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Short-wave excitations in non-local Gross-Pitaevskii model

Research Article

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Abstract: We show that a non-local form of the Gross-Pitaevskii equation describes not only long-wave excitations, but also the short-wave ones in Bose-condensate systems. At certain parameter values, the excitation spectrum mimics the Landau spectrum of quasi-particle excitations in superfluid helium with roton minimum. The excitation wavelength, at which the roton minimum exists, is close to the inter-particle interaction range. We determine how the roton gap and the effective roton mass depend on the interaction potential parameters, and show that the existence domain of the spectrum with a roton minimum is reduced if one accounts for an inter-particle attraction.

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1. Introduction

The accumulation of a macroscopic number of particles in the ground state at low temperature was predicted by Einstein in his papers on the properties of the ideal quantum gas [1] on the grounds of the approach developed by Bose [2]. The Bose-Einstein condensation (BEC) effect was used by London [3] and Tisza [4] to describe the superfluidity of liquid helium, discovered by Kapitsa [5] and Allen [6]. Later on, Landau developed a theory of superfluidity [7, 8] which did not depend on BEC. Nevertheless, the relation between superfluidity and BEC is not understood yet. The existence of BEC in the superfluid phase of helium was proved by inelastic neutron scattering experiments [9]. There is also a theoretical consideration of the Bose particle condensation due to the experimental discovery of BEC in the atomic gases [10–12] at the end of the last century. The current state of the problem is reviewed in [13, 14].

Landau's theory of liquid helium superfluidity is based on the form of the quasiparticle excitation spectrum, which was postulated in his approach [7, 8]. Landau assumed that at small momenta the spectrum is sound-like and the energy of such a phonon excitation is linear in momentum. At higher momenta, of order $p_0 \approx \frac{\hbar}{a_0}$, where a_0 is an interatomic scale, Landau found that the spectrum has a minimum and the excitations with momenta close to p_0 are called rotons. The shape of the energy spectrum of the elementary excitations in a multiparticle Bose system was first obtained in a microscopic consideration

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by Bogolyubov [15] using a weakly non-ideal gas model. Later on, the spectral structures of systems of interacting particles were studied by e.g. [16–21]. Bogolyubov [15] and other authors have shown that, due to the presence of the condensate, the excitation spectrum of a system of interacting Bose particles with small momenta is analogous to the spectrum postulated by Landau. Paper [15], and many others on Bose system theory, assumes that the particle interaction is point-like and can be described by means of a single interaction constant. In order to preserve the stability of the system, this constant is made positive, so that the interaction is repulsive. In this model the elementary excitation energy monotonically increases with momentum and the roton minimum is absent. The actual interaction between particles is, however, complicated and cannot be described with only one parameter. Usually (e.g. in helium) the long-distance interaction is the Van der Waals attraction and at short distances one observes a very strong repulsion leading to momentum dependence of the matrix element of the potential and, consequently, the shape of the quasiparticle spectrum becomes much more complicated than that for point-like interaction. One can choose such a momentum dependence of the matrix element that the Landau spectrum with the roton minimum is reproduced qualitatively [22].

An alternative description of the weakly interacting, low-temperature bosons is given by the equation obtained by Gross and Pitaevskii [23–25]. This equation describes the particle dynamics in BEC. In particular, it gives a framework for studying the condensate oscillations and obtaining the elementary excitation spectra. Knowledge of the latter is necessary in order to obtain the thermodynamic functions of the system.

It is often assumed that the condensate wave function $\Phi(r, t)$ varies slowly over the distances of order r_0, which is the range of the inter-atomic interaction potential $U(r)$. This condition allows to express the Gross-Pitaevskii (GP) equation as a non-linear differential equation.

Unfortunately, in such a case, the imposed assumption restricts consideration to the long-wave excitations in BEC. Under these circumstances, it is possible to derive the Bogolyubov sound (long-wave) spectrum of the excitations, in which the energy increases monotonically with momentum [25]. Meanwhile, a superfluid system can also have some well-defined long-lived short-wave excitations with de Broglie wavelengths on the order of the inter-particle distance (or interaction potential range) [26]. It was pointed out that in the superfluid helium the rotons are the excitations of this type. Taking into account the non-local effects in the GP equation, one can qualitatively describe also the maxon-roton part of the dispersion curve observed for superfluid helium.

