf{r}_{j}|), \qquad (2.1)$$

where the first term on the right-hand side is the kinetic energy operator, with  $\mathbf{p}_j = -i\hbar\nabla_j$  being the momentum operator, and the second term is the potential energy which consists of a sum of the pairwise interaction potentials  $\Phi(|\mathbf{r}_i - \mathbf{r}_j|)$ .

An effective method to study such a system is the socalled collective variables method, in which, instead of considering a set of Cartesian coordinates, one takes an *infinite* set of the quantities

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-i\mathbf{k}\mathbf{r}_j}, \quad \mathbf{k} \neq 0,$$
(2.2)

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which are the Fourier transforms of density fluctuations. In Eq. (2.2), the components of the wave-vector  $\mathbf{k}$  run over  $2\pi n/L$ , where  $n = 0, \pm 1, \pm 2, \ldots$ , and  $L^D = V$ .

This method was first introduced by Bohm [15] who limited the 'spectrum' of wave-vectors by a certain value  $k_c$  in order to choose the *ND* collective variables from the infinite set of  $\rho_{\mathbf{k}}$  which is the number of Cartesian coordinates in the original formulation.

Bogoliubov and Zubarev [16] proposed an alternative approach, in which the number of collective variables remains infinite, but the transformation to the collective variables is accompanied by the Jacobian transition. Hamiltonian (2.1) in the  $\rho_{\mathbf{k}}$ -representation consists of an infinite sum of harmonic oscillators, which describe density fluctuations of a Bose fluid, and anharmonic corrections:

$$\hat{H} = \sum_{\mathbf{k}\neq 0} \frac{\hbar^2 k^2}{2m} \left( -\frac{\partial^2}{\partial \rho_{\mathbf{k}} \partial \rho_{-\mathbf{k}}} + \frac{1}{4} \rho_{\mathbf{k}} \rho_{-\mathbf{k}} - \frac{1}{2} \right) + \frac{N(N-1)}{2V} \nu_0 + \frac{N}{2V} \sum_{\mathbf{k}\neq 0} \nu_k (\rho_{\mathbf{k}} \rho_{-\mathbf{k}} - 1) + \Delta \hat{H}, \quad (2.3)$$

$$\Delta \widehat{H} = \sum_{\substack{\mathbf{k}\neq0\\\mathbf{k}+\mathbf{k}'\neq0}} \sum_{\substack{\mathbf{k}'\neq0\\\mathbf{k}+\mathbf{k}'\neq0}} \frac{\hbar^2(\mathbf{k}\mathbf{k}')}{2m\sqrt{N}} \rho_{\mathbf{k}+\mathbf{k}'} \frac{\partial^2}{\partial \rho_{\mathbf{k}} \partial \rho_{\mathbf{k}'}} +$$

$$+\sum_{n\geq 3}\frac{(-)^n}{4n(n-1)(\sqrt{N})^{n-2}}>$$

$$\sum_{\substack{\mathbf{k}_1 \neq 0 \\ \mathbf{k}_1 + \mathbf{k}_2 + \dots + \mathbf{k}_n = 0}} \sum_{\substack{\mathbf{k}_n \neq 0 \\ \mathbf{k}_1 + \mathbf{k}_2 + \dots + \mathbf{k}_n = 0}} \frac{\hbar^2}{2m} (k_1^2 + \dots + k_n^2) \rho_{\mathbf{k}_1 \dots} \rho_{\mathbf{k}_n},$$
(2.4)

where  $\nu_k = \int e^{-i\mathbf{k}\mathbf{R}} \Phi(R) d\mathbf{R}$  is the Fourier transform of the interaction potential. The operator  $\Delta \hat{H}$ , whose form is omitted here (see, e.g., Ref. [17]), consists of all types of anharmonic oscillations starting from the third order and including the specific anharmonic terms linear in  $\rho_{\mathbf{k}}$ and quadratic in  $\partial/\partial \rho_{\mathbf{k}}$ .

