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

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Abstract
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 the 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 condi-
tions.

The theory of point bosons [1, 2, 3, 4, 5, 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 $\gamma$, and the thermodynamic quantities can
be determined from the 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 of importance 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]

$$ p = \sum_{i=1}^{N} (k_i - \dot{k}_i), \quad (1) $$

where $k_i$ are the solutions for the ground state, and $\dot{k}_i$ 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 ($v_{th} = \sqrt{m^{-1} \partial P/\partial \rho}$, $P = -\partial E_0/\partial L$, $\rho = N/L$) coincides
with the microscopic one ($v_{mic}^{\rho} = \partial E(p)/\partial p|_{p \to 0}$) [3].

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

$$ p = \sum_{i=1}^{N} (|\dot{k}_i| - |k_i|). \quad (2) $$
However, in such approach the equality $v_s^{th} = v_s^{mic}$ is strongly violated \cite{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

$$\sum_j \frac{\partial^2}{\partial x_j^2} \Psi + 2c \sum_{i<j} \delta(x_i - x_j) \Psi = E \Psi.$$  \hspace{1cm} (3)

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

$$\psi_{\{k\}}(x_1, \ldots, x_N) = \sum_P a(P) \ e^{i \sum_{l=1}^N k_{P_l} x_l},$$  \hspace{1cm} (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 \cite{5}:

$$\Psi_{\{|k|\}}(x_1, \ldots, x_N) = \sum_{\{\varepsilon\}} C(\varepsilon_1, \ldots, \varepsilon_N) \psi_{\{k\}}(x_1, \ldots, x_N),$$  \hspace{1cm} (5)

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

$$E = k_1^2 + k_2^2 + \ldots + k_N^2.$$  \hspace{1cm} (6)

Under the periodic BCs, $k_j$ satisfy the Lieb–Liniger’s equations \cite{2} that are usually written in the Yang–Yang’s form \cite{4}

$$Lk_i = 2\pi I_i - 2 \sum_{j=1}^N \arctan \frac{k_i - k_j}{c}, \quad i = 1, \ldots, N.$$  \hspace{1cm} (7)

We will use the Lieb–Liniger’s equations in the Gaudin’s form \cite{5}:

$$Lk_i = 2\pi n_i + 2 \sum_{j=1}^N \arctan \left( \frac{c}{k_i - k_j} \right)_{j\neq i}, \quad i = 1, \ldots, N,$$  \hspace{1cm} (8)

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

Under the zero BCs, $k_j$ satisfy the Gaudin’s equations \cite{5}:

$$L|k_i| = \pi n_i + \sum_{j=1}^N \left( \arctan \frac{c}{|k_i| - |k_j|} + \arctan \frac{c}{|k_i| + |k_j|} \right)_{j\neq i}, \quad i = 1, \ldots, N,$$  \hspace{1cm} (9)

where $n_i$ are integers, $n_i \geq 1$ \cite{5, 11}. The ground state corresponds to $n_i = 1$ for all $i$. We denote $\rho = N/L$, $\gamma = c/\rho$.

Equations (8) has the unique real solution $\{k_i\}$ \cite{6}, and equations (9) have the unique real solution $\{|k_i|\}$ \cite{11}.

The quasiparticles are commonly described with the help of the Yang–Yang’s $I_i$-numbering \cite{7}. Below we will introduce the quasiparticles with the help of the Gaudin’s $n_i$-numbering \cite{5, 9}, since this way is simpler and more physical \cite{12}, and allows one to sight the Bose properties of quasiparticles \cite{7}. These two ways of introduction of quasiparticles are equivalent. For example, under the periodic BCs, the “particle” $\{I_i\} = (1 - \frac{N+1}{2}, \ldots, N - 1 - \frac{N+1}{2}, N - \frac{N+1}{2} + j)$ with the help of the $n_i$-numbering is
written as \( \{n_i\} = (0, \ldots, 0, j) \). In the \( n_i \)-language, the “hole” \( \{I_i\} = (1 - \frac{N+1}{2}, \ldots, N - 2 - \frac{N+1}{2}, N - \frac{N+1}{2}, N+1 - \frac{N+1}{2}) \) is \( \{n_i\} = (0, \ldots, 0, 1, 1) \). A way of introduction of quasiparticles with the help of the \( n_i \)-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]

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

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

\[
P = \sum_{j=1}^{N} k_j,
\]

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

\[
|\gamma_N\rangle = 0
\]

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 \( \leq 0.1\% \). In this case, the error depends strongly on \( \gamma \) and \( N \): \( |v_s^{mic} - v_s^{th}| \approx \frac{0.01}{\gamma N} \).