The GP equation with non-local interactions has been used before, e.g. in papers [27–34]. In Ref. [27] the non-local GP equation was applied to study the stability of the interacting Bose-Einstein condensate particles; in Ref. [28] it was used to study the vortex excitations in these systems. The effects of small non-locality in the GP equation and the analysis of the nanoscale structure formation using this approach was carried in Refs. [29, 30]. The roton-maxon spectrum in the atomic systems with BEC and possessing the long distance interactions due to dipole-dipole forces was considered in [31, 33]. In [32] the quasi-local GP equation was applied for studies of BEC in gases with pairwise attractive interactions. It was proved that the collapse is absent in this model. The modulational instability of the background in case of a one-dimentional non-local GP equation was studied in [34]. It was found that a modulationally stable background may exist and dark-soliton solutions can be found. The stability was verified through computation of the full spectrum of the eigenvalues for small perturbations. This result is important in context of our research.

In this paper we show that the non-local form of the GP equation can describe the short-wave excitations in a Bose-system with condensate, as well as the long-wave excitations, even when the dipole-dipole forces are absent, provided that we release the constraint on the spatial change scale of the macroscopic wave function. At certain values of the interaction potential parameters, the excitation spectrum mimics the Landau spectrum for the quasi-particles in the superfluid helium which has the roton minimum. We consider the following two cases:

- the repulsion at finite interaction range ("semi-transparent sphere model");
- the Van der Waals attraction of particles at long distances, in addition to the repulsion at short distances.

We study the influence of the inter-particle interaction on the dispersion curve in the short-wave domain to show that the inter-particle attraction narrows down the existence domain of a stable spectrum, i.e. inter-particle interaction reduces the range of parameters where a spectrum with roton minimum may exist.

2. Non-local form of Gross-Pitaevskii equation

A system of many Bose particles in the second quantization picture is described, accounting for pairwise interactions, by the Hamiltonian

$$H = \int d\mathbf{r}\hat{\psi}^{+}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\Delta\right)\hat{\psi}(\mathbf{r}) + \frac{1}{2}\iint d\mathbf{r}d\mathbf{r}'\hat{\psi}^{+}(\mathbf{r})\hat{\psi}^{+}(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}). \quad (1)$$

The equation of motion for the field operator in the Heisenberg picture reads

$$i\hbar\frac{\partial\hat{\psi}(\mathbf{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\hat{\psi}(\mathbf{r},t) + \psi(\mathbf{r},t)\int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')\left|\hat{\psi}(\mathbf{r}',t)\right|^2. \quad (2)$$

Due to a large number of particles in the condensate, one may consider the operator $\hat{\psi}(\mathbf{r},t)$ in Eq. (2) as a non-operator function $\psi(\mathbf{r},t)$. Further, it is convenient to define a function $\Phi(\mathbf{r},t)$:

$$\psi(\mathbf{r},t) = \Phi(\mathbf{r},t)\exp(-i\mu t), \quad (3)$$

where μ is the equilibrium chemical potential[1]. Then the equation for Φ reads

$$i\hbar\frac{\partial\Phi(r,t)}{\partial t} = -\left(\frac{\hbar^2}{2m}\Delta + \mu\right)\Phi(r,t) + \Phi(r,t)\int dr'U(r-r')\left|\Phi(r',t)\right|^2. \quad (4)$$

The value of the the equilibrium chemical potential is determined by the equilibrium state of the system

$$\mu = \int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')\left|\Phi_0(\mathbf{r}')\right|^2, \quad (5)$$

with $\Phi_0(\mathbf{r})$ the equilibrium value of the condensate wave function. Taking into account that the equilibrium condensate density in absence of external fields $n_0 = |\Phi_0(\mathbf{r})|^2$ does not depend on the coordinate, one can express Eq. (4) as

