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Quasimomentum of an elementary excitation for a system of point bosons under zero boundary conditions

Presented by Academician of the NAS of Ukraine V.M. Loktev

As is known, an elementary excitation of a many-particle system with boundaries is not characterized by a definite momentum. We obtain the formula for the quasimomentum of an elementary excitation for a one-dimensional system of N spinless point bosons under zero boundary conditions (BCs). In this case, we use Gaudin's solutions obtained with the help of the Bethe ansatz. We have also found the dispersion laws of the particle-like and hole-like excitations under zero BCs. They coincide with the known dispersion laws obtained under periodic BCs.

Keywords: *point bosons, elementary excitation, quasimomentum, zero boundary conditions.*

The theory of point bosons [1—6] based on the Bethe ansatz is a valuable part of the physics of many-particle systems, since the system of equations for quasimomenta k_j can be solved exactly at any coupling constant γ, and the thermodynamic quantities can be determined from Yang—Yang's equations [4] at any temperature. This allows one to test the solutions for real nonpoint bosons, the equations for which can rarely be solved.

In the present work, we will study a one-dimensional (1D) system of spinless point bosons in the exactly solvable approach based on the Bethe ansatz. For the real systems, the boundary conditions (BCs) are closer to the zero ones ($\Psi(x_1,\ldots,x_N)=0$ on the boundaries), than to the periodic BCs. Therefore, it is important to find the ground-state energy and the dispersion law under the zero BCs. The ground state was already studied [5, 7], but the dispersion law was not found. To find it, one needs to determine the energy and the quasimomentum of a quasiparticle. These problems will be considered in our work. The main difficulty consists in obtaining the formula for the quasimomentum, because the ordinary method with the use of the operator of momentum fails under the zero BCs.

Under the periodic BCs [2], a quasiparticle possesses the momentum [3, 6, 8, 9]

$$p=\sum_{j=1}^{N}(k'_j-k_j), \qquad (1)$$

where k_j are the solutions for the ground state, k'_j are the solutions for the state with one quasiparticle. This definition of the momentum of a quasiparticle is self-consistent: the thermodynamic velocity of sound ($v_s^{th} = \sqrt{m^{-1}\partial P / \partial \rho}$, $P = -\partial E_0 / \partial L$, $\rho = N / L$) coincides with the microscopic one ($v_s^{mic} = \partial E(p) / \partial p |_{p\to 0}$) [3].

Under the zero BCs, the quasimomentum of a quasiparticle was obtained similarly to (1) [7, 10]:

$$p = \sum_{j=1}^{N} (| k'_j | - | k_j |). \qquad (2)$$

However, in such approach, the equality $v_s^{th} = v_s^{mic}$ is strongly violated [7]. Below, we will define the quantity p in such a way that this difficulty disappears.

Initial equations. Consider N spinless point bosons placed on a line of length L. The Schrödinger equation for such system reads

$$-\sum_j \frac{\partial^2}{\partial x_j^2}\Psi + 2c\sum_{l<j}\delta(x_l - x_j)\Psi = E\Psi. \qquad (3)$$

We use the units with $\hbar = 2m = 1$. Under the periodic BCs, for each of the domains $x_1 \leqslant \leqslant x_2 \leqslant \ldots \leqslant x_N$, a solution of the Schrödinger equation is the Bethe ansatz [2, 5]

$$\psi_{\{k\}}(x_1, \ldots, x_N) = \sum_P a(P) e^{i\sum_{l=1}^{N} k_{P_l} x_l}, \qquad (4)$$

where k_{P_l} is one of $k_1, \ldots, k_N$, and P means all permutations of k_l . Under the zero BCs, the solution is a superposition of counter-waves [5]:

$$\Psi_{\{|k|\}}(x_1, \ldots, x_N) = \sum_{\{\varepsilon\}} C(\varepsilon_1, \ldots, \varepsilon_N)\psi_{\{k\}}(x_1, \ldots, x_N), \qquad (5)$$