We now consider the system under the zero BCs. Relation [3] yields

\[
\sum_{j=1}^{N} |k_j| = \frac{\pi}{L} \sum_{j=1}^{N} n_j + \frac{1}{L} \sum_{i,j=1, i\neq j}^{N} \arctan \frac{c}{|k_i| + |k_j|}.
\]
Introduce the quantity
\[
P(\{ |k_i| \}) = \sum_{j=1}^{N} |k_j| - \frac{1}{L} \sum_{l,j=1}^{N} \arctan \frac{c}{|k_l| + |k_j|} |j\neq l|, \tag{15}
\]
then relations (14) and (15) yield
\[
P(\{ |k_i| \}) = \frac{\pi}{L} \sum_{j=1}^{N} n_j. \tag{16}
\]

Since \(P\) (15), (16) 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 \(P\) (15), (16) 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 \(\leq N\) (the same limitation exists also for a system of nonpoint bosons [12]). This limitation agrees with (16). The smallest quasimomentum of the system corresponds to the ground state:
\[
P_0 = P(n_{i\leq N} = 1) = \frac{\pi}{L} \sum_{j=1}^{N} 1 = \frac{\pi N}{L} = \pi \rho. \tag{17}
\]

The quasimomentum of a particle-like excitation is
\[
p_{r-1} = P(n_{i\leq N-1} = 1, n_N = r) - P(n_{i\leq N} = 1) = \sum_{j=1}^{N} (|\hat{k}_j| - |k_j|) - \frac{1}{L} \sum_{l,j=1}^{N} \left( \arctan \frac{c}{|k_l| + |k_j|} - \arctan \frac{c}{|k_l| + |k_j|} \right) |j\neq l|, \tag{18}
\]
where \(\{ |\hat{k}_j| \}\) 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
\[
p_{r-1} = \pi (r - 1)/L, \tag{19}
\]
where \(r\) is equal to the value of \(n_N\) for the state with one particle-like excitation: \(r = n_N = 2, 3, 4, \ldots ; n_{j\leq N-1} = 1\). 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 \(v_s^{\text{th}} = v_s^{\text{mic}}\) is satisfied with an error of \(\lesssim 1\%\) for \(\rho = 1; \gamma = 0.1, 1, 10\); \(N = 200, 1000, 5000\).

This error depends on \(\gamma\) and \(N\) approximately as \(\frac{|v_s^{\text{mic}} - v_s^{\text{th}}|}{v_s^{\text{mic}}} \approx 0.5 \sqrt{\gamma N}\). 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 \(\sqrt{\gamma N} \to \infty\). That is, 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 \(v_s^{\text{th}} = v_s^{\text{mic}}\) 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 \(v_s^{\text{th}} = v_s^{\text{mic}}\). 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 \(N \gtrsim 100\); for the zero BCs, this occurs for larger \(N\): \(N \gtrsim 1000\).

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
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 [13] and the formula for the energy of a quasiparticle is [3]

$$E = \sum_{j=1}^{N} (\hat{k}_j^2 - k_j^2).$$

Under the periodic BCs we use formulae (13), (20). We find the solutions $\{\hat{k}_j\}$ and $\{k_j\}$ from Eqs. (8) under the periodic BCs and from Eqs. (9) under the zero BCs. In this case, $\{\hat{k}_j\}$ corresponds to the state with one quasiparticle ($n_{j \leq N-1} = 0$, $n_N = r$ for the periodic BCs and $n_{j \leq N-1} = 1$, $n_N = r > 1$ for the zero BCs), whereas $\{k_j\}$ corresponds to the ground state ($n_{j \leq N} = 0$ for the periodic BCs and $n_{j \leq N} = 1$ 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 Fig. 1, 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 the 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 Fig. 1 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 $n_j$: $n_{l \leq j \leq l+1} = 1$, $n_{l+1 < j \leq N} = 2$, where $l = 0, 1, \ldots, N - 2$. Under the periodic BCs, holes are the states with $n_{l \leq j \leq l+1} = 0$, $n_{l+1 < j \leq N} = 1$ ($l = 0, 1, \ldots, N - 2$) and the states with $n_{1 \leq j \leq k} = -1$, $n_{k < j \leq N} = 0$ ($k = 0, 1, \ldots, N - 2$).
2, 3, . . . , 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 (Fig. 1) 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 \( T = 0 \)) [12]:

\[
\frac{\sqrt{\gamma}}{2\pi} \ln \frac{N\sqrt{\gamma}}{\pi} \ll 1. \tag{21}
\]

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. [7] at \( N = 1000 \); therefore, the dispersion law \( E(p)|_{N=1000} \) coincides with the above-found one \( E(p)|_{N=\infty} \) and is close to the Bogoliubov law, if \( \gamma \lesssim 1 \). We remark that the dispersion law for \( \gamma = 10 \) (see Fig. 1) is closer to the Bogoliubov law, than to the Girardeau’s one. Though it would be expected the contrary, since the Girardeau’s formula is exact at \( \gamma = +\infty \), whereas the Bogoliubov formula loses its meaning at such \( \gamma \).

The reason for the applicability of the Bogoliubov solutions at not small \( \gamma \) 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 (15).

The question is, how to 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 the Gaudin’s wave function (5) to a localized wave package with a definite momentum.

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