$$i\hbar\frac{\partial\Phi(\mathbf{r},t)}{\partial t} = -\left(\frac{\hbar^2}{2m}\Delta + n_0U_0\right)\Phi(\mathbf{r},t) + \Phi(\mathbf{r},t)\int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')\left|\Phi(\mathbf{r}',t)\right|^2, \quad (6)$$

where $U_0 = \int d\mathbf{r}'U(\mathbf{r}-\mathbf{r}')$. We call Eq. (6) the *non-local Gross-Pitaevskii equation* (NGP). If one is interested only in the long-wave perturbations, and assumes that the characteristic spatial scale of the condensate wave function is much greater than the inter-particle interaction potential range, then the square of the wave function can be taken out of the integral in the right hand side of Eq. (6). The equation then takes the form

$$i\hbar\frac{\partial\Phi(\mathbf{r},t)}{\partial t} = -\left(\frac{\hbar^2}{2m}\Delta + n_0U_0\right)\Phi(\mathbf{r},t) + U_0\Phi(\mathbf{r},t)\left|\Phi(\mathbf{r},t)\right|^2. \quad (7)$$

This is the usual way to apply the GP equation. Small oscillations described by Eq. (7) have the dispersion law (for derivation see [25])

$$\varepsilon_k = \sqrt{\left(\frac{\hbar^2k^2}{2m}\right)\left(2U_0n_0 + \frac{\hbar^2k^2}{2m}\right)}, \quad (8)$$

where k is the wave number. The dispersion law (8) was derived by Bogolyubov [15] in a different approach with the use of the second quantization method. The excitation energy due to Eq. (8) depends linearly on the wave number for small k and monotonically increases with k, approaching the free particle dispersion law. One should stress that spectrum (8) is valid only for the long-wave oscillations due to the approximation used for deriving Eq. (7).

Meanwhile, the derivation of the GP equation in form (6) does not assume that the excitations are of the long-wave type. Thus, Eq. (6) is also valid for description of the excitations which wave length is of order of the inter-particle interaction. This equation can be applied in order to study the dispersion law of the collective excitations of a Bose condensate in a short-wave spectral domain and to analyze the spatial behavior of the condensate wave function at distances comparable to the inter-atomic potential range.

3. Hydrodynamic form of non-local Gross-Pitaevskii equation

Equation (6) can be rewritten in the form of hydrodynamic equations if the condensate wave function is taken

[1] Any macroscopic wave function of a Bose system can be expressed in form (3) by factoring out the time-dependent term with the equilibrium chemical potential μ. In this case the wave function Φ has time dependence only for the non-equilibrium states.

as $\Phi = \eta e^{i\varphi}$, where φ, η are the phase and the absolute value of the condensate wave function and $\eta^2 = n$ is the particle number density in the condensate.
Taking the above into account, Eq. (7) leads to

$$\frac{\partial n}{\partial t} + \nabla(n\mathbf{v}) = 0, \tag{9}$$

$$\begin{aligned}\frac{\hbar}{m}\frac{\partial\varphi}{\partial t} &= -\frac{\mathbf{v}^2}{2} + \frac{\hbar^2}{4m^2}\left(\frac{\Delta n}{n} - \frac{(\nabla n)^2}{2n^2}\right) \\ &+ \frac{n_0 U_0}{m} - \frac{1}{m}\int d\mathbf{r}' U\left(\mathbf{r}-\mathbf{r}'\right) n(\mathbf{r}'),\end{aligned} \tag{10}$$

where the superfluid velocity is introduced as

$$\mathbf{v} = \frac{\hbar}{m}\nabla\varphi. \tag{11}$$

Eq. (9) is the continuity equation, and Eq. (10) is analogous to the Josephson equation in the theory of superconductivity. Taking a gradient of both sides of Eq. (10) and taking into account the definition of the velocity (11),

$$\frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}\nabla)\mathbf{v} = \nabla w, \tag{12}$$

where

$$w = \frac{\hbar^2}{2m}\frac{\Delta\eta}{\eta} - \frac{1}{m}\int d\mathbf{r}' U\left(\mathbf{r}-\mathbf{r}'\right) n(\mathbf{r}'). \tag{13}$$