The investigations of the method of collective variables itself and many-body Bose systems based on Hamiltonian (2.3) have been carried out in many works and by using different approaches. Most of them treat the operator  $\Delta \hat{H}$  perturbatively [16–25]. In this work, we propose an absolutely different approach which is described in the next section.

#### 3. Hamiltonian of a Bose-fluid in the Deformed Space

Note firstly that the collective variables  $\rho_{\mathbf{k}}$  are complex quantities:

$$\begin{aligned} \rho_{\mathbf{k}} &= \rho_{\mathbf{k}}^{c} - i\rho_{\mathbf{k}}^{s} \,, \\ \rho_{\mathbf{k}}^{c} &= \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \cos \mathbf{k} \mathbf{r}_{j} \,, \quad \rho_{\mathbf{k}}^{s} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \sin \mathbf{k} \mathbf{r}_{j} \,. \end{aligned}$$

Because  $\rho_{\mathbf{k}}^* = \rho_{-\mathbf{k}}$  (i.e.,  $\rho_{\mathbf{k}}^c = \rho_{-\mathbf{k}}^c$  and  $\rho_{\mathbf{k}}^s = -\rho_{-\mathbf{k}}$ ), some variables with the wave-vector  $\mathbf{k}$  have the same (up to a sign) values as variables with the wave-vector  $-\mathbf{k}$ . This means that the independent variables are  $\rho_{\mathbf{k}}$ , but the wave-vector space is limited to the half-space.

Taking this into account, we present the harmonic part of Hamiltonian (2.3) via the generalized coordinates and momenta as follows:

$$\hat{H} = \sum_{\mu=c,s} \sum_{\mathbf{k}\neq 0} \left( \frac{\hat{P}_{\mathbf{k},\mu}^2}{2m_k} + \frac{m_k \omega_k^2 \hat{Q}_{\mathbf{k},\mu}^2}{2} \right) + \frac{N(N-1)}{2V} \nu_0 - \sum_{\mathbf{k}\neq 0} \left( \frac{\hbar^2 k^2}{4m} + \frac{N}{2V} \nu_k \right),$$
(3.1)

where the generalized momentum operator  $\widehat{P}_{\mathbf{k},\mu}$  is conjugated to the generalized coordinate  $\widehat{Q}_{\mathbf{k},\mu}$ ; in the  $\rho_{\mathbf{k}}$  representation,  $\widehat{Q}_{\mathbf{k},c} = \rho_{\mathbf{k}}^c$  and  $\widehat{Q}_{\mathbf{k},s} = \rho_{\mathbf{k}}^s$ . The prime at the sum means that the sum is limited to the half-space. By comparing Eqs. (3.1) and (2.3), we find

$$m_k = \frac{2m}{k^2}, \quad \omega_k = \frac{\hbar k^2}{2m} \alpha_k, \quad \alpha_k = \sqrt{1 + \frac{2N}{V} \nu_k / \frac{\hbar^2 k^2}{2m}}.$$
(3.2)

We note that the operator  $\widehat{P}_{\mathbf{k},\mu}$  has the dimension of action  $\hbar$ , while  $\widehat{Q}_{\mathbf{k},\mu}$  is dimensionless.

We now proceed as follows. Instead of considering the anharmonic part  $\Delta \hat{H}$  of (2.1) directly, we take it into account indirectly by deforming the commutation relations. Thus, we consider only the harmonic Hamiltonian (3.1), while the anharmonic part  $\Delta \hat{H}$  will follow from a deformation of the Heisenberg algebra of the generalized coordinates and momenta,

$$\widehat{Q}_{\mathbf{k},\mu}\widehat{P}_{\mathbf{k},\mu} - \widehat{P}_{\mathbf{k},\mu}\widehat{Q}_{\mathbf{k},\mu} = i\hbar \big(1 + \beta_k \widehat{P}_{\mathbf{k},\mu}^2/\hbar^2\big), \qquad (3.3)$$

where the dimensionless deformation parameter  $\beta_k$  depends on the absolute value of the wave-vector,  $k = |\mathbf{k}|$ ; all operators  $\hat{Q}_{\mathbf{k},\mu}$  and  $\hat{P}_{\mathbf{k}',\mu'}$  with different indices commute.

