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Exact methods in the analysis of the non-equilibrium dynamics of integrable models: application to the study of correlation functions for non-equilibrium 1D Bose gas

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Abstract. In this paper we study the non-equilibrium dynamics of one-dimensional Bose gas from the general perspective of the dynamics of integrable systems. After outlining and critically reviewing methods based on the inverse scattering transform, intertwining operators, q-deformed objects, and extended dynamical conformal symmetry, we focus on the form-factor based approach. Motivated by possible applications in nonlinear quantum optics and experiments with ultracold atoms, we concentrate on the regime of strong repulsive interactions. We consider dynamical evolution starting from two initial states: a condensate of particles in a state with zero momentum and a condensate of particles in a Gaussian wavepacket in real space. Combining the form-factor approach with the method of intertwining operators we develop a numerical procedure which allows explicit summation over intermediate states and analysis of the time evolution of non-local density–density correlation functions. In both cases we observe a tendency toward the formation of crystal-like correlations at intermediate timescales.

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Contents

1. Introduction

Quantum many-body systems in low dimensions cannot typically be described using mean-field approaches. This makes analysis of their non-equilibrium dynamics particularly challenging. However following demand from recent experiments, certain progress has been achieved in developing theoretical methods which can address this problem. In this paper we use a Bethe ansatz solution to study the non-equilibrium dynamics of the one-dimensional Bose gas interacting via contact interaction. This microscopic model of δ-interacting bosons is called the Lieb–Liniger (LL) model [1]–[3]. It belongs to a general class of models which can be studied using a Bethe ansatz solution [4]. These exactly solvable models are characterized by an infinite number (in the thermodynamic limit) of conserved quantities which originate from the nature of the collision processes. In the LL model the two-particle collisions cannot change the momenta of scattering particles, and only give rise to a phase shift. Moreover any many-body collision is factorizable into a sequence of two-body scattering events. While implications of the exact solution for thermodynamic properties have been discussed before [1, 4, 5], their consequences for non-equilibrium dynamics are not known. This will be the central question of our paper.

Systems of one-dimensional Bose gases with contact interactions have been recently realized using ultracold atoms [6]–[10], and current experiments allow wide control over parameters of the microscopic Hamiltonian (see [11, 12] for a recent review). For example, the effective strength of the repulsive interaction can be tuned either by changing the density of the atomic cloud, or by modifying the strength of the transverse confinement, or by changing the scattering length using magnetically tuned Feshbach resonance. In particular a very interesting regime can be achieved when repulsion is so strong that bosonic atoms become essentially impenetrable [13] and the system undergoes effective fermionization [6]–[8]. Recent studies of thermodynamic properties demonstrated excellent agreement between experiments and the exact solution [8, 10]. However parameters of the Hamiltonian can also be changed dynamically. In this case one needs to study the dynamics starting with the initial state which is not an eigenstate of the Hamiltonian. Generally such dynamics involves superposition of coherent evolutions of all eigenstates of the system. This is the problem that we address in this paper.

Another class of systems where the LL model appears naturally is those of light propagation in one-dimensional photonic fibers. It has been known since the 1960s (see e.g. [14]) that propagation of classical pulses of electromagnetic waves in a one-dimensional nonlinear medium can be described by the nonlinear Schrödinger equation, which can be interpreted as the operator equation of motion arising from the LL microscopic Hamiltonian. In this case the nonlinearity is proportional to the nonlinear polarizability of the medium, $\chi^{(3)}$ (see e.g. [15]). A typical propagation problem for one-dimensional nonlinear fiber corresponds to the classical limit of the quantum LL model subject to non-equilibrium boundary and/or initial conditions [16]. Earlier analysis assumed that photon nonlinearities come from the interaction of photons with two-level atoms, in which case nonlinearity corresponds to the attractive interaction in the LL model [17]. Corresponding quantum models have bound states which eventually lead to the formation of solitons and a classical regime [18]. Earlier analysis of optical systems also assumed a regime of weak nonlinearities, since increasing nonlinearities in two-level systems would lead to strong photon losses. However recent techniques utilizing electromagnetically induced

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transparency [19] make it possible not only to realize effective repulsion between photons but also to increase dramatically the strength of nonlinearities [20]. Optical realizations of the LL model should allow direct measurements of both the first-order and the second-order coherences [21], $g^{(1)}(t,\tau) = \langle \Psi^\dagger(t)\Psi(t+\tau)\rangle$ and $g^{(2)}(t,\tau) = \langle \rho(t)\rho(t+\tau)\rangle$, where $\Psi(t)$ is the amplitude of the propagating electromagnetic field and $\rho(t) = \Psi^\dagger(t)\Psi(t)$ is the field intensity, measuring the number of photons.