Notice that the system of equations (9), (12) coincides with the hydrodynamics equations for the superfluid helium at zero temperature [26].
In a linear approximation, the right hand side of Eq. (12) can be expressed as

$$\nabla w = \frac{-\nabla p}{m n_0}.$$

The pressure and the density are then related in a non-local way:

$$p = -\frac{\hbar^2}{2}\eta_0\Delta\eta + n_0\int d\mathbf{r}' U\left(\mathbf{r}-\mathbf{r}'\right) n(\mathbf{r}'). \tag{14}$$

This non-local relationship between pressure and density was used in the phenomenological approach of [35] (neglecting the quantum term) to describe the rotons in the superfluid helium. From our consideration, it follows that the non-locality kernel, which relates the pressure and the density in a phenomenological approach, is determined by the inter-particle interaction potential.

4. Small oscillation spectrum with non-local effects

In analogy to the derivation of the spectrum (8) from Eq. (7), the non-local GP equation (6) leads to the following dispersion law for small oscillations

$$\varepsilon_k = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)\left(2\,U_k n_0 + \frac{\hbar^2 k^2}{2m}\right)}, \tag{15}$$

which differs from (8) due to the appearance of a potential Fourier component $U_k = \int d\mathbf{r}\, U(\mathbf{r})\, e^{i\,kr}$ (dependent on the wave vector) instead of U_0.
Usually, at short distances, a strong repulsion occurs, so the interaction potential grows rapidly, leading to a divergence of the Fourier component U_k. To overcome this obstacle, one may suppose that the potential remains finite at short distances [36, 37]. As the simplest case, we will use the "semitransparent sphere model" potential

$$U(\mathbf{r}) = \begin{cases} U_{\max}, & r \leqslant a, \\ 0, & r > a, \end{cases} \tag{16}$$

and consider $U_{\max}$ and a as two independent parameters of the dimension of energy and length, correspondingly. In this case the Bose-condensate excitation spectrum (15) depends on the only dimensionless parameter

$$\xi = \frac{\hbar^2}{8\pi\; n_0\; a^5\; m\; U_{\max}}. \tag{17}$$

The Fourier component of the potential (16) reads

$$U_k = \frac{4\pi a U_{\max}}{k^2}\, j_1(ka), \tag{18}$$

where $j_1(x) = x^{-1}\sin x - \cos x$ is the Riccati-Bessel function.
Putting this expression into Eq. (15), one obtains the energy spectrum

$$\varepsilon = \varepsilon_0\sqrt{f(z)}, \tag{19}$$

where

$$f(z) = z^{-1}(\sin z - z\cos z) + \xi z^4, \tag{20}$$

$$\varepsilon_0 = \hbar\sqrt{4\pi\; n_0\; a\; \frac{U_{\max}}{m}}, \tag{21}$$

$$z = ka. \tag{22}$$

Notice that the dimensionless parameter ξ (17) depends strongly on the potential range $\xi \propto a^{-5}$, and grows rapidly with decreasing a.

The dependence of condensate excitation frequency on the wave number is shown in Fig. 1. At parameter values $\xi > \xi_h = 3.4{\cdot}10^{-3}$, the dispersion curve lacks local minima and the energy monotonically increases with wave number (upper curve in Fig. 1).
At $\xi_l < \xi < \xi_h$ (with $\xi_l = 0.92 \cdot 10^{-3}$) the dispersion curve acquires a roton minimum (middle curve in Fig. 1) and its depth increases with decreasing ξ. In this range the excitation spectrum mimics that of superfluid helium with a roton minimum as Landau postulated and, in the vicinity of the roton minimum, can be written as [7, 8, 26]

$$\varepsilon_k = \Delta + \frac{\hbar^2(k-k_0)^2}{2m_*}, \tag{23}$$

where Δ is the roton gap, k_0 is the roton wave number in the spectrum minimum and m_* is the effective mass.