To summarize, we have a 'simplified' Hamiltonian, by making it harmonic, and sent all 'inconveniences' into the commutations relations by deforming them. By doing so, we do not follow the Ziman advice [26] who stated that if one has to make approximation, it is better to omit some terms in the Hamiltonian rather than to touch mysterious commutation relations.

In what follows, we skip the question of the form of the  $\hat{P}_{\mathbf{k},\mu}$  operator in the  $\rho_{\mathbf{k}}$  representation. We assume instead that Hamiltonian (3.1) with the commutation relations (3.3) describes the properties of a Bose fluid as effectively and as well as the original Hamiltonian (2.3) provided the deformation parameter  $\beta_k$  is properly chosen. Obviously, we do not expect the two Hamiltonians to give the completely identical description of the Bose system.

# 4. Energy Levels and Wave Functions of a Bose Fluid

We introduce new canonically conjugated operators  $\hat{q}_{\mathbf{k},\mu}$ ,  $\hat{p}_{\mathbf{k},\mu}$  obeying the standard Heisenberg algebra:

$$\widehat{Q}_{\mathbf{k},\mu} = \widehat{q}_{\mathbf{k},\mu}, \quad \widehat{P}_{\mathbf{k},\mu} = \frac{\hbar}{\sqrt{\beta}} \tan\left(\frac{\widehat{p}_{\mathbf{k},\mu}\sqrt{\beta}_k}{\hbar}\right),$$
$$\widehat{q}_{\mathbf{k},\mu}\widehat{p}_{\mathbf{k},\mu} - \widehat{p}_{\mathbf{k},\mu}\widehat{q}_{\mathbf{k},\mu} = i\hbar.$$
(4.1)

Hamiltonian (3.1) in terms of the new operators takes the form

$$+\frac{N(N-1)}{2V}\nu_0 - \sum_{\mathbf{k}\neq 0} \left(\frac{\hbar^2 k^2}{4m} + \frac{N}{2V}\nu_k\right).$$
(4.2)

The eigenfunctions and eigenvalues of this operator are known [9, 10, 17]. The energy levels can therefore be readily obtained as

 $E_{\ldots,\,n_{\mathbf{k},c},\,\ldots;\,\ldots,\,n_{\mathbf{k},s},\,\ldots} =$ 

=

$$=\sum_{\mu=c,s}\sum_{\mathbf{k}\neq 0} \frac{\hbar^2 k^2}{2m} \alpha_k \left[ \left( n_{\mathbf{k},\mu} + \frac{1}{2} \right) \sqrt{1 + \left( \frac{\beta_k \alpha_k}{2} \right)^2} + \right]$$

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$$+\frac{\beta_k \alpha_k}{2} \left( n_{\mathbf{k},\mu}^2 + n_{\mathbf{k},\mu} + \frac{1}{2} \right) \right] + \frac{N(N-1)}{2V} \nu_0 -$$

$$-\sum_{\mathbf{k}\neq 0} \left( \frac{\hbar^{2} \kappa^{2}}{4m} + \frac{N}{2V} \nu_{k} \right), \qquad (4.3)$$

where the quantum numbers  $n_{\mathbf{k},\mu} = 0, 1, 2, \dots, \mu = c, s$ .

The wavefunctions in the momentum representation  $\hat{p}_{\mathbf{k},\mu} = p_{\mathbf{k},\mu}, \, \hat{q}_{\mathbf{k},\mu} = i\hbar\partial/\partial p_{\mathbf{k},\mu}$ :

$$\psi_{\ldots,n_{\mathbf{k},c},\ldots;\ldots,n_{\mathbf{k},s},\ldots}(\ldots,p_{\mathbf{k},\mu},\ldots) =$$

$$=\prod_{\mathbf{k}\neq 0}'\prod_{\mu=c,s}\psi_{n_{\mathbf{k},\mu}}(p_{\mathbf{k},\mu}),\qquad(4.4)$$