There are three main reasons why we undertake a detailed analysis of the non-equilibrium quantum dynamics of the LL model. The *first* reason is that dynamics of integrable models, such as the LL model, should exhibit special features originating from an infinite number of integrals of motion. One manifestation of constraints on the phase space available for dynamics should be the absence of thermalization and ergodicity [9, 22, 23]. Conservation laws originating from integrability also lead to the so-called Mazur inequalities [24], which should result in special transport properties. For example, the possibility of an infinite Drude weight has been discussed for several integrable models of lattice fermions [25]. Our *second* motivation for analysis of the LL model is to use it as a testing ground for developing new theoretical methods and techniques, which can then be applied to a broader class of models and systems. Our work should provide a general framework for understanding dynamics of integrable systems and for future developments of non-perturbative methods in the study of non-equilibrium dynamics. We emphasize that our analysis uses special properties of exactly solvable models, and that the methods that we apply here are fundamentally different from the more conventional perturbative approaches discussed in [26, 27]. Finally we point out that recent progress in the areas of ultracold atoms, quantum optics, and low dimensional strongly correlated materials makes it possible to fabricate concrete physical systems, which can be accurately described by the LL model. Thus our *third* reason for analyzing this model is that theoretical predictions for the time-dependent evolution of correlation functions can be measured directly in experiments. Specific systems in which one can realize dynamical experiments discussed in our paper are one-dimensional Bose gases in optical lattices and magnetic microtraps (see [28, 29] for a review). Realization of such experiments should provide a unique opportunity to study non-equilibrium dynamics of strongly correlated exactly solvable systems.

In this paper we calculate the time evolution of the density–density correlation function for two different condensate-like initial states: when all particles are in a state with zero momentum and when all particles are in a Gaussian wavepacket in real space. There are two reasons for focusing on these two states. Firstly, both of these states correspond to important physical systems: a zero-momentum state represents a good starting point for discussions of the dynamics of a Bose condensate when the interaction is suddenly switched on (which can be done in real experiments), whereas the Gaussian wavepacket in real space is a prototypical example of the photonic pulse in quantum optics. The second reason is related to the fact that the time evolution of these two states can be accessed analytically to a large extent and quite easily handled numerically. We emphasize here that this is *not* the case for a generic initial state. Therefore further progress in the understanding of the dynamics of the generic initial state would be highly desirable.

This paper is organized as follows. Section 2 provides a brief *critical* overview of several different methods which can be used to describe non-equilibrium dynamics of

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integrable quantum systems such as the LL model. Section 3 provides an in-depth discussion of one of these approaches, the so-called form-factor technique, which relies on numerical summation over intermediate states. The overlap with the initial states in the strongly interacting regime is found using the method of intertwining operators. In section 4 we focus on the non-equilibrium dynamics of the many-body system described by the LL model. There we choose two particular initial states as explained above. A summary of our results and conclusions is given in section 5. To provide additional background to the readers, in the appendix we provide basic facts about the algebraic Bethe ansatz formalism and the inverse scattering transform for the model of one-dimensional Bose gas with both repulsive and attractive interactions.

2. A review of methods for investigating the non-equilibrium dynamics of integrable models

In this paper we analyze the time evolution of correlation functions in integrable models when the initial state is not an eigenstate of the Hamiltonian. Here we give an overview of (some of) the possible approaches to studying non-equilibrium dynamics of integrable systems. We only discuss approaches which explicitly use the property of integrability and exclude more conventional techniques which rely on approximations and perturbative expansions, such as the Keldysh formalism [26]. Although the focus of this paper is on the 1D Bose gas, methods discussed here can be applied to other exactly solvable models, e.g. for the Gaudin-type integrable models [30].

