Exact crystalline solution for a one-dimensional few-boson system with point interaction

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Received 21 August 2021, revised 19 January 2022
Accepted for publication 15 February 2022
Published 3 March 2022

Abstract
We study the exact solutions for a one-dimensional system of \( N = 2 \); 3 spinless point bosons for zero boundary conditions. In this case, we are based on M Gaudin's formulae obtained with the help of Bethe ansatz. We find the density profile \( \rho(x) \) and the nodal structure of a wave function for a set of the lowest states of the system for different values of the coupling constant \( \gamma \geq 0 \). The analysis shows that the ideal crystal corresponds to the quantum numbers (from Gaudin’s equations) \( n_1 = \cdots = n_N = N \) and to the coupling constant \( \gamma \ll 1 \). We also find that the ground state (GS) of the system \( (n_1 = \cdots = n_N = 1) \) corresponds to a liquid for any \( \gamma \) and any \( N \gg 1 \). In this case, the wave function of the GS is nodeless, and the wave function of the ideal crystal has nodes.

Keywords: Bose crystal, one dimension, point bosons, ground state

(Some figures may appear in colour only in the online journal)

1. Introduction

The one-dimensional (1D) crystals were observed in the form of stripes in a two-dimensional (2D) system in many experiments (see, e.g., [1–3] and references therein). Recently, the stripe 1D Bose crystals were found in a three-dimensional (3D) system placed in the field of a trap [4–7]. The 1D Bose crystals are of great theoretical interest since a 1D system is much simpler than 2D and 3D ones, which facilitates the finding of solutions. On the whole, the analytic or numerical search for an \textit{accurate} solution for a crystal is a very complicated problem. All
solutions we know for a crystal are approximate. In what follows, we will obtain (seemingly, for the first time) the exact solution for the ideal Bose crystal of \( N = 2 \); point atoms in one dimension.

The solutions for 1D Bose crystals without the external field were investigated in many works \([1–3, 8–16]\). In particular, Gross obtained a crystalline solution for a 1D Bose system in the mean-field approximation \([8]\). Nepomnyashchii \([9]\) considered the crystal-like 1D solution for a 3D Bose system with a condensate of atoms with momentum \( \hbar \mathbf{k} \) (where \( \mathbf{k} \) is a vector of the reciprocal lattice of a 1D crystal). In the work by Shevchenko, a possibility of the appearance of a 1D superfluidity along the line of dislocations in a 3D Bose crystal was studied \([10]\). Arkhipov et al. numerically found a crystalline regime for the ground state (GS) of a 1D Bose system with the dipole–dipole repulsive interaction \([11]\). The crystalline 1D solutions for a 2D system of dipoles were obtained within various methods in works \([1–3, 12–15]\). The approximate 1D crystalline solution corresponding to a fragmented condensate of atoms was found for a \( j \)-dimensional periodic system; \( j = 1; 2; 3 \) \([16]\) (the 1D nature of this solution can be seen from the fact that the axis \( x \), say, can always be directed along the vector \( \mathbf{k} \) describing the crystal).

In the last decade, the 1D crystalline solutions were obtained for 3D \([5, 7, 17]\) and 1D \([18–23]\) systems of dipoles in a trap (see also the review on few-boson 1D systems \([24]\)). The GS of a 1D dipolar system corresponds to a crystal in the case of the strong repulsion of dipoles, which takes place at a large constant of dipole–dipole interaction \([18–23]\) or at a small distance between dipoles \([19, 20]\). However, for a 1D Bose system with the point interaction, GS corresponds to a gas (liquid) at any parameters of the system. This was shown for an infinite system with periodic boundary conditions (BCs) in the classical work by Lieb and Liniger \([25]\). This property is true also for zero BCs, since the GS energy of a 1D system of point bosons is the same in the thermodynamic limit for periodic and zero BCs \([26, 27]\). In what follows, we will show that GS of a finite 1D system of point bosons with zero BCs also corresponds always to a gas (liquid).

According to the well-known result by Landau, the infinite 1D crystal must be destroyed by fluctuations \([28, 29]\). This conclusion is valid for the 1D crystalline ordering in a system of any dimensionality: 1, 2 or 3. However, as early as Frenkel noted that Landau’s conclusion is not quite correct for real (finite) crystals, because for a finite 1D system the transition from the sum \( \sum_{j=1}^{\infty} T/k_j^2 \) to the integral \( (TL/2\pi) \int_{0}^{\infty} dk/k^2 \) is not proper \([30]\) (this was also noted in \([29]\)). In nature, all systems are finite. Therefore, the Landau’s result significantly reduces the stability region of 1D crystals, but does not forbid their existence. In addition, the GS of a 1D system of point bosons corresponds to a liquid even at small \( N, L \) (see the upper curve in figure 5 below) for which Landau’s forbidding clearly does not work. Therefore, it is clear that the liquid character of GS of a 1D system of point bosons is not related to Landau’s forbidding.