$$\psi_n(p_{\mathbf{k},\mu}) = \frac{\beta_k^{1/4}}{\sqrt{\hbar}} \sqrt{\frac{\Gamma(\nu+n+1)\Gamma(n+2\nu)}{n!\Gamma(1/2)\Gamma(\nu+n+1/2)\Gamma(2\nu+2n)}} \times \left(-\frac{d}{dp} + \nu \tan p\right) \cdots \left(-\frac{d}{dp} + (\nu+n-1)\tan p\right) \cos^{\nu+n} p,$$
(4.5)

where

$$\nu = \frac{1}{2} + \frac{1}{\beta_k \alpha_k} \sqrt{1 + \left(\frac{\beta_k \alpha_k}{2}\right)^2},$$

$$p = p_{\mathbf{k},\mu} \sqrt{\beta_k} / \hbar, \quad n = n_{\mathbf{k},\mu}.$$
(4.6)

Note that the wavefunctions are orthonormalized:

$$\int_{-\pi\hbar/(2\sqrt{\beta_k})}^{\pi\hbar/(2\sqrt{\beta_k})} \psi_{n'}(p_{\mathbf{k},\mu})\psi_n(p_{\mathbf{k},\mu}) \, dp_{\mathbf{k},\mu} = \delta_{n',n} \,. \tag{4.7}$$

The ground-state wave function and the wave function of the first excited state are

$$\psi_0(p_{\mathbf{k},\mu}) = \frac{\beta_k^{1/4}}{\sqrt{\hbar}} \sqrt{\frac{\Gamma(\nu+1)}{\Gamma(1/2)\Gamma(\nu+1/2)}} \cos^{\nu} p ,$$
  
$$\psi_1(p_{\mathbf{k},\mu}) = \frac{\beta_k^{1/4}}{\sqrt{\hbar}} \sqrt{\frac{2\Gamma(\nu+2)}{\Gamma(1/2)\Gamma(\nu+1/2)}} \cos^{\nu} p \sin p . \quad (4.8)$$

We emphasize that the eigenvalues are quadratic in the quantum number  $n_{\mathbf{k},\mu}$ , as it is in the theory of an

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anharmonic oscillator treated perturbatively to the order of  $\hbar^2$  [17, 27].

In the case of no deformation  $(\beta_k \to 0)$ , the quantity  $\nu \to 1/\beta_k \alpha_k \to \infty$ , and we obtain

$$\cos^{\nu} p \mathop{=}_{\beta_k \to 0} \left( 1 - \frac{p_{\mathbf{k},\mu}^2 \beta_k}{2\hbar^2} + \cdots \right)^{1/\beta_k \alpha_k} \mathop{=}_{\beta_k \to 0} e^{-p_{\mathbf{k},\mu}^2/2\hbar^2 \alpha_k} \,.$$

Using the asymptotic expression  $\Gamma(\nu + a) \sim \sqrt{2\pi}e^{-\nu}\nu^{\nu+a-1/2}, \nu \to \infty$ , Eq. (4.5) yields the wave function of the harmonic oscillator in the momentum representation (as it should be):

$$\psi_{n_{\mathbf{k},\mu}}(p_{\mathbf{k},\mu}) = \left(\frac{1}{\pi\hbar^2 \alpha_k}\right)^{1/4} \times \frac{1}{\sqrt{n_{\mathbf{k},\mu}! 2^{n_{\mathbf{k},\mu}}}} \left(-\frac{d}{d\eta} + \eta\right)^{n_{\mathbf{k},\mu}} e^{-\eta^2/2}, \qquad (4.9)$$

where  $\eta = p_{\mathbf{k},\mu}/\hbar\sqrt{\alpha_k}$ . Note also that the limits of integration over  $p_{\mathbf{k},\mu}$  in Eq. (4.7) which are  $\left(-\pi\hbar/(2\sqrt{\beta_k}), \pi\hbar/(2\sqrt{\beta_k})\right)$  go to  $(-\infty, +\infty)$  as the deformation parameter  $\beta_k \to 0$ .