The Hamiltonian of the 1D interacting Bose gas in a finite size system has the following form [4]:

$$H_c = \int_0^L \mathrm{d}x \, [\partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)]. \tag{1}$$

Here $\Psi(x)$ is a bosonic field in the second-quantized notation, c is an interaction constant, and L is the size of the system. The equation of motion for this Hamiltonian is the nonlinear Schrödinger (NS) equation. The first-quantized version of this Hamiltonian corresponds to the Lieb–Liniger model of Bose gas interacting with the contact interaction. The Bethe ansatz solution of this model has been given in [1]–[3], [5].

Below we discuss several possible approaches to the study of non-equilibrium dynamics of nonlinear integrable models, such as the LL model (1).

2.1. The quantum inverse scattering method

One approach to analyzing the dynamics of model (1) would be to use the formalism of the inverse scattering problem. This method relies on the solution of the quantum version of the Gelfand–Levitan–Marchenko equation (see the appendix). From the inverse scattering transform (see e.g. [31] for a review) it is known that the solution is given by the following infinite series representation:

$$\Psi(x) = \sum_{N=0}^{\infty} \int \prod_{i=1}^{N} \frac{\mathrm{d}p_i}{2\pi} \prod_{j=0}^{N} \frac{\mathrm{d}k_j}{2\pi} g_N(\{p\},\{k\};x) R^\dagger(p_1)\cdots R^\dagger(p_N) R(k_N)\cdots R(k_0) \tag{2}$$

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where the operators $R(p)$ diagonalize the problem on the infinite interval $[-\infty,\infty]$. The function g_N can be cast into different forms [32]. One specific representation is given by

$$g_N(\{p\},\{k\};x)=\frac{(-c)^N\exp[\mathrm{i}x(\sum_0^N k_i-\sum_1^N p_i)]}{\prod_{m=1}^N(p_m-k_m-\mathrm{i}\epsilon)(p_m-k_{m-1}-\mathrm{i}\epsilon)}. \tag{3}$$

The above perturbative expansion is a quantum version of the Rosales expansion [33, 34]. Thus,

$$\Psi(x)=\int\frac{\mathrm{d}\xi_1}{2\pi}R(\xi_1)\mathrm{e}^{\mathrm{i}\xi_1 x}+c^2\int\frac{\mathrm{d}\xi_1}{2\pi}\int\frac{\mathrm{d}\xi_2}{2\pi}\int\frac{\mathrm{d}\xi_3}{2\pi}\frac{R^\dagger(\xi_2)R(\xi_1)R(\xi_3)\mathrm{e}^{\mathrm{i}(\xi_1-\xi_2+\xi_3)}}{(\xi_2-\xi_1-\mathrm{i}\epsilon)(\xi_3-\xi_2+\mathrm{i}\epsilon)}+\cdots. \tag{4}$$

The inverse expression (the direct Gelfand–Levitan transform) is also available (see [35] for the finite interval),

$$R^\dagger(\xi)=\frac{1}{\sqrt{2\pi}}\int\mathrm{d}x\,\Psi^\dagger(x)\mathrm{e}^{-\mathrm{i}qx}+\frac{1}{\sqrt{2\pi}}\int\mathrm{d}x_1\,\mathrm{d}x_2\,\mathrm{d}x_3\,g_2(x_1,x_2,x_3;q)\Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x_3)+\cdots, \tag{5}$$

where e.g. [36] $g_2(x_1,x_2,x_3;q)=c\theta(x_2-x_3)\theta(x_3-x_1)\exp(-\mathrm{i}q(x_1+x_2-x_3))$, $g_4(x_1,x_2,x_3,x_4,x_5;q)=c^2\theta(x_3-x_5)\theta(x_5-x_2)\theta(x_2-x_4)\theta(x_4-x_1)\exp(-\mathrm{i}q(x_1+x_2+x_3-x_4-x_5))$. Here the operators of the reflection coefficient $R(\xi),R^\dagger(\xi)$ diagonalize the Hamiltonian and satisfy the Zamolodchikov–Faddeev algebra (see the appendix for more details):

$$[H,R^\dagger(\xi)]=\xi^2R^\dagger(\xi), \tag{6}$$

$$R(\xi)R(\xi')=S(\xi'-\xi)R(\xi')R(\xi),\qquad R(\xi)R^\dagger(\xi')=S(\xi-\xi')R^\dagger(\xi')R(\xi)+2\pi\delta(\xi-\xi') \tag{7}$$