In the present work, we will investigate the exact crystalline solution and the nature of the lowest state for a 1D system of spinless bosons with point interaction.

2. Solution for a 1D Bose crystal

It is impossible to find the exact solution for a 2D or 3D crystal, at least at present. Some authors believe that certain Monte Carlo methods provide a numerically exact solution. As far as we see, in practice they give only an approximate solution. Moreover, any ‘exact’ Monte Carlo method gives no analytic solution for a wave function (WF) and observable quantities. However, in the case of a 1D system, the exact crystalline solution can be found for a point interatomic interaction. To this end, we use a theory based on the Bethe ansatz \([25, 31–34]\) (see also the recent reviews \([27, 35, 36]\)).
Consider the system of $N$ spinless point bosons not placed in an external field, under zero BCs ($\Psi = 0$ on the boundaries). The Schrödinger equation for such a system reads

$$-\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} \Psi + 2\epsilon \sum_{i<j} \delta(x_i - x_j) \Psi = E \Psi. \quad (1)$$

Here, $\hbar = 2m = 1$. Using the analysis in [32, 33], we find that, for $N = 2$, any pure state of such a system is described by WF

$$\Psi_{(k)}(x_1, x_2)|_{x_1 \leq x_2} = 4 \left(1 + \frac{c^2}{k_1^2 - k_2^2}\right) \sin k_1 x_1 \sin k_2 x_2$$
$$+ 4 \left(1 + \frac{c^2}{k_2^2 - k_1^2}\right) \sin k_2 x_1 \sin k_1 x_2$$
$$+ 4 \left(\frac{c}{k_1 - k_2} - \frac{c}{k_1 + k_2}\right) \sin k_1 x_1 \cos k_2 x_2$$
$$+ 4 \left(\frac{c}{k_2 - k_1} - \frac{c}{k_1 + k_2}\right) \sin k_2 x_1 \cos k_1 x_2. \quad (2)$$

If $x_1 > x_2$, the solution for WF follows from (2) by the permutation of $x_1$ and $x_2$. For any $N \geq 2$, the quantities $k_1, \cdots, k_N$ satisfy the Gaudin’s equations [32, 33]

$$L_k j = \pi n_j + \sum_{i=1}^{N} \left(\arctan \frac{c}{k_j - k_i} + \arctan \frac{c}{k_j + k_i}\right) |_{i \neq j}, \quad j = 1, \cdots, N, \quad (3)$$

where $n_j$ are integers, $n_j \geq 1$ [32, 33, 37], $c \geq 0$ is the interatomic interaction constant, and $L$ is the size of the system. Different states correspond to different collections of $\{n_j\} \equiv (n_1, \cdots, n_N)$. In particular, $n_j = 1$ for GS. For the excited states, $n_j \geq 1$ for all $j = 1, \cdots, N$; in this case, $n_j > 1$ at least for one $j$ [26, 32, 33, 38]. We note that, in (2)–(6), $k_1, \cdots, k_N$ denote the quantities $|k_1|, \cdots, |k_N|$, respectively.

For $N = 3$, WF of any pure state reads [32, 33]

$$\Psi_{(k)}(x_1, x_2, x_3)|_{x_1 \leq x_2 \leq x_3} = \sum_{\varepsilon_1, \varepsilon_2, \varepsilon_3 = \pm 1} A(\varepsilon_1, \varepsilon_2, \varepsilon_3)$$
$$\times \sum_{p} a(k_1, k_2, k_3) e^{i\varepsilon_1 k_1 x_1 + i\varepsilon_2 k_2 x_2 + i\varepsilon_3 k_3 x_3}, \quad (4)$$

where $\sum_{p}$ is the sum over all possible permutations of the numbers $\varepsilon_1 k_1, \varepsilon_2 k_2, \varepsilon_3 k_3$,

$$a(k_1, k_2, k_3) = \left(1 + \frac{ic}{\varepsilon_1 k_1 - \varepsilon_2 k_2}\right) \left(1 + \frac{ic}{\varepsilon_2 k_2 - \varepsilon_3 k_3}\right) \left(1 + \frac{ic}{\varepsilon_3 k_3 - \varepsilon_1 k_1}\right). \quad (5)$$

$$A(\varepsilon_1, \varepsilon_2, \varepsilon_3) = \varepsilon_1 \varepsilon_2 \varepsilon_3 \left(1 - \frac{ic}{\varepsilon_1 k_1 + \varepsilon_2 k_2}\right) \left(1 - \frac{ic}{\varepsilon_2 k_2 + \varepsilon_3 k_3}\right) \left(1 - \frac{ic}{\varepsilon_3 k_3 + \varepsilon_1 k_1}\right). \quad (6)$$