where $k_j = \varepsilon_j | k_j |$, $\varepsilon_j = \pm 1$. Under any BCs, the energy of the system is

$$E = k_1^2 + k_2^2 + \ldots + k_N^2. \qquad (6)$$

Under the periodic BCs, k_j satisfy Lieb—Liniger's equations [2] that are usually written in Yang—Yang's form [4]

$$Lk_j = 2\pi I_j - 2\sum_{l=1}^{N} \arctan\frac{k_j - k_l}{c}, \quad j = 1, \ldots, N. \qquad (7)$$

We will use Lieb—Lininger's equations in the Gaudin's form [5]:

$$Lk_j = 2\pi n_j + 2\sum_{l=1}^{N} \arctan\frac{c}{k_j - k_l}\bigg|_{l\neq j}, \quad j = 1, \ldots, N, \qquad (8)$$

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where n_j are integers. For the ground state of the system, $n_j = 0$ for all $j = 1, \ldots, N$. The systems of equations (7) and (8) are equivalent [5]. In this case, $I_j = n_j + j - \frac{N+1}{2}$.

Under the zero BCs, k_j satisfy the Gaudin's equations [5]:

$$L|k_j| = \pi n_j + \sum_{l=1}^{N}\left(\arctan\frac{c}{|k_j|-|k_l|} + \arctan\frac{c}{|k_j|+|k_l|}\right)|_{l\neq j}, \quad j = 1, \ldots, N, \tag{9}$$

where n_j are integers, $n_j \geqslant 1$ [5,11]. The ground state corresponds to $n_j = 1$ for all j. We denote $\rho = N/L$, $\gamma = c/\rho$.

Equations (8) has the unique real solution $\{k_j\}$ [6], and Eqs. (9) have the unique real solution $\{|k_j|\}$ [11].

The quasiparticles are commonly described with the help of Yang—Yang's I_j-numbering (7). Below, we will introduce the quasiparticles with the help of Gaudin's n_j-numbering (8), (9), since this way is simpler and more physical [12] and allows one to sight the Bose properties of quasiparticles [7]. These two ways of introduction of quasiparticles are equivalent. For example, under the periodic BCs, the "particle" $\{I_j\} = \left(1-\frac{N+1}{2}, \ldots, N-1-\frac{N+1}{2}, N-\frac{N+1}{2}+l\right)$ with the help of the n_j-numbering is written as $\{n_j\} = (0, \ldots, 0, l)$. In the n_j-language, the "hole" $\{I_j\} = \left(1-\frac{N+1}{2}, \ldots, N-2-\frac{N+1}{2}, N-\frac{N+1}{2}, N+1-\frac{N+1}{2}\right)$ is $\{n_j\} = (0, \ldots, 0, 1, 1)$. A way of introduction of quasiparticles with the help of the n_j-numbering was proposed in [7].

Definition of the quasimomentum of an elementary excitation. We now find how the quasimomentum of an elementary excitation can be determined under the zero BCs. Under the periodic BCs, the relation [2]

$$\sum_{j=1}^{N}\left(-i\frac{\partial}{\partial x_j}\right)\cdot\psi_{\{k\}}(x_1, \ldots, x_N) = \left(\sum_{j=1}^{N}k_j\right)\psi_{\{k\}}(x_1, \ldots, x_N) \tag{10}$$

holds in the whole domain $x_1, \ldots, x_N \in [0, L]$. Therefore, the system has the total momentum

$$P = \sum_{j=1}^{N}k_j, \tag{11}$$

and the momentum of a quasiparticle is given by formula (1). Under the zero BCs, the relation

$$\sum_{j=1}^{N}\left(-i\frac{\partial}{\partial x_j}\right)\Psi_{\{|k|\}}(x_1, \ldots, x_N) = f(|k_1|, \ldots, |k_N|)\Psi_{\{|k|\}}(x_1, \ldots, x_N)$$