where the scattering matrix is $S(\xi-\xi')=(\xi-\xi'-\mathrm{i}c)/(\xi-\xi'+\mathrm{i}c)$. These relations make the problem of finding the time evolution easy: the factor $\exp[\mathrm{i}x(\sum_0^N k_i-\sum_1^N p_i)]$ in equation (3) simply needs to be replaced by the factor $\exp[\mathrm{i}x(\sum_0^N k_i-\sum_1^N p_i)-\mathrm{i}t(\sum_0^N k_i^2-\sum_1^N p_i^2)]$. Application of this formalism to non-equilibrium problems is also straightforward: one has to decompose the initial state, written in terms of bosonic $\Psi(x)$-operators, into a series of Zamolodchikov–Faddeev operators $R(\xi)$, generated by the inverse transform, and then find the time evolution according to (6) using the direct transform.

Strictly speaking, this expansion is valid only for an infinite interval. For finite intervals it gives rise to singularities in expressions for the correlation functions, which, however, can be corrected by careful consideration of expressions in each order [32]. This series can be summed up explicitly only for the infinite value of the coupling c [37, 32]. Unfortunately this approach is very difficult to use for calculating the time dependence of the correlation functions at finite c even in equilibrium. We are not aware of the reproducibility of the asymptotic results which would correspond to the Luttinger liquid power laws. On the other hand the advantage of this approach is the possibility of generalizing it to other specific boundary or initial conditions. In principle this formalism should allow one to include impurities [38] and can be extended to multi-component generalizations of the NSE [39].

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2.2. The intertwining operator

Some integrable (and sometime quasi-exactly solvable) models have the following property:

$$IH_0 = H_c I \tag{8}$$

where two *different* Hamiltonians $H_{0,c}$ are connected (intertwined) by the action of some operator I, called the *intertwining* operator. In general, if H_0 and H_c belong to two different representations of the same algebra, then intertwining operators exchange these two representations of the same algebras (or, stated mathematically, establish a certain homomorphism between them). If H_0 is a Hamiltonian for free, *non-interacting* particles, and H_c is the Hamiltonian for the *interacting* system with interaction constant given by c, then the evolution of observables in the interacting model can be related to the evolution of the non-interacting one. Hence the *dynamics* of the interacting Hamiltonian can be mapped to the dynamics of the non-interacting Hamiltonian using

$$\mathrm{e}^{\mathrm{i}H_c t} = I\mathrm{e}^{\mathrm{i}H_0 t}I^{-1}. \tag{9}$$

A few comments are in order. The existence of the intertwining operator for integrable models follows from the following facts: (i) the Bethe states of all integrable models are parametrized by the integer numbers which label the eigenfunctions of non-interacting problems; therefore the wavenumbers of a interacting model are analytically connected to the wavenumbers of the non-interacting one; (ii) in the language of the coordinate Bethe ansatz a system of N particles is described by the wavefunction defined in the N-dimensional space divided by the hyperplanes on which the collision processes occur. Outside these hyperplanes a system behaves as a non-interacting one. Amplitudes of transition between $N!$ different regions (outer spaces of the hyperplanes) are the same for all eigenstates because of the permutation symmetry. These transition amplitudes define a unitary transformation which is nothing but the intertwining operator. However, one should note that in general the operator I is not unitary. Thus, the wavefunctions of exactly solvable models are not orthonormalized; their overlaps are given by the determinants of some matrix via the Gaudin–Slavnov formula [5, 4]. Defining orthonormalized wavefunctions, one can construct a unitary version of the operator I.

2.2.1. Degenerate affine Hecke algebra: first-quantized notation. In the case of the Lieb–Liniger model the intertwining operator can be related to the representation of the degenerate affine Hecke algebra [40]. For the XXZ spin chains there should exist a similar operator for intertwining between different representations of the $U_q(sl_2)$ and Temperley–Lieb algebras. One reason for expecting this is because the LL model and the XXX spin chain share essentially the same R-matrix satisfying the Yang–Baxter equation. Some earlier discussion on the XXZ chain is contained in [41].