WFs (2) and (4) are not normalized. Note that WF (2) is real, and WF (4) is purely imaginary. In order to obtain $\Psi_{(k)}(x_1, x_2, x_3)$ for the configuration $x_3 \leq x_1 \leq x_2$ (for example), one needs to make in (4) changes $x_1 \rightarrow x_3, x_2 \rightarrow x_1, x_3 \rightarrow x_2$. 


Figure 1. Nodal lines \((\Psi(x_1, x_2) = 0)\) for a system of \(N = L = 2\) point bosons under the zero BCs for the state with \(n_1 = n_2 = 2\): at \(\gamma = 0\) (solid lines), \(\gamma = 0.1\) (rhombus), \(\gamma = 1\) (squares), \(\gamma = 10\) (triangles), and \(\gamma = 100\) (circles).

We remark that, in the analysis below, the values of \(kj\) for different \(c, N, L, nj\) are found by numerically solving equation (3) by the Newton method.

The analysis of functions (2) and (4) for \(N = 2; 3\) indicates that the ground-state WF is nodeless for any coupling constant \(\gamma \equiv c/g \geq 0\) (but \(\gamma < \infty\)), where \(g = N/L\) is the concentration (we follow the terminology [39], according to which the nodal points, nodal lines, and nodal surfaces of any dimensionality are called nodes). For the low-lying states with the given collection of numbers \(n_j\) (we studied all states with \(1 \leq n_1, \cdots, n_N \leq N + 1\)), the evolution of the nodal structure of WF occurs in the following way, as \(\gamma\) increases. For \(\gamma = 0\), the nodal surfaces divide the space \(0 \leq x_1, \cdots, x_N \leq L\) into \(l\) segments, where the value of \(l\) depends on the collection \(\{n_j\}\). At \(0 < \gamma < \infty\) for some collections \(\{n_j\}\), several of those segments can separate themselves into parts. In this case, for each collection \(\{n_j\}\), the number of segments \(l\) is the same for all \(0 < \gamma < \infty\). As \(\gamma\) increases, only the shape of segments slightly changes (see figures 1 and 3). Presumably, these properties hold true for the high-lying states as well.

Thus, the nodal structure of WF is the same for all \(0 < \gamma < \infty\). As \(\gamma\) increases, some segments merge, while others divide themselves into parts. In this case, the maxima of \(|\Psi|^2\) smoothly shift. The transition from \(\gamma \gg 1\) to \(\gamma = \infty\) leads to the addition of the nodal lines \(x_j = x_l\) (here, \(j \neq l\) and \(j, l = 1, \cdots, N\)). In general, for each state \((n_1, \cdots, n_N)\) the distribution of atoms in a rough approximation is approximately the same for all \(0 \leq \gamma \leq \infty\). This means that the structure of any solution, including the crystalline one, for a given \(\gamma > 0\) can be very approximately understood by examining the solution for free bosons \((\gamma = 0)\) with the same \(n_1, \cdots, n_N\) (we stress that we keep in mind the structure of the solution in a crude approximation: the nodal structure of WF and approximate distribution of atoms; to understand the details of the solution, one needs, of course, to find the solution for a given \(\gamma > 0\), as one can see in figure 4). We suppose that this property is true for any \(N \geq 2\) and any dimension of the space. However, for a non-point interaction this property is not valid, at least for the 1D systems (e.g. GS of a 1D system can correspond to either a crystal, or liquid, depending on the coupling constant [18–23]).

Interestingly, the ideal crystal (the state of the \(N\)-particle system for which the density profile \(\rho(x) = N \int dx_2 \cdots dx_N |\Psi(x, x_2, \cdots, x_N)|^2\) contains \(N\) identical equidistant peaks) corresponds to the quantum numbers \(n_1 = n_2 = \cdots = n_N = N\) and to values \(\gamma \lesssim 1\) (see figures 2 and 4). In
Figure 2. Density profile $\rho(x)$ of a system of point bosons under the zero BCs at $N = L = 2$, $\gamma = 1$, for the following states: $n_1 = n_2 = 1$ (solid line); $n_1 = 1, n_2 = 2$ (triangles); $n_1 = n_2 = 2$ (stars); $n_1 = 2, n_2 = 3$ (squares); and $n_1 = 3, n_2 = 4$ (circles).