As we have mentioned in Introduction, the deformation parameter can be positive or negative. During the course of calculations, however, we will encounter nonanalytic expressions of the form  $\beta_k^{1/2}$ ,  $\beta_k^{1/4}$ , etc. which are complex-valued for negative  $\beta_k$ . Hence, the wave functions are functions of the imaginary argument. In order to avoid these complications, we assume from now on that  $\beta_k > 0$ ; we relax this assumption in the final results, in particular, for observable quantities.

The wave functions (up to a normalization constant) for negative deformation parameters  $\beta_k = -|\beta_k|$  are obtained from (4.5) by formally changing  $\nu \to -\nu$ . In particular,

$$\psi_0(p_{\mathbf{k},\mu}) = \frac{|\beta_k|^{1/4}}{\sqrt{\hbar}} \sqrt{\frac{\Gamma(\nu+1/2)}{\Gamma(1/2)\Gamma(\nu)}} \frac{1}{\cosh^{\nu} p} \,,$$

$$\psi_1(p_{\mathbf{k},\mu}) = \frac{|\beta_k|^{1/4}}{\sqrt{\hbar}} \sqrt{\frac{2\Gamma(\nu+1/2)}{\Gamma(1/2)\Gamma(\nu-1)}} \frac{\sinh p}{\cosh^\nu p} \ . \tag{4.10}$$

Here, 
$$p = p_{\mathbf{k},\mu} \sqrt{|\beta_k|} / \hbar$$
,  
 $\nu = -\frac{1}{2} + \frac{1}{\alpha_k |\beta_k|} \sqrt{1 + \left(\frac{\alpha_k \beta_k}{2}\right)^2}$ , (4.11)

the momentum  $-\infty < p_{\mathbf{k},\mu} < \infty$ , and the energy spectrum is again given by Eq. (4.3) but is limited from above,  $n_{\mathbf{k},\mu} < \nu$ .

#### 5. Ground-State Energy

The ground-state energy follows from Eq. (4.3) by setting all quantum numbers  $n_{\mathbf{k},\mu} = 0$ ; we get, after simple calculations,

$$E_{0} = \frac{N(N-1)}{2V}\nu_{0} - \sum_{\mathbf{k}\neq 0} \frac{\hbar^{2}k^{2}}{8m} (\alpha_{k}-1)^{2} + \sum_{\mathbf{k}\neq 0} \frac{\hbar^{2}k^{2}}{4m} \alpha_{k} \left(\sqrt{1 + \left(\frac{\beta_{k}\alpha_{k}}{2}\right)^{2}} + \frac{\beta_{k}\alpha_{k}}{2} - 1\right).$$
(5.1)

In Eq. (5.1), the first two terms reproduce the groundstate energy obtained within the Bogoliubov approximation [28], and the last term, which is due to anharmonic oscillations, is negative if  $\beta_k < 0$ . Such a decrease of the ground-state energy of liquid <sup>4</sup>He is also obtained if one treats the anharmonic part  $\Delta \hat{H}$  of Hamiltonian (2.3), by directly using perturbation theory [25].

Below, we present the results of numerical calculations of the ground-state energy  $E_0$  for liquid <sup>4</sup>He using Eq. (5.1). The best 'test' for expression (5.1), as well as for other results, is to apply it to a model possessing an exact analytical solution or allowing a correct perturbative treatment. The main question for such a comparison is to fix the deformation parameter  $\beta_k$ .

#### 6. Elementary Excitation Spectrum

Let us calculate the energy of the first excited state with the wave vector  $\mathbf{q}$ , i.e., the quantum number  $n_{\mathbf{q},c} = 1$ while  $n_{\mathbf{k},\mu} = 0$  for  $\mathbf{k} \neq \mathbf{q}, \mu \neq c$ ; or  $n_{\mathbf{q},s} = 1$  and  $n_{\mathbf{k},\mu} = 0$ for  $\mathbf{k} \neq \mathbf{q}, \mu \neq s$ . Using Eq. (4.3), we get

$$E_{\dots,0,n_{\mathbf{q},c}=1,0,\dots;\dots,0,\dots} =$$

$$E_{\dots,\,0,\,\dots;\,\dots,\,0,\,n_{\mathbf{q},\,s}=1,\,0,\,\dots;\,\dots,\,0,\,\dots}=E_0+E_q\,,$$

where the elementary excitation spectrum

$$E_q = \frac{\hbar^2 q^2}{2m} \alpha_q \left[ \sqrt{1 + \left(\frac{\beta_q \alpha_q}{2}\right)^2 + \beta_q \alpha_q} \right].$$
(6.1)