is not satisfied. Therefore, the system has no definite momentum. To find the formula for the quasimomentum of an excitation, we use the following property. It is known that the momentum (quasimomentum) of a quasiparticle is quantized by the law $p_j = \hbar 2\pi j/L$ $(j = \pm1, \pm2, \ldots)$ under the periodic BCs [13], and $p_j = \hbar\pi j/L$ $(j = 1, 2, \ldots)$ under the zero BCs [14,15]. Starting from these relations, one can guess the formula for the momentum (quasimomentum).

Consider a periodic system. Equations (8) yield

$$\sum_{j=1}^{N} k_j = \frac{2\pi}{L}\sum_{j=1}^{N} n_j. \tag{12}$$

It is seen that the quantity $P = \sum_{j=1}^{N} k_j$ is quantized in the same way as the momentum of an ensemble of quasiparticles [13]. Therefore, it is natural to identify P with the total momentum of the system (in the reference system, where the center of masses is at rest). We obtain that $P_0 = \sum_{j=1}^{N} k_j = 0$ is for the ground state and $P_1 = \sum_{j=1}^{N} k_j = 2\pi r / L$ for the state with one particle-like excitation ($n_{j \leqslant N-1} = 0$, $n_N = r \neq 0$). The momentum of a particle-like excitation

$$p = P_1 - P_0 = \sum_{j=1}^{N}(k_j^{'} - k_j) = \frac{2\pi n_N}{L} = \frac{2\pi r}{L} \tag{13}$$

corresponds to formula (1) and to momentum quantization $p_j = 2\pi j/L$ [13]. We have solved system (8) numerically, found the energies of the ground and excited states, and obtained that the equality $v_s^{th} = v_s^{mic}$ holds with high accuracy: for $\rho = 1$, $N = 200, 1000, 5000$ and $\gamma = 0.1$, 1, 10, the equality $v_s^{th} = v_s^{mic}$ holds with an error of $\leqslant 0.1$ %. In this case, the error depends strongly on γ and N: $\frac{|v_s^{mic} - v_s^{th}|}{v_s^{th}} \simeq \frac{0.01}{\gamma N}$.

We now consider the system under the zero BCs. Relation (9) yields

$$\sum_{j=1}^{N} |k_j| = \frac{\pi}{L}\sum_{j=1}^{N} n_j + \frac{1}{L}\sum_{l,j=1}^{N} \arctan\frac{c}{|k_j| + |k_l|}\bigg|_{l \neq j}. \tag{14}$$

Introduce the quantity

$$P(\{|k_i|\}) = \sum_{j=1}^{N} |k_j| - \frac{1}{L}\sum_{l,j=1}^{N} \arctan\frac{c}{|k_j| + |k_l|}\bigg|_{l \neq j}, \tag{15}$$

then relations (14) and (15) yield

$$P(\{|k_i|\}) = \frac{\pi}{L}\sum_{j=1}^{N} n_j. \tag{16}$$

Since P is quantized similarly to the quasimomentum of the ensemble of quasiparticles for an interacting system under the zero BCs [15], it is natural to identify P with this quasimomentum. It is essential that the quasiparticles are introduced for a system of point bosons in such a way that the total number of quasiparticles is $\leqslant N$ (the same limitation exists also for a system of nonpoint bosons [12]). This agrees with (16). The smallest quasimomentum of the system corresponds to the ground state:

$$P_0 = P(n_{j \leqslant N} = 1) = \frac{\pi}{L}\sum_{j=1}^{N} 1 = \frac{\pi N}{L} = \pi\rho. \tag{17}$$