In Figure 2 we present the density profiles $\rho(x)$ at $N = 2$ for the GS ($n_1 = n_2 = 1$) and states close to the crystal one. Figure 4 shows the evolution of the density profile for $N = 3$, as $\gamma$ increases. In Figures 2 and 4, $\Psi$ is normalized to 1. For $N > 3$, the ideal crystal should also correspond to the quantum numbers $n_j \leq N = N$ since, for free bosons, the crystal corresponds namely to such $n_j$ (as can be shown), and with an increase in $\gamma$ the nodal structure almost does not change (see above). The formula $n_j \leq N = N$ is also related to results by Syrwid and Sacha [40]. In this article, the averaged density $\tilde{\rho}(x)$ is found for the state $n_1 = \ldots = n_N = J$ at $J = 2; 3; 4$ and $N = 6; 7$ (see also review [27]). As far as we understand, $\tilde{\rho}(x)$ from [40] is equivalent to $\rho_N(x_N)$ from [41]: it is the probability density of finding the $N$th particle at the point $x_N$ provided that the coordinates of $N - 1$ remaining particles have been measured, and the averaging over many measurements has been carried out. Perhaps, under the zero BCs $\tilde{\rho}(x)$ coincides with $\rho(x)$, if $\tilde{\rho}(x)$ is obtained by averaging over an infinite number of measurements. Each solution in [40] contains $J$ immovable domains associated by the authors with $J - 1$ solitons. In our opinion, the analysis in [40] is not sufficient for the proof of solitonic properties of such solutions. In particular, the classical solitonic analogs of such solutions have not been found. Rather, these are domain solutions. The solution with $J = N$ corresponding to the ideal crystal was not considered in [40]. However, the results in [40] indicate that for $J = N$ there should be $N$ domains. This agrees with the above results, though we have found the ordinary density $\rho(x)$ instead of $\tilde{\rho}(x)$ (under periodic BCs, the density is constant: $\rho(x) = \text{const}$; therefore, to determine the structure of a solution, one needs to find more complicated functions instead of $\rho(x)$, for example, the binary distribution function $g_2(x_1, x_2)$ or $\tilde{\rho}(x)$; however, under the zero BCs, we have $\rho(x) \neq \text{const}$ and it is usually sufficient to find only $\rho(x)$ to understand the structure of a solution).

Based on available information, we suppose that the ideal crystal corresponds solely to the quantum numbers $n_1 = n_2 = \ldots = n_N = N$ (i.e. any other collection $\{n_j\}$ does not correspond to the ideal crystal, for any $\gamma$).

By the node theorem [39], if the states $\Psi_j$ are associated with the numbers $j = 1, 2, \ldots, \infty$ in the order of increasing energies $E_j$, then the nodes of the function $\Psi_j$ divide the phase space $x_1, \ldots, x_N$ into $l \leq j$ segments. In this case, the lowest state must be non-degenerate, and the higher states can be degenerate [39]. The theorem was proved for one particle in the 2D space,
Figure 3. Nodal lines \(\langle \Psi(x_1, x_2, x_3) \rangle_{x_3=L/2} = 0\) for a system of \(N = L = 3\) point bosons under the zero BCs for the state with \(n_1 = n_2 = n_3 = 3\); for \(\gamma = 0\) (solid lines), \(\gamma = 1\) (squares), \(\gamma = 10\) (triangles), and \(\gamma = 100\) (circles). Here, we show the cross-section of a 3D nodal network by the plane \(x_3 = L/2\).

Figure 4. Density profile \(\rho(x)\) of a system of point bosons under the zero BCs for the state with \(n_1 = n_2 = n_3 = 3\), \(N = L = 3\): for \(\gamma = 0\) (stars), \(\gamma = 1\) (squares), \(\gamma = 10\) (triangles), and \(\gamma = 100\) (circles).

but the proof can be easily generalized to the case of any \(N > 1\) and any dimension of the space. Our results for \(N = 2; 3\) are in agreement with this theorem. Additionally, we have established for the lowest states of a 1D system of \(N = 2; 3\) point bosons that, for any collection \(\{n_j\}\), the number of segments \(l\) is independent of \(\gamma\) (if \(0 < \gamma < \infty\)), and the shape of segments depends weakly. For illustration, we remark that the nodes can ‘draw’ whimsical patterns in the profile of the probability density \(\langle \psi_j(x_1, \cdots, x_N) \rangle^2\), see figures 5 and 6 in [42].