As one can see, in the case of no deformation, this expression reduces to the elementary excitation spectrum due to Bogoliubov [28]:

$$E_q^B = \frac{\hbar^2 q^2}{2m} \alpha_q \,. \tag{6.2}$$

Equation (6.1) is the exact solution of the Schrödinger equation with Hamiltonian (4.2). Obviously, one cannot obtain here such a phenomenon as the decay of the elementary excitation spectrum, because there are no terms in Hamiltonian (4.2) describing the scattering of elementary excitations and their decay. The fact that the elementary excitations fall into two parts causes the liquid <sup>4</sup>He spectrum to have an end point at  $k \simeq 2.7$  Å<sup>-1</sup>. Our formula Eq. (6.1), as well as Bogoliubov's equation (6.2), reduces to the free particle spectrum  $\hbar^2 k^2/2m$  because, as we shall see further, the deformation parameter  $\beta_k \to 0$  as  $k \to \infty$ .

#### 7. Structure Factor in the Ground State

By definition, the structure factor (of a fluid) is the average of squared density fluctuations:

$$S_k = \langle |\rho_{\mathbf{k}}|^2 \rangle \,. \tag{7.1}$$

Let us calculate this average using the wave function of the ground state, Eq. (4.8):

$$S_{k} = \langle \widehat{Q}_{\mathbf{k},c}^{2} + \widehat{Q}_{\mathbf{k},s}^{2} \rangle = -\hbar^{2} \left\langle \frac{d^{2}}{dp_{\mathbf{k},c}^{2}} + \frac{d^{2}}{dp_{\mathbf{k},s}^{2}} \right\rangle =$$

$$\pi \hbar / (2\sqrt{\beta_{k}})$$

$$d^{2}a/\mu (m_{k})$$

$$= -2\hbar^2 \int_{-\pi\hbar/(2\sqrt{\beta_k})}^{+\pi\pi} \psi_0(p_{\mathbf{k},\mu}) \frac{d^2\psi_0(p_{\mathbf{k},\mu})}{dp_{\mathbf{k},\mu}^2} dp_{\mathbf{k},\mu} =$$

=

$$= -2\hbar\sqrt{\beta} \int_{-\pi/2}^{\pi/2} \psi_0 \frac{d^2\psi_0}{dp^2} dp \,. \tag{7.2}$$

By evaluation of the last integral, we get

$$S_k = \frac{\beta_k \nu^2}{\nu - 1/2} \,, \tag{7.3}$$

and, by taking Eq. (4.6) into account,

$$S_{k} = \frac{1}{\alpha_{k}} \frac{\left[\sqrt{1 + (\beta_{k}\alpha_{k}/2)^{2}} + \beta_{k}\alpha_{k}/2\right]^{2}}{\sqrt{1 + (\beta_{k}\alpha_{k}/2)^{2}}}.$$
(7.4)

At  $\beta_k = 0$ , we obtain the Bogoliubov–Zubarev results,  $S_k = 1/\alpha_k$  [16].

The structure factor can also be calculated in a different way, by taking the variational derivative of the free

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energy (which gives the ground-state energy  $E_0$  at zero temperature) with respect to  $\nu_k$ :

$$S_k - 1 = \frac{2V}{N} \frac{\delta E_0}{\delta \nu_k} \,.$$

By using Eq. (5.1) for  $E_0$ , we get expression (7.4) after simple transformations.

Finally, we note that the structure factor  $S_k$  is an analytic function of the deformation parameter  $\beta_k$  which can be positive or negative.