The quasimomentum of a particle-like excitation is

$$p_{r-1} = P(n_{j \leqslant N-1} = 1, n_N = r) - P(n_{j \leqslant N} = 1) =$$
$$= \sum_{j=1}^{N} \left(|k_j^{'}| - |k_j| \right) - \frac{1}{L} \sum_{l,\, j=1}^{N} \left(\arctan \frac{c}{|k_j^{\prime}| + |k_l^{\prime}|} - \arctan \frac{c}{|k_j| + |k_l|} \right) \Big|_{l \neq j} \qquad (18)$$

where $\{|k_j'|\}$ and $\{|k_j|\}$ are solutions of Gaudin's equations (9) for the states with one particle-like excitation and without excitations, respectively. Relations (16), (18) yield

$$p_{r-1} = \pi(r-1)/L\,, \qquad (19)$$

where r is equal to the value of n_N for the state with one particle-like excitation: $r = n_N = 2, 3, 4, \ldots$; $n_{j \leqslant N-1} = 1$. We have obtained the quantity with the required law of quantization: $p_j = \pi j/L$ [14, 15]. The numerical analysis has shown that the equality $v_s^{th} = v_s^{mic}$ is satisfied with an error of $\leqslant 1\%$ for $\rho = 1$; $\gamma = 0.1, 1, 10$; $N = 200, 1000, 5000$. This error depends on γ and N approximately as $\frac{|v_s^{mic} - v_s^{th}|}{v_s^{th}} \simeq \frac{0.5}{\sqrt{\gamma}N}$. In this case, the linearity of the dispersion law requires $\sqrt{\gamma}N \gg 1$. It is significant that, for the zero and periodic BCs, the error disappears as $N \to \infty$. In other words, this error is due to the finiteness of a system (for very large N, one more error related to a numerical method should appear). The equality $v_s^{th} = v_s^{mic}$ must be exact in the thermodynamic limit and may be violated for not large N, L. Thus, in the thermodynamic limit, our formulae agree with the exact equality $v_s^{th} = v_s^{mic}$. Hence, formulae (18) and (19) for the quasimomentum are exact, at least as $N, L \to \infty$.

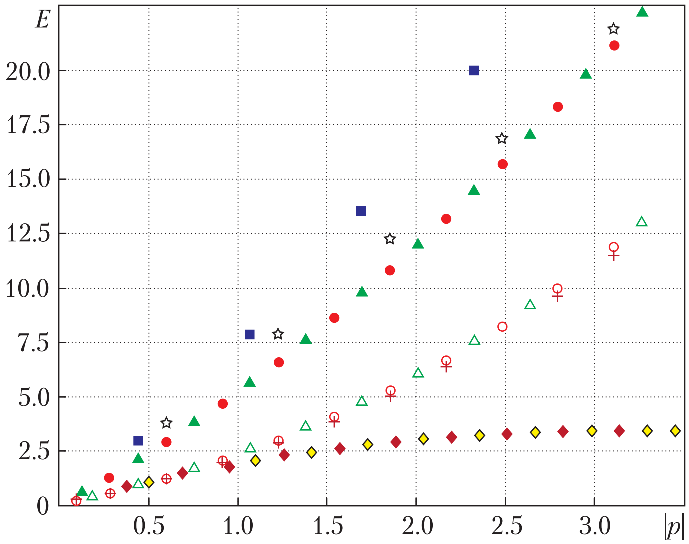
We note that, for the zero BCs, the error is larger by 1—2 orders of magnitude, than in the periodic BCs case. We suppose that this is connected with a nonuniformity of the wave function near boundaries. In particular, for a periodic system, the solution for the ground-state energy E_0 becomes close to Bogoliubov's asymptotic solution $E_0(N \to \infty)$ [13], if $N \geqslant 100$; for the zero BCs, this occurs for larger N: $N \geqslant 1000$.

Thus, we have obtained the formula for the quasimomentum of a quasiparticle for the system under the zero BCs. Apparently, quasimomentum (15), (16) corresponds to an accidental integral of motion. It would be of interest to clarify which operator corresponds to quasimomentum (15).