From a physical standpoint, the properties described above mean the following. Each \(n_j > 1\) corresponds to a quasiparticle with a quasimomentum \(p_j = \hbar \pi (n_j - 1)/L\) [38]. At the weak and strong coupling, we have, respectively, Bogolyubov–Feynman quasiparticles [43–45] and Girardeau–Lieb particle excitations [46, 47]. Therefore, each state \(\{n_j\}\) corresponds to some
collection of quasiparticles \( \{ p_j \} \). According to the above analysis, for each state with a collection of quasiparticles \( \{ p_j \} \), the distribution of atoms (maxima of \( |\Psi|^2 \)) is approximately the same for all \( 0 \leq \gamma \leq \infty \). The ideal crystal corresponds to \( n_1 = \cdots = n_N = N \), i.e. to \( N \) identical quasiparticles with the quasimomentum \( p_j = \hbar \pi (N - 1) / L \equiv \bar{p}_c \). In other words, the crystal is formed by the condensate of \( N \) quasiparticles with the quasimomentum \( \bar{p}_c \). It is the lowest (ground) state of the crystal. The close states for which some \( n_j \) are slightly different from \( N \) correspond presumably to a crystal with excitations or defects.

It is worth noting that the quasiparticles in a 1D system of point bosons are usually divided into ‘holes’ and ‘particles’, following the work by Lieb [47]. However, it was recently shown that, at weak coupling, the hole is a set of interacting phonons (‘particles’) with the lowest momentum [48]. This does not contradict the solitonic properties of holes (these properties have been found at weak coupling for the holes with a large momentum \( p \gg \hbar \pi / L \) [41, 49–52]).

Thus, under the zero BCs, there exist the following states with a condensate of quasiparticles: the hole state with a quasimomentum \( \hbar \pi l / L \) (where \( l \sim N \)) is a condensate of \( l \) phonons with a quasimomentum \( \hbar \pi / L \). The \( j \)-domain state [40] is a condensate of \( N \) phonons with a quasimomentum \( \hbar (j - 1) \pi / L \). The above-obtained solution for the ideal crystal corresponds to a condensate of \( N \) short-wave phonons with a quasimomentum \( \hbar (N - 1) \pi / L \). Such states have not been found in experiments, to our knowledge. Most probably, all (or almost all) of them are unstable without the support of an external field with a similar domain structure. It is natural to expect that each of the mentioned above states with a condensate of phonons with a quasimomentum \( \hbar \pi n_1 / L \) (for \( m = 1; j - 1; N - 1 \)) is also characterized by a condensate of atoms with the same quasimomentum.

3. The lowest state of a Bose crystal: basic models

Let us concisely consider how the GS of a Bose crystal is described in the literature. Several ansätze for the ground-state WF of a crystal were investigated (see reviews [53–55]). The historically first and most widely used is a localized-Jastrow ansatz [56–61]

\[
\Psi^c_0 = C e^{i \theta} \sum_{p_c} e^{\sum_{j=1}^N \varphi(r_j - R_j)},
\]

where \( N \) is the number of atoms in the system, \( r_j \) and \( R_j \) are, respectively, the coordinates of atoms and lattice sites, \( \varphi(r) = -\alpha^2 r^2 / 2 \), and \( p_c \) denotes all possible permutations of the coordinates \( r_j \). \( \varphi(r) \) is usually written in the Bijl–Jastrow approximation \( \varphi(r) = \sum_{i<j} \varphi_j(r) \). A wave-Jastrow ansatz reads [62, 63]

\[
\Psi^c_0 = C e^{i \sum_{j=1}^N \theta(r_j)},
\]

where the function \( \theta(r) \) is periodic with the periods of a crystal. In ansätze (7) and (8), the function \( S_0 \) is usually written in the Bijl–Jastrow approximation \( S_0 = \sum_{i<j} S_0(r_i - r_j) \) [64, 65]. Ansatz (8) is a wave type solution and corresponds to a condensate of atoms with WF \( \Psi_0(r) \approx e^{-i \theta(r)} \). In the case of the localized ansatz (7), a condensate of atoms is absent [66–68].

Later, a ‘shadow’ ansatz was proposed [69–71]:

\[
\Psi_0(r) = \int e^{-\Xi(r,s)} ds, \quad r \equiv r_1, \cdots, r_N.
\]
Here, \( s \equiv s_1, \ldots, s_N \) are ‘shadow’ variables, and \( \Xi(r, s) = \sum_{j<k} u_r(\mathbf{r}_j - \mathbf{r}_k) + \sum_i u_{rs}(\mathbf{r}_i - s_i) + \sum_{j<k} u_s(s_j - s_k) \). If \( u_r, u_{rs}, u_s \) are represented in the form of appropriate Fourier series, then WF (9) is translationally invariant.