The construction of I for the 1D Bose gas relies on the notion of the Dunkl operator

$$\hat{d}_i = -\mathrm{i}\partial_i + \mathrm{i}\frac{c}{2}\sum_{j<i}(\epsilon(x_i - x_j) - 1)s_{i,j} + \mathrm{i}\frac{c}{2}\sum_{j>i}(\epsilon(x_i - x_j) + 1)s_{i,j} \tag{10}$$

where $\epsilon(x)$ is a signature function, operator $s_{i,j}$ provides a representation of Artin's relations for the braids, exchanges coordinates of particles i and j and satisfies $x_i s_{i,j} = s_{i,j}x_j$. The operators $\hat{d}_i, s_j \equiv s_{j,j+1}$ form a representation of the degenerate affine Hecke

algebra. Another representation of the same algebra is formed by the ordinary differential (difference) operator $-\mathrm{i}\partial_i$ and the integral operator Q_i [42] representing the scattering matrix and acting on the arbitrary function $f(\ldots, x_i, x_{i+1}, \ldots)$ as

$$Q_i f(\ldots, x_i, x_{i+1}, \ldots) = f(\ldots, x_{i+1}, x_i, \ldots) - c\int_0^{x_i - x_{i+1}} f(\ldots, x_i - t, x_{i+1} + t, \ldots)\,\mathrm{d}t. \quad (11)$$

The intertwining operator I interchanges these two representations of the affine Hecke algebra, $(\hat{d}_i, s_{i,j})$ and $(-\mathrm{i}\partial_i, Q_i)$, and thus intertwines the Dunkl operator $\hat{d}_i$ and the ordinary partial differential operator. Explicitly

$$I = \sum_{w\in S_N} \theta(x_{w^{-1}(1)} < \cdots x_{w^{-1}(N)}) s_{w^{-1}} Q_w \quad (12)$$

where $s_{w^{-1}} = s_{i_p}\cdots s_{i_2} s_{i_1}$ and $Q_w = Q_{i_1} Q_{i_2}\cdots Q_{i_p}$ $(1 \le i_1, i_2, \ldots, i_p \le N-1)$ and where w is a transposition from the symmetric group S_N [40].

All conserved quantities $\mathcal{I}_n$ for the 1D Bose gas system are given by the powers of the Dunkl operator, $\mathcal{I}_n = \sum_i \pi(\hat{d}_i^n)$, where $\pi(.)$ is the projection onto a symmetric subspace. Thus, the Hamiltonian (1) is just equal to $\mathcal{I}_2$.

As a side remark we note that these facts are convenient for the formulation of the generalized Gibbs ensemble (GGE) approach to the non-equilibrium dynamics of the LL model [22]. In particular, the GGE density matrix of the 1D Bose gas should be related to the non-interacting density matrix by the intertwining relation. As discussed in [43], the GGE conjecture should work when eigenvalues of the integrals of motion are parametrized by either $\{0, 1\}$ (fermionic-like systems) or by integers $\{0, 1, 2, \ldots\}$ (bosonic-like systems). The case of the Bose gas belongs to the second class. We therefore conjecture that the GGE approach is applicable to the 1D Bose gas (LL model), at least for the local observables.

2.2.2. Graphical representation: the Gutkin approach. An interesting approach to the 1D Bose gas based on the intertwining operator has been developed by Gutkin in a series of papers [41, 42, 44, 45]. It was later applied to the problem of propagation of an optical pulse in nonlinear media in [46].

In this approach the intertwining operator is expanded as a series of different contributions labeled by the so-called collision graphs[3]. The evolution of the quantum field $\Psi(x,t)$ governed by the NSE is given entirely in terms of the evolution of the field $\Psi_0(x,t)$ for the free Schrödinger equation, $\mathrm{i}\partial_t\Psi_0(x,t) = -\partial_x^2\Psi_0(x,t)$, and by the quantities a_Γ (defined in terms of some distributions) entering the expansion of the intertwining operator over a set of collision graphs

$$I = \sum_{\Gamma, n=q(\Gamma)} \int \mathrm{d}^n x \int \mathrm{d}^n y\, a_\Gamma(x_1, x_2, \ldots, x_n, y_1, y_2, \ldots y_n) \times \Psi_0^\dagger(x_1)\Psi_0^\dagger(x_2)\cdots\Psi_0^\dagger(x_n)\Psi_0(y_1)\Psi_0(y_2)\cdots\Psi_0(y_n) \quad (13)$$

[3] The graph Γ with q vertices and p oriented edges is called a collision graph if (a) for every vertex there is an edge coming into it or going out of it; (b) there is at most one edge between any two vertices; (c) all vertices can be labeled in an ordered way from 1 to q such that the edges go from smaller to larger number.