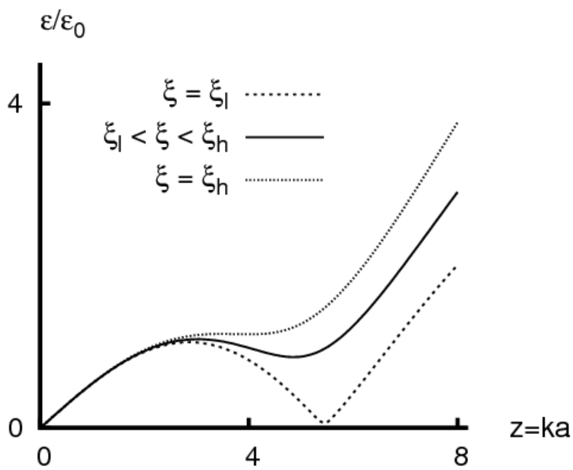

Figure 1. Condensate excitation spectrum for the “semitransparent sphere model” interaction; $\xi_h = 3.4 \cdot 10^{-3}$, $\xi_l = 0.92 \cdot 10^{-3}$.

The roton minimum position $z_0 = k_0 a$ in our model is determined by $f'(z_0) = 0$. Dependence of z_0 on the parameter ξ is shown in Fig. 2. With increasing ξ, the roton minimum position gets shifted toward smaller wave numbers, changing from its maximum $z_{\max} = 5.45$ (for $\xi_l = 0.92 \cdot 10^{-3}$) to minimum $z_{\min} = 3.72$ (for $\xi_h = 3.4 \cdot 10^{-3}$). It follows that the excitation wave length λ, at the dispersion curve minimum lies in the range

$$1.15\,a < \lambda < 1.69\,a. \tag{24}$$

Thus one may conclude that the existence of a dispersion curve minimum is caused by the finiteness of the inter-particle interaction range and is not connected with any specific superfluid properties of system. It is noteworthy that, in helium, the repulsive range of the inter-atomic interaction potential may be estimated as $a = 2.56$ Å and the roton wave length is $\lambda_r = 3.3$ Å, such that the relation $\lambda_r = 1.28\,a$ fits into the interval (24).

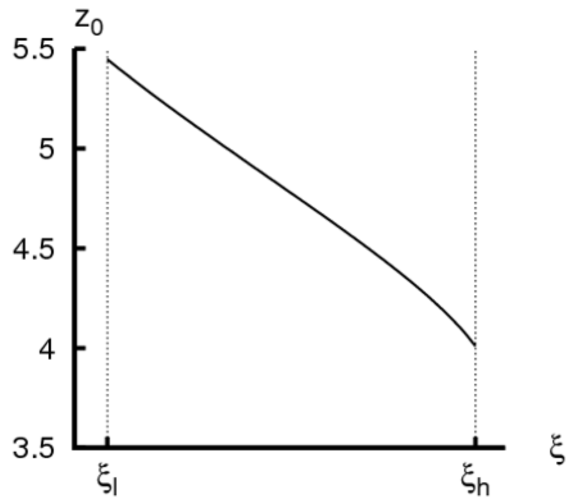

Figure 2. Roton minimum position z_0 as a function of parameter ξ.

Dependence of the roton gap $\Delta = \varepsilon_0\sqrt{f(z_0)}$ on the parameter ξ in spectrum (23) is shown in Fig. 3. At $\xi = \xi_l$ the gap is zero. It grows with ξ, achieving its maximum

$$\frac{\Delta_{\max}}{\varepsilon_0} = 1.17$$

at $\xi = \xi_h$.
At the value $\xi = \xi_l = 0.92 \cdot 10^{-3}$, the excitation energy minimum equals to zero (lower curve in Fig. 1); this means an instability of a many-particle system for given parameters of the interaction potential. Thus, only in the range $\xi_l < \xi < \xi_h$ the excitation spectrum mimics that of superfluid Helium with a roton minimum (23).
The effective mass of the roton in this case is

$$m_* = \frac{2\hbar^2}{a^2\varepsilon_0}\,\frac{\sqrt{f(z_0)}}{f''(z_0)}. \tag{25}$$

The dependence of the dimensionless effective mass

$$M_* \equiv \frac{m_* a^2 \varepsilon_0}{2\hbar^2}$$

on the parameter ξ is illustrated in Fig. 4. The effective mass varies from zero at ξ_l up to $M_* \approx 9.663$ at ξ_h.