Finally, a translationally invariant ansatz is given by [72–74]

\[
\Psi_0 = C \cdot e^{S_0},
\]

\[
S_0 = \sum_{j < k} S_2(\mathbf{r}_j - \mathbf{r}_k) + \sum_{j < k < l} S_3(\mathbf{r}_j - \mathbf{r}_k, \mathbf{r}_k - \mathbf{r}_l) + \cdots
\]

\[
+ \sum_{j_1 < j_2 < \cdots < j_N} S_N(\mathbf{r}_{j_1} - \mathbf{r}_{j_2}, \mathbf{r}_{j_2} - \mathbf{r}_{j_3}, \cdots, \mathbf{r}_{j_{N-1}} - \mathbf{r}_{j_N}).
\]

Function (9) is a partial case of WF (10), (11). The latter sets the general form of the exact (isotropic or not) translationally invariant WF of the GS of the Bose system. In other words, the gaseous, crystalline, and liquid GSs of a periodic Bose system are described by WF (10), (11). In practice, it is usually restricted to the simplest Bijl–Jastrow approximation; sometimes, a three-particle correction \( S_3 \) is additionally taken into account.

All ansätze (7)–(11) are applicable to 1D, 2D and 3D crystals. Ansätze (7)–(9) are approximate, and ansatz (10) and (11) is exact. Ansätze (7) and (8) can be treated as approximate solutions for a crystal with zero BCs. Ansätze (9)–(11) are used under periodic BCs. All available in the literature calculations (analytical and numerical) with ansätze (7)–(11) are approximate. Therefore, it is still hard to make a reliable choice between ansatz (7) and ansatz (8), say.

Ansätze (7)–(11) describe crystalline states corresponding to the genuine (nodeless) GS of the Bose system. In 2D and 3D cases, a nodeless crystalline solution is seemingly possible for any reasonable interatomic potential: non-point or point-like. However, for a 1D system the nodeless solutions (7)–(11) are possible only for a non-point potential. Indeed, we have found above (section 2) for the 1D system of spinless point bosons that the WF of the ideal crystal indispensably has nodes. The structure of the WFs of the crystal for \( N = 2; \ 3 \) shows that, in the thermodynamic limit \( (N, L \to \infty, N/L = \text{const.)} \), the exact WF of the ideal 1D crystal with the zero BCs is, seemingly, quite close to the function

\[
\Psi_0^c = C e^{S_0} \prod_{j=1}^N \sin(k_c x_j),
\]

where \( k_c = N\pi/L = \pi/a \), \( a \) is the period of the lattice, and \( S_0 \) is equal to the sum of a two-particle term \( \sum_{p < j} S_2(x_p - x_j) \) and the many-particle correlation corrections. The function \( S_c(x_1, \cdots, x_N) \) is unknown and can be found from the Schrödinger equation. The product of sines in (12) directly sets the crystal lattice.

One can comprehend the structure (12) from a qualitative reasoning. Consider a 1D system of \( N \) free bosons under the zero BCs. In this case, GS is described by the nodeless \( \Psi_0 = C \prod_{j=1}^N \{ \sin(\pi x_j/L) \} \), and the crystal is set by the multi-node WF (12) with \( S_0 = S_c = 0 \). It is an ideal crystal with one atom per cell. It was shown above that if we ‘switch on’ the point interaction and increase its strength, then the number and location of cells do not virtually change. Only the probability density distribution for atoms in the cell changes. It holds for the interatomic interaction of zero range and, apparently, small nonzero one. Therefore, we can crudely see the general structure of WF of the crystal in the case of a strong coupling by considering the corresponding WF for zero coupling. Namely, the crystal is formed by a condensate of \( N \) quasiparticles with a quasimomentum \( p_c = \hbar N(N-1)/L \). At zero coupling, this
corresponds to $N$ free bosons with a quasimomentum $p_c$. We suppose that formula (12) qualitatively correctly describes the structure of GS of a macroscopic finite crystal (everywhere, except for a narrow near-boundary region, where the size of cells can be different), if the interaction has a small radius ($\ll \bar{d}$; $\bar{d}$ being the average interatomic distance) and is repulsive. In this case, the factor $e^{\epsilon_0}$ describes the interatomic correlations, and the factor $e^{\epsilon_c}$ corresponds to the influence of the interatomic interaction on the distribution of atoms in the cell.

We remark that, at the interatomic interaction with nonzero range, the ‘replacement’ of the solution for a strong coupling by the corresponding one for zero coupling may lead to an error. Since for such a 1D system with strong coupling, the crystal may correspond to a nodeless $\Psi_0^c$ (the genuine GS of the system) [11, 18–23], whereas the crystal-like solution $\Psi_0^c = C \prod_{j=1}^{N} \{\sin(\pi x_j/a)\}$ obtained for zero coupling has many nodes.