Let us find the dispersion law $E(p)$ of particle-like excitations for a system under the zero and periodic BCs. Under the zero BCs, we are based on (19), and the formula for the energy of a quasiparticle is [3]

$$E = \sum_{j=1}^{N} ((k_j^{'})^2 - k_j^2). \qquad (20)$$

Under the periodic BCs, we use formulae (13), (20). We find the solutions $\{k_j'\}$ and $\{k_j\}$ from Eqs. (8) under the periodic BCs and from Eqs. (9) under the zero BCs. In this case, $\{k_j'\}$ corresponds to the state with one quasiparticle ($n_{j \leqslant N-1} = 0$, $n_N = r$ for the periodic BCs and



Dispersion curves $E(p)$ obtained by the numerical solution of Eqs. (8), (9) within the Newton method for $N = L = 1000$. 1) $\gamma = 1$: $E(p)$ of particle-like excitations under the periodic BCs (open circles), under the zero BCs (open triangles), and the Bogoliubov law [13] $E = \sqrt{p^4 + 4\gamma\rho^2 p^2}$ (crosses); 2) $\gamma = 10$: $E(p)$ of particle-like excitations under the periodic BCs (circles), under the zero BCs (triangles), the Bogoliubov law (stars), and Girardeau's law [1] $E = p^2 + 2\pi\rho\,|\,p\,|$ (squares); 3) $\gamma = 1.725$: $E(p)$ of hole-like excitations under the periodic (open diamonds) and zero (diamonds) BCs

$n_{j\leqslant N-1} = 1$, $n_N = r > 1$ for the zero BCs), whereas $\{k_j\}$ corresponds to the ground state ($n_{j\leqslant N} = 0$ for the periodic BCs and $n_{j\leqslant N} = 1$ for the zero BCs). We have solved Eqs. (8), (9) numerically and determined the dispersion law $E(p)$ for the zero and periodic BCs. As is seen from Figure, the dispersion laws $E(p)$ under the periodic and zero BCs *coincide*. The numerical solution of systems (8) and (9) indicates that the ground-state energy (E_0) under the zero BCs exceeds E_0 under the periodic BCs by only a small surface contribution $\Delta E_0 \sim E_0 / N$ [7]. For interacting nonpoint bosons, the picture is similar: at any repulsive interatomic potential, the values of E_0 and $E(p)$ of a 1D system under the zero BCs [15] coincide with E_0 and $E(p)$ of a periodic system [13]. Moreover, for a 1D system of interacting bosons, it was found in the harmonic-fluid approximation that the sound velocity is identical under the periodic and zero BCs [14].

We have also calculated the dispersion law of hole-like excitations. It is seen from Figure that the dispersion law is the same under the zero and periodic BCs. Visually, it coincides with the dispersion law of holes obtained by Lieb [3]. Under the zero BCs, holes correspond to the states with the following quantum numbers n_j: $n_{1\leqslant j\leqslant l} = 1$, $n_{l<j\leqslant N} = 2$, where $l = 0, 1, \ldots, N-2$. Under the periodic BCs, holes are the states with $n_{1\leqslant j\leqslant l} = 0$, $n_{l<j\leqslant N} = 1$ ($l = 0, 1, \ldots, N-2$) and the states with $n_{1\leqslant j\leqslant k} = -1$, $n_{k<j\leqslant N} = 0$ ($k = 2, 3, \ldots, N$). Formula (16) implies that the quasimomentum of a hole under the zero BCs is $p = \pi\,(N-l)/L$; the largest quasimomentum is $p = \pi N/L = \pi\rho$. Under the periodic BCs, the hole has momentum (1), (12), which takes values from $p = -2\pi\rho$ to $p = 2\pi\rho$. Note that, as shown in work [12], a hole is a set of interacting particle-like excitations.

We note that the formulae for the quasimomentum and the solutions for the dispersion laws, obtained above under the zero BCs, are new results.