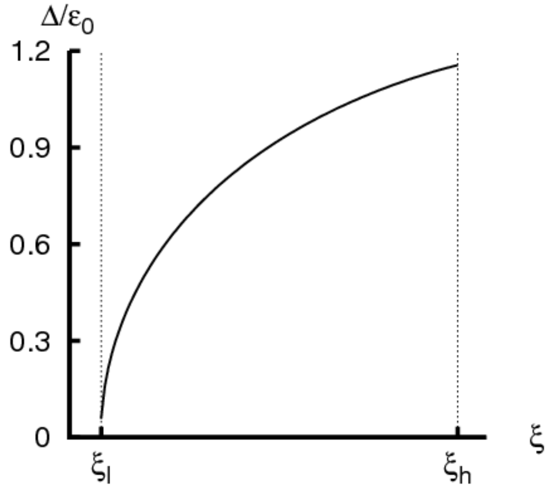

Figure 3. Roton gap versus parameter ξ.

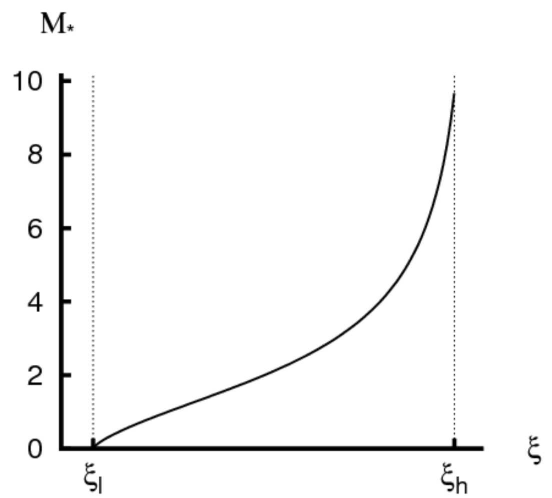

Figure 4. The dependence of the dimensionless effective mass of the roton $M_* \equiv m_* a^2 \varepsilon_0/(2\hbar^2)$ on the parameter ξ.

5. Attraction influence on the small oscillation spectrum

In the majority of the papers devoted to a non-ideal Bose-gas, as in [15], it is supposed that the inter-particle interaction is repulsive. It is hence of interest to investigate the influence of long-distance inter-particle attraction on the elementary excitation spectrum. Toward this end we calculate the spectrum for the interaction potential

$$U(\mathbf{r}) = \begin{cases} U_{\max}, & r \leqslant a, \\ -\frac{C}{r^6}, & r > a, \end{cases} \tag{26}$$

where C is positive. This potential accounts for a Van der Waals long-distance attraction of particles. The Fourier component of this potential reads

$$U_k = \frac{4\pi a U_{\max}}{k^2}\left[j_1(ka) - \alpha\, g(ka)\right]. \tag{27}$$

Using this expression, one obtains from (15) the energy spectrum

$$\varepsilon = \varepsilon_0\sqrt{f(z) - \alpha\, g(z)}, \tag{28}$$

with a dimensionless parameter

$$\alpha = \frac{C}{U_{\max} a^6}.$$

An auxiliary function

$$g(z) = \frac{z}{4}\left[\left(1 - \frac{z^2}{6}\right)\sin z + \frac{z}{3}\left(1 - \frac{z^2}{2}\right)\cos z + \frac{z^4}{6}\left(\frac{\pi}{2} - \mathrm{Si}(z)\right)\right], \tag{29}$$

($\mathrm{Si}(z)$ stands for integral sine) describes the impact of the attractive part of the inter-particle potential on the elementary excitation spectrum. This function is shown in Fig. 5. Function $g(z)$ is positive for wave numbers $0 < z < 2.45$ and negative for $2.45 < z < 5.40$. For $z > 5.40$ function $g(z)$ is positive and rises sharply.
One may notice that the interval $2.45 < z < 5.40$, where function (29) is negative, overlaps with the domain of the roton minimum existence. It follows that the attraction leads to the growth of the excitation energy in the domain of the roton minimum existence and smears this minimum. In the range of small wave numbers, and also for very large $z > 5.40$, attraction lowers the excitation energy. Thus the long-distance atomic attraction smoothes the dispersion curve and narrows the range over which the excitation spectrum has extrema (rotons and maxons). Attraction reduces the upper bound ξ_h and increases the lower one ξ_l, narrowing the range over which a Landau-like excitation spectrum $\delta\xi \equiv \xi_h - \xi_l$ exists. Dependence of $\delta\xi$ for a spectrum with roton minimum on attraction strength