It is currently accepted in the literature that the lowest states of 2D and 3D Bose crystals are described by wave functions without nodes. However, we do not exclude the existence in nature of Bose crystals whose lowest state corresponds to a wave function with many nodes (which is similar to (12), but is 2D or 3D). However, there is yet no reliable evidence (theoretical or experimental) of the existence of such crystals. In particular, symmetry analysis is not enough to ascertain whether the GS of a Bose system is a crystal or a liquid [75].

4. Discussion

It is worth noting that the field of a trap can strongly change the structure of GS, since the trap field decreases the symmetry of the Hamiltonian $\hat{H}$. In particular, when switching on the trap field, $\hat{H}$ ceases to commute with the operator of the total momentum. In this case, the translational symmetry disappears. If the trap field is very strong and corresponds to an ideal crystal, then it is clear that the genuine GS of a system corresponds most likely to the same crystal. On the whole, we may expect that GS corresponds to the most symmetric WF from the set of eigenfunctions of the boundary-value problem [76]. Therefore, a decrease in the symmetry of the Hamiltonian should lead to a decrease in the symmetry of GS.

4.1. Structure of the ground state of the 1D system of point bosons

In section 2, we considered the exact solutions for systems of $N = 2; 3$ spinless point bosons. The results indicate that the ideal crystal corresponds to WF with a lot of nodes, whereas the nodeless GS is characterized by the most smooth density profile $\rho(x)$ and, therefore, corresponds to a liquid (gas). At $N \gg 1$, GS of such a system also corresponds to a liquid (gas) for any $\gamma \geq 0$. This is seen from that the GS energy $E_0$ [25, 26, 32, 77] for $\gamma \ll 1$ is close to Bogolyubov’s one [43, 44], and the curves $E_0(g)|_{N,\gamma = \text{const}} \sim g^2$ and $E_0(\gamma)|_{N, g = N/L = \text{const}}$ [25] for $0 < \gamma < \infty$ contain no features, which indicate a possible transition to the crystal regime. Finally, at $\gamma = \infty$, the system is a gas of impenetrable bosons [46].

The results listed in the previous paragraph are obtained mainly for periodic BCs and in the thermodynamic limit ($N, L \to \infty, N/L = \text{const}$). We now investigate the function $E_0(\gamma)$ for finite $N \gg 1$ and the zero BCs. Dimensional reasoning implies that the energy $E_0$ of a 1D system of $N \gg 1$ point bosons can be represented in the form [25]

$$E_0 = Ng^2 e_0(\gamma),$$

(13)

where $e_0$ depends only on $\gamma$. We verified this property for the zero BCs. To make it, we numerically found the numbers $k_j$ for GS ($n_j \leq N$) from equation (3) at $N = 10; 100; 1000$ and $c = 0.01; 1; 100$. The analysis confirmed that, for a fixed $N$, the quantity $e_0$ in (13) depends only on $\gamma$. If the system would transit from the gaseous (liquid) state to a crystal one at a change
Figure 5. Function $e_0(\gamma)$ (13) for a 1D system of spinless point bosons with the zero BCs for $N = 10$ (dotted line), $N = 100$ (dashed line), and $N = 1000$ (solid line). Dash-dotted line marks the limiting value $e_0(\gamma \to \infty, N = 1000) = \left(1 - \frac{1}{3N^2}\right) \frac{\pi^2}{3}$ obtained by Girardeau for periodic BCs [46]. Here, $\lg \equiv \log_{10}$.

in the parameters ($L$, $c$ or $g$), then we would observe a jump on the curve $e_0(\gamma)$ (or $\partial e_0(\gamma)/\partial \gamma$, or $\partial^2 e_0(\gamma)/\partial \gamma^2$) for some $\gamma = \gamma_c$. Since the regimes $\gamma \ll 1$ and $\gamma \gg 1$ correspond to a gas (Bogolyubov gas and the Tonks–Girardeau gas, respectively), there should be two points $\gamma_c$, and they should be fairly close to each other: $\gamma_c \sim 1–10$ for both ones. However, the curves $e_0(\gamma)$ (see figure 5) contain no similar peculiarities (we obtained these curves by changing $\gamma$ with a sufficiently small step $\gamma \to 1.1 \gamma$). The signs of a smooth transition of the crossover type are also absent.

Thus, the GS of the 1D system of spinless point bosons corresponds to a liquid (gas) for any parameters of the system. In the case of non-point interaction, the GS of a 1D system can correspond not only to liquid (gas) but also to a crystal (see below).