Interestingly, the dispersion law of particle-like excitations (see Figure) differs at $\gamma = 1$ from the Bogoliubov law only by 5 %. In this case, the available criterion of applicability of the Bogoliubov model in the 1D case for the zero and periodic BCs is as follows (at $T = 0$) [15]:

$$\frac{\sqrt{\gamma}}{2\pi}\ln\frac{N\sqrt{\gamma}}{\pi} \ll 1. \qquad (21)$$

According to (21), it should be $\gamma \to 0$ as $N \to \infty$. But the solutions E_0 and $E(p)$ for point bosons are close to the Bogoliubov solutions even at $N \to \infty$, $\gamma \sim 1$ (as for the periodic BCs, see [2, 3]; for the zero BCs, it was found [7] that the solutions E_0 and $E(p)$ obtained in the limit $N \to \infty$ coincide (with an error of 1 %) with E_0 and $E(p)$ found by directly numerically solving Eqs. (9) at $N = 1000$; therefore, the dispersion law $E(p)|_{N\to\infty}$ coincides with the above-found one $E(p)|_{N\to1000}$ and is close to the Bogoliubov law, if $\gamma \leqslant 1$). We remark that the dispersion law for $\gamma = 10$ (see Figure) is closer to the Bogoliubov law, than to Girardeau's one. Though it would be expected the contrary, since Girardeau's formula is exact at $\gamma = +\infty$, whereas the Bogoliubov formula loses its meaning at such γ. The reason for the applicability of the Bogoliubov solutions at not small γ is yet unclear.

It was obtained [7] that the dispersion laws of particle-like excitations under the zero and periodic BCs are strongly different. However, this difference is unphysical: it arose because, under the zero BCs, formula (2) was used instead of formula (18).

The question is how can one measure the dispersion law in a system under the zero BCs? Apparently, this can be made with the help of an ordinary scattering. But we do not know how to pass from Gaudin's wave function (5) to a localized wave package with a definite momentum.

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КВАЗІІМПУЛЬС ЕЛЕМЕНТАРНОГО ЗБУДЖЕННЯ
ДЛЯ СИСТЕМИ ТОЧКОВИХ БОЗОНІВ
З НУЛЬОВИМИ МЕЖОВИМИ УМОВАМИ

Як відомо, елементарне збудження багаточастинкової системи з межами не має визначеного імпульсу. Ми отримали формулу для квазіімпульсу елементарного збудження одновимірної системи N безспінових точкових бозонів з нульовими межовими умовами (МУ). При цьому ми спирались на розв'язки Годена, отримані за допомогою анзаца Бете. Також ми знайшли закони дисперсії частинкоподібних та діркоподібних збуджень за нульових МУ. Вони збігаються з відомими законами дисперсії, знайденими для періодичних МУ.

Ключові слова: *точкові бозони, елементарне збудження, квазіімпульс, нульові межові умови.*

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КВАЗИИМПУЛЬС ЭЛЕМЕНТАРНОГО ВОЗБУЖДЕНИЯ
ДЛЯ СИСТЕМЫ ТОЧЕЧНЫХ БОЗОНОВ
С НУЛЕВЫМИ ГРАНИЧНЫМИ УСЛОВИЯМИ

Как известно, элементарное возбуждение многочастичной системы с границами не имеет определенного импульса. Мы получаем формулу для квазиимпульса элементарного возбуждения одномерной системы N бесспиновых точечных бозонов с нулевыми граничными условиями (ГУ). При этом мы используем решения Годена, полученные с помощью анзаца Бете. Также мы нашли законы дисперсии частицеподобных и дыркоподобных возбуждений при нулевых ГУ. Они совпадают с известными законами дисперсии, найденными при периодических ГУ.

Кючевые слова: *точечные бозоны, элементарное возбуждение, квазиимпульс, нулевые граничные условия.*