#### 8. Deformation Parameter

The deformation parameter  $\beta_k$  for liquid <sup>4</sup>He can be estimated using Eqs. (6.1) and (7.4) and experimental values for  $E_k$  and/or  $S_k$ . If the interaction potential  $\nu_k$ is known, one can use either Eq. (7.4) with the structure factor from the diffraction experiments [29–32] or Eq. (6.1) along with the elementary excitation spectrum  $E_q$  measured in the scattering experiments [33, 34].

We consider Eqs. (6.1) and (7.4) as a system of two equations for two unknowns  $\alpha_k$  and  $\beta_k$ . Equation (6.1) yields

$$\frac{\beta_k \alpha_k}{2} = \frac{2}{3} \eta_k - \sqrt{\frac{1}{3} + \left(\frac{\eta_k}{3}\right)^2},$$
(8.1)

where

$$\eta_k = E_k / \alpha_k \frac{\hbar^2 k^2}{2m} \,. \tag{8.2}$$

By substituting Eq. (8.1) into Eq. (7.4), one obtains, after a simple algebra,

$$\frac{E_k}{\eta_k \hbar^2 k^2 / (2mS_k)} - \eta_k = \frac{\left[\frac{2}{3}\eta_k - \sqrt{\frac{1}{3} + \left(\frac{\eta_k}{3}\right)^2}\right]^2}{\sqrt{1 + \left[\frac{2}{3}\eta_k - \sqrt{\frac{1}{3} + \left(\frac{\eta_k}{3}\right)^2}\right]^2}}.$$
(8.3)

We have got an equation for the unknown  $\eta_k$  provided the elementary excitation spectrum  $E_k$  and the structure factor  $S_k$  are known (from experiments). Now, using Eq. (8.2), one finds  $\alpha_k$  and, hence, using Eq. (3.2), also the Fourier transform of the interaction potential  $\nu_k$ . Having  $\alpha_k$  and  $\eta_k$ , one readily calculates  $\beta_k$  from Eq. (8.1).

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A simple analysis of Eq. (8.3) shows that, for large wave vectors, for which  $E_k \to \hbar^2 k^2/2m$ ,  $S_k \to 1$ , and the quantity  $\eta_k \to 1$ . Then, from Eq. (8.1) one concludes that, because  $\alpha_k \to 1$ , the deformation parameter  $\beta_k \to 0$  as  $k \to \infty$ .

For small wave-vectors,  $k \to 0$ , when  $E_k = \hbar kc$ , and  $S_k = \hbar k/2mc$ , where c is the sound velocity in a liquid, the quantity  $\eta_k \to 1$ . Hence, also the deformation parameter  $\beta_k \to 0$  as  $k \to 0$ . Furthermore, by using Eq. (8.2), we obtain the leading term at small wave-vectors:

$$\alpha_k = \frac{2mc}{\hbar k}, \quad k \to 0.$$
(8.4)

From Eqs. (8.4) and (3.2), one easily finds the zero component of the Fourier transform of the interaction potential

$$\nu_0 = \frac{mc^2}{\rho} \,. \tag{8.5}$$

Let us look at the asymptotic behavior of  $\beta_k$  as  $k \to 0$ in more details. As we know [20, 30, 35, 36], the second terms of the small k expansions of the spectrum  $E_k$  and of the structure factor  $S_k$  are proportional to  $k^3$ . In particular, due to this contribution,  $E_k$  turns upward and  $S_k$  turns downward:

$$E_{k} = \hbar kc \left[ 1 + \gamma_{E} \left( \frac{\hbar k}{mc} \right)^{2} + \cdots \right],$$
$$S_{k} = \frac{\hbar k}{2mc} \left[ 1 - \gamma_{S} \left( \frac{\hbar k}{mc} \right)^{2} + \cdots \right], \quad k \to 0,$$

where  $\gamma_E \simeq 1$  [34] and  $\gamma_S \simeq 1.42$  [30]. Now, it follows from Eq. (8.3) that  $\eta_k$  goes to 1 as  $k^2$ :

$$\eta_k = 1 - \frac{\gamma_S - \gamma_E}{2} \left(\frac{\hbar k}{mc}\right)^2 + \cdots, \quad k \to 0.$$