In this work, we do not distinguish between gas and liquid. Indeed, the main difference between a gas and a liquid is that liquid keeps its volume (due to surface tension), while gas does not. This difference disappears for the 1D system since it has no surface (consequently, there is no surface tension). In principle, a gaseous and liquid state could differ in the properties of the distribution functions (e.g. the function $g_2(x_1, x_2)$). But then, the transition from one phase to the other when $\gamma$ varies would lead to a change of the function $e_0(\gamma)$. However, as we noted above, features of such a change are absent. Therefore, we believe that for the 1D system of point bosons, the gaseous and liquid states do not differ.

4.2. Mechanisms of formation of 1D Bose crystals

As was mentioned in the introduction, the crystalline regime was found for the lowest state of a 1D Bose system with dipole–dipole interaction [11, 18–23]. In particular, for the singular potential $U(x_j, x_l) = g_d (x_j - x_l)^3$ crystalline solutions were obtained for the concentrations exceeding some critical one: $n > n_c$ [11, 19, 20]. For the nonsingular potential $U(x_j, x_l) = \frac{g_d}{(x_j - x_l)^{1+\alpha}}$, crystalline solutions were found for a strong interaction $(g_d > g_c)$ [18–23] and are almost independent of the magnitude of the trap field [23]. We remark that for $g_d > g_c$ there should exist two solutions corresponding to the ideal crystal: the nodeless solution obtained in [11, 18–23]
and a solution of the type (12) with a large number of nodes. We may expect that they are characterized by a similar structure of $g_2(x_1, x_2)$, but by different energies.

The overall picture of the conditions under which the lowest state of a 1D system of interacting bosons corresponds to a crystal is still not completely clear. Crystalline solutions for a 1D system were explored in works [8, 11, 16, 18–23] (see also [9, 78]). In this case, the analysis in [8, 9, 16, 78] is approximate. The numerical solutions for few-boson systems [18–23] and the exact solution in the present work are, seemingly, reliable. Perhaps, a solution [11] by the Monte Carlo method is also close to exact. In other words, only the solutions for the point-like and dipole–dipole [11, 18–23] interactions are reliable. We conjecture that the main reason for the crystallization of the lowest state of the dipole system is the strong atomic repulsion on small (but nonzero) interatomic distances $|x_j - x_l|$. Because of that repulsion, every two adjacent particles strive to stay as far away from each other as possible, which seemingly corresponds to a crystal state. In this case, the crystalline ordering is energetically most preferred and arises in the genuine nodeless GS. We suppose that the long-range character of the interaction plays a small role in this instance: most of all, crystallization will also occur in the case of a short (or mid) range potential with radius $b > d$ (e.g. $U(x_j, x_l) = \frac{g_2}{(x_j - x_l)^2 + \alpha^2}$ for $|x_j - x_l| \leq b$, and $U(x_j, x_l) = 0$ for $|x_j - x_l| > b$); to our knowledge, only the case of $b = \infty$ was investigated in the literature. In the case of point interaction, the above mechanism does not work since a $j$th and $l$th particles interact only when $|x_j - x_l| = 0$. In that case, a crystal is created by the nodes of WF. It is an entirely different mechanism. In addition, the approximate analysis in [8, 16, 78] indicates that the crystalline solution can be energetically most favored given the interaction is non-point: in this case, the Fourier transform $\nu(k)$ of the potential is negative at some $k$’s, which can make the crystal energetically preferred over a liquid. It gives, in general, a third possible mechanism for crystal formation. Under such a mechanism, the crystalline energy minimum in the space of states may be absolute or local. If this minimum is absolute, the third mechanism is equivalent (or close) to the first from the mentioned above mechanisms. If the minimum is local, the third mechanism can be equivalent to the second (node) mechanism. To clearly understand the conditions required for crystallization, one needs to investigate the solutions for various potentials in detail. It is a task for the future.

5. Conclusion

We note a few of the results obtained above. We have found the exact crystalline solution for a 1D system of point bosons. It corresponds to small and intermediate values of the coupling constant ($\gamma \lesssim 1$). The results of the earlier work [40] indicate that such a solution should exist. It is of importance that the ideal crystal corresponds to the wave function with nodes and (at $N \gg 1$) is formed by the condensate of short-wave phonons. Interestingly, at $0 < \gamma < \infty$ the nodal structure of the wave function is invariable at a change of $\gamma$ (we have investigated $(N + 1)^N$ lowest states for $N = 2, 3$).

Acknowledgments

The author acknowledges support by the National Academy of Sciences of Ukraine grant ‘Effects of external fields and spatial inhomogeneities on the electronic properties of Dirac and superconducting materials’ (program KPKVK 6541230).
Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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