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and similarly for the operator I^{-1} with a_Γ replaced by the related distribution b_Γ. There is a special choice of a_Γ and b_Γ for which the operator I is unitary. For details about this approach we refer the reader to the original papers by Gutkin.

The advantage of this approach is the possibility of finding the propagator of the nonlinear problem and thus, potentially, solving the initial state evolution problem for an arbitrary initial state. Computationally one only needs to deal with the free fields $\Psi_0(x)$ and their time evolution with a free (non-interacting) Hamiltonian. We note that the collision graph expansion is highly non-perturbative and cannot be rewritten as an expansion in powers of c, in contrast to the Gelfand–Levitan based expansion of section 2.1. A disadvantage of this approach is the rapidly growing complexity of collision graph expansion with increasing number of particles. Also it is not known at present whether some of the most relevant graphs can be summed in order to develop useful approximation schemes.

2.2.3. The second-quantized approach. In series of papers [47] Sasaki and Kebukawa developed a field-theoretical approach to the LL model. Although they did not present it in this context, the second-quantized form of the intertwining operator can be recognized in their construction[4]. In this approach one considers the LL Hamiltonian written in the usual second-quantized form,

$$H_c = \sum_p \frac{p^2}{2m} a_p^\dagger a_p + \sum_{p,q,r} \frac{c}{2L} a_{p+r}^\dagger a_{q-r}^\dagger a_q a_p. \tag{14}$$

Here $a_p^\dagger, a_p$ are bosonic creation and annihilation operators corresponding to momenta $p_i = 2\pi\hbar n_i/L$ (n_i should be an integer). The second-quantized analog of the Bethe ansatz wavefunction for N particles has the form

$$|\Psi_{q_1,q_2,\ldots q_N}\rangle = B_{q_1,q_2,\ldots q_N} \sum_{p_{i,j};1\le i<j\le N} \prod_{1\le i<j\le N} d(p_{i,j};k_{i,j}) \prod_{i=1}^{N} a^\dagger_{\sum_{j=1,j\neq i}^N p_{i,j}+q_i} |0\rangle \tag{15}$$

where $B_{q_1,q_2,\ldots q_N}$ is a normalization factor, $p_{i,j} = p_i - p_j = -p_{j,i}$ and q_i $(i = 1,\ldots,N)$ are defined as an integer $\times\, 2\pi\hbar/L$, $d_(p_{i,j};k_{i,j}) = -k_{i,j}/(p_{i,j} - k_{i,j})$ and $k_{i,j} = -k_{j,i}$ are solutions of the Bethe ansatz equations

$$\cot\left(\frac{Lk_{i,j}}{2\hbar}\right) = \frac{\hbar}{mc}(k_i - k_j) = \frac{\hbar}{mc}\left(2k_{i,j} + \sum_{l\neq i,j}(k_{i,l} - k_{j,l}) + q_i - q_j\right),$$
$$1 \le i < j \le N. \tag{16}$$

The eigenvalues in this notation are given by $E_{q_1,\ldots,q_N} = \sum_{i=1}^N k_i^2/2m = \sum_{i=1}^N \sum_{j\neq i}(k_{i,j} + q_i)^2/2m$.

It is interesting that the authors of [47] found a *unitary* operator which transforms eigenstates of the non-interacting system H_0 into eigenstates of the interacting

[4] It is also interesting to note that later on the same authors constructed a similar second-quantized approach to the fermionic Yang–Gaudin model as well.

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Hamiltonian H_c. In the second-quantized form this unitary operator is given by

$$U = \sum_{q_1 \le q_2 \le \cdots q_n} \sum_{p_{i,j}; 1 \le i < j \le n} B_{q_1,q_2,\ldots,q_n} A_{q_1,q_2,\ldots,q_n} \prod_{1 \le i < j \le n} d(p_{i,j}; k_{i,j}) \prod_{i=1}^{n} a^{\dagger}_{\sum_{j=1; j \ne i}^{n} p_{i,j} + q_i} \prod_{i=1}^{n} a_{q_i} \tag{17}$$

where $A_{q_1,\ldots,q_N}$ are normalization factors for non-interacting eigenstates. Explicit calculations show that this unitary operator is indeed equivalent to the intertwining operator from previous subsections.

This approach has advantages for initial states which can be readily represented using the formalism of second quantization. For the case of a large coupling constant it gives the same result as the one used later on in the text.

2.3. *q*-bosons

In a series of recent papers [48, 49] a system of q-bosons hopping on a 1D lattice has been studied. This model is defined by its Hamiltonian

$$H_q = -\tfrac{1}{2} \sum_{n=1}^{M} (b_n^{\dagger} b_{n+1} + b_n b_{n+1}^{\dagger} - 2N_n) \tag{18}$$

where the periodic boundary condition is imposed. Operators B_n, $B_n^{\dagger}$ and N_n satisfy the q-boson algebra

$$[N_i, b_j^{\dagger}] = b_j^{\dagger} \delta_{ij}, \qquad [N_i, b_j] = -b_i \delta_{ij}, \qquad [b_i, b_j^{\dagger}] = q^{-2N_i} \delta_{ij} \tag{19}$$

where $q = \mathrm{e}^{\gamma}$. The operator of the total number of particles $N = \sum_{j=1}^{M} N_j$ commutes with the Hamiltonian H_q.

The continuum limit of the model is defined using the limiting procedure

$$\delta \to 0, \qquad M\delta = L, \qquad \gamma = \frac{c\delta}{2}. \tag{20}$$

When applied to the system of q-bosons this procedure gives

$$H = \int_0^L \mathrm{d}x \, \left[\partial_x b^{\dagger}(x) \partial_x b(x) + c b^{\dagger}(x) b^{\dagger}(x) b(x) b(x) \right], \tag{21}$$

where $[b(x), b^{\dagger}(y)] = \delta(x - y)$ are the canonical Bose fields. Therefore 1D Bose gas with a contact interaction can be regarded as a continuum limit of the q-boson lattice model. Apparently a solution of the inverse scattering problem for the NSE should be related to the one for the q-boson model. An explicit form of this relationship is not known, although it should exist[5].

This approach can be used to study non-equilibrium dynamics. Solutions of the particular evolution problem for q-bosons can be transformed into solutions of the NS problem via the limiting procedure (20). An attempt to construct the evolution operator for a single-mode q-boson system has been made in [50]. Even for this simple case the q-path integral has an involved structure which includes integration with the

[5] The authors are grateful to M Zvonarev for discussions on this issue.

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measure corresponding to non-flat phase space and complicated action having a non-trivial dynamical phase. All this makes the possibility of explicit evaluation of the q-path integral questionable. It is interesting to note that the dynamics in this phase space is naturally constrained by integrals of motion. This is reminiscent of recent suggestions of the importance of the GGE for the dynamics of integrable models [22].

2.4. Extended conformal symmetry

It is known that the low energy description of the 1D Bose gas can be formulated as a bosonic Luttinger liquid [51, 52]. This description operates with a linear spectrum of bosonic modes and treats the interaction part essentially exactly. From the more formal point of view, in this low energy description the thermodynamic limit of the NS system represents a conformal field theory (CFT) with the central charge $c = 1$. This means, in particular, that the low energy (bosonic Luttinger) Hamiltonian is a linear combination of the zero-momentum generators $L_0, \bar{L}_0$ (for the right moving and for the left moving parts) of the conformal symmetry algebra, i.e. the Virasoro algebra

$$[L_n, L_m] = (n-m)L_{n+m} + \tfrac{1}{12}n(n^2-1)\delta_{n+m,0} \tag{22}$$

and the same for $\bar{L}_n$, ($[L_n, \bar{L}_m] = 0, \forall n, m$). The space of states is the so-called Verma module (representation space) for this Virasoro algebra. The Kac table defines a conformal tower for this $c = 1$ CFT which allows one to compute any correlation functions. One could also include finite size corrections and effects of irrelevant perturbations [53, 54].

The non-equilibrium dynamics cannot be correctly described in terms of the low energy, Luttinger liquid theory only. There are two reasons for this: first, if the initial state represents a 'large' perturbation over equilibrium, which includes the overlap with the whole spectrum, the excitations involving the nonlinear part of the spectrum should be important; second, even for relatively weak perturbations, which do not thermalize because of integrability, the dynamics at large times leads to growing correlations over the entire momentum space. So irrelevant contributions from the interaction part of the Hamiltonian should become important at long times.

It appears that nonlinearity of the dispersion as well as irrelevant (from the equilibrium point of view) parts of the interaction can be included using the *extended* conformal symmetry called $\mathcal{W}_{1+\infty}$. The $\mathcal{W}_{1+\infty}$ algebra is a representative of a class of nonlinear algebras which appeared in conformal field theories. It is a product of a quantum version of an algebra of area-preserving diffeomorphisms of a 2D cylinder and the Abelian Kac–Moody algebra. The presence of dynamical symmetry $\mathcal{W}_{1+\infty}$ is a general property of gapless one-dimensional systems. The chiral generators W_n^α of $\mathcal{W}_{1+\infty}$ are labeled by the momentum index $n, k = 2\pi n/L$, and by the conformal spin index $\alpha = 0, 1, 2, \ldots \infty$. They satisfy

$$[W_n^\alpha, W_m^\beta] = (\beta n - \alpha m)W_{n+m}^{\alpha+\beta-1} + q(\alpha, \beta, n, m)W_{n+m}^{\alpha+\beta-3} + \cdots + \delta^{\alpha\beta}\delta_{n+m,0}cd(\alpha, n) \tag{23}$$

where $q(\alpha, \beta, n, m)$ and $d(\alpha, n)$ are known polynomials of their arguments [55].

For many interesting cases the Hamiltonian can be written as linear and bilinear combinations of Cartan generators of the $\mathcal{W}_{1+\infty}$ algebra[6]. The representation theory of

[6] Cartan generators of any algebra are those which commute with each other. In our case this means that $[W_0^\alpha, W_0^\beta] = 0, \forall \alpha, \beta$.

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$W_{1+\infty}$ in the Verma module can be constructed in the same way as the representation theory for the Virasoro algebra [56] starting from the highest weight state and building a tower of descendant states. Using this representation theory one can construct the action of $\mathcal{W}_{1+\infty}$ generators on bosonic Fock space. One can therefore establish a correspondence between Bethe ansatz eigenstates and a certain combination of states of representation module of the $\mathcal{W}_{1+\infty}$. The evolution operator is factorized as a product of factors corresponding to different Cartan generators:

$$U(t) = \mathrm{e}^{\mathrm{i}Ht} = \prod_{\alpha} \mathrm{e}^{\mathrm{i}\beta_\alpha W^\alpha t} \tag{24}$$

where β_α are functions of the interaction strength and a level. When the initial state can be expressed as a linear combination of descendant states, the application of $U(t)$ is straightforward.

In practice it is difficult to deal with the whole nonlinear dispersion, so, for practical purposes, one can keep only next-to-linear terms in this expansion. In this case the Hamiltonian will include only a finite number of $\mathcal{W}_\infty$ generators. For example, in the strong coupling regime, corrections to the Hamiltonian to the first order in the inverse power of the interaction strength are as follows:

$$H = \frac{2\pi\rho}{LK}(W_0^1 + \bar{W}_0^1) + \frac{2\pi}{L^2K}[W_0^2 + \bar{W}_0^2] + \cdots. \tag{25}$$

The advantage of this approach is the simplicity of including higher order corrections originating from nonlinearity of the dispersion, and the potential for solving the problem exactly. The disadvantage of this method comes from its limitation to treating gapless systems only. Details of this approach together with several related questions will be presented in a separate work [57].

2.5. Form factors and decomposition of the initial state

This is the most direct approach which we will use further in this paper. In this approach we decompose the initial state into a form in terms of the eigenstates of the Hamiltonian. The latter form a complete and orthogonal set of states. To compute the time evolution of the correlation functions we have to combine several ingredients: (i) find a complete basis of many-body wavefunctions; (ii) know the exact eigenvalues; (iii) determine matrix elements (or *form factors*) of various operators in the basis of exact eigenfunctions; (iv) find a decomposition of the initial state in the complete set of exact many-body states; (v) develop an effective procedure for summation over