Finally, using Eq. (8.1), we find

$$\beta_k = -\frac{\gamma_S - \gamma_E}{4} \left(\frac{\hbar k}{mc}\right)^3, \quad k \to 0.$$

Evidently, this also follows directly from Eq. (6.1), because

$$\alpha_k = \frac{2mc}{\hbar k} \left[ 1 + \frac{\gamma_E + \gamma_S}{2} \left( \frac{\hbar k}{mc} \right)^2 + \cdots \right], \quad k \to 0.$$

We emphasize that expressions (8.4) and (8.5) coincide with the corresponding expressions of the Bogoliubov theory [28], because the deformation parameter  $\beta_k$  goes to zero at small wave-vectors k.

Finally, it is worth to note the following. Assume that Eq. (8.3) has a solution also for intermediate values of the wave vector k. This means that the proposed method to calculate anharmonic contributions by deforming the Heisenberg commutation relations in the theory of liquid <sup>4</sup>He is not contradictory.

#### 9. Conclusions

We conclude that the proposed method to study a Bose fluid by using the approximate Hamiltonian (3.1) together with the deformed commutation relations for the coordinates and momenta (3.3), instead of the model Hamiltonian (2.3), is correct.

One can also consider other deformations of the Heisenberg algebra. For instance, instead of  $\beta_k \hat{P}_{\mathbf{k},\mu}^2/\hbar^2$ in Eq. (3.3), we can use  $\beta'_k \hat{Q}_{\mathbf{k},\mu}^2$ . However, by a simple transformation,  $1/m_k \rightarrow m_k \omega_k^2$  and vice versa, we obtain exactly the same results except that  $\beta_k \alpha_k$  changes to  $\beta'_k/\alpha_k$ ; in other words, it is only a matter of different notations. There exist, of course, more complicated deformations such as, for instance, a linear combination  $(\beta_k \hat{P}_{\mathbf{k},\mu}^2/\hbar^2 + \beta'_k \hat{Q}_{\mathbf{k},\mu}^2)$  with two deformation parameters. The main message is, however, that one *can* account for anharmonic contributions by deforming the commutation relations, and that such an approach is selfconsistent.

It would be interesting to investigate other problems by using this method such as, for instance, the motion of a <sup>3</sup>He impurity in liquid <sup>4</sup>He or the motion of a polaron in an anharmonic crystal. It is also interesting to test the present approach on the exactly solvable model of a one-dimensional Bosegas with the  $\delta$ -function-like repulsive potential [37]. We will present such investigations in separate papers.

This article has been written on the special occasion of the 100th anniversary of the famous scientist Mykola Bogoliubov, whose brilliant and original ideas demonstrate the power and universalism of the mathematics applied to studies of complex and subtle physical phenomena. The author remembers, with the great pleasure, Bogoliubov's seminar and discussions in the Bogoliubov group on the manybody Bose systems which took place almost 40 years ago.

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#### ДЕФОРМОВАНА АЛГЕБРА ГАЙЗЕНБЕРГА В ТЕОРІЇ РІДКОГО <sup>4</sup>Не

І.О. Вакарчук

#### Резюме

Запропоновано метод врахування ангармонізмів коливань густини бозе-рідини через деформацію алгебри Гайзенберга. Гамільтоніан бозе-рідини в зображенні колективних координат має головну частину, яка описує гармонічні коливання густини і частину, що описує ангармонізми всіх порядків, котру враховують за допомогою стандартної теорії збурень. Припускаємо, що в гамільтоніані можна брати до уваги лише головну частину, а "незручні" ангармонічні доданки врахувати опосередковано через деформацію переставних співвідношень між узагальненими координатами та імпульсами. Для деформації квадратичної за імпульсами знайдено точні вирази для енергетичних рівнів і хвильових функцій. Обчислено енергію основного стану, спектр елементарних збуджень, структурний фактор при температурі абсолютного нуля. Параметр деформації, залежний від хвильового вектора, знайдено з рівняння узгодження розрахованих фізичних величин зі спостережуваними. Обчислено потенціальну енергію двочастинкової взаємодії атомів рілини.