$$\alpha = \frac{C}{U_{\max} a^6},$$

is shown in Fig. 6.
Notice that experimental spectrum of quasi-particle excitations in the superfluid helium at large momentum p ($p \equiv \hbar k > 3$ Å^{-1}) increases slowly such that the derivative of $\varepsilon(p)$ is close to zero at the boundary of the spectrum [38]. This behavior can be understood with help of

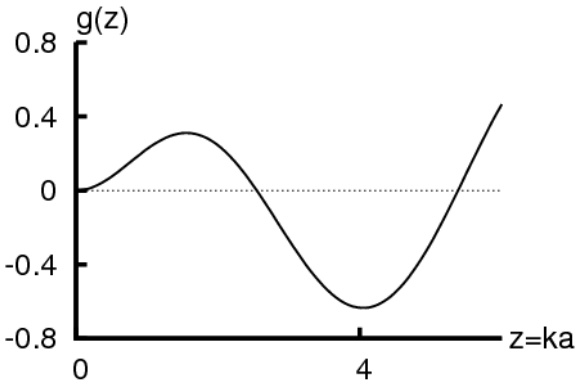

Figure 5. Function $g\,(z)$ in the domain of z of physical interest.

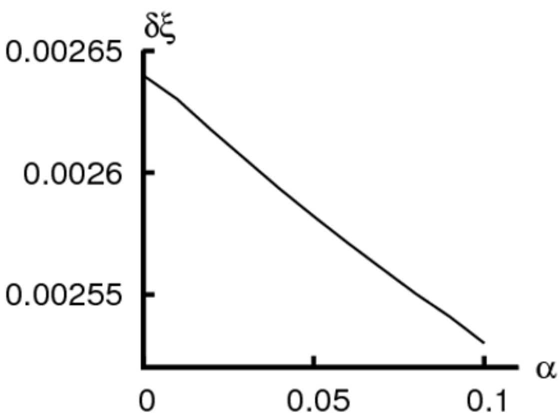

Figure 6. Range $\delta\xi$ as a function of the interaction strength α.

a long-range attraction. Recall that function $g(z)$ is positive and increasing for $z > 5.40$. Thereby, due to (28), it opposes the dispersion curve growing at large momentum.

We should draw attention to how small the attraction part of the potential is for helium – it is the smallest among the rare gases. Specifically, the depth of the potential well for helium is $\varepsilon = -10.5$ K, compared to $\varepsilon = -35.9$ K for neon, $\varepsilon = -121$ K for argon, $\varepsilon = -173$ K for krypton. It seems that, due to this fact, the maxon-roton part of the dispersion curve in liquid helium is the most pronounced not only in a superfluid phase, but in a normal phase as well. Notice a feature of the superfluid phase: the lifetime of the maxon-roton excitations are much larger than that in normal liquids.

6. Conclusions

It is shown that the Gross-Pitaevskii equation, with allowance for non-local effects caused by the finiteness of the inter-particle interaction range, can describe the short-wave excitation spectrum for which the wavelength is of inter-particle interaction range order.

For a Bose-system the spectrum for arbitrary wave number is obtained; it has a shape of the Landau spectrum of superfluid helium. We estimated the range of parameters where such a spectrum exists. Computation shows that the roton minimum in the dispersion curve is caused by the finiteness of the inter-particle interaction range; the wave length of this minimum is close to the repulsion range of the interaction. We studied the influence of the long-distance inter-particle attraction on the dispersion curve, showing that it results in smoothing of the excitation spectrum and in narrowing the range of the existence of a maxon-roton type curve. Our analysis showed that the attraction part of the potential for the helium atoms is small in comparison with that for other atoms; it seems that this fact induces a pronounced maxon-roton part of the liquid helium dispersion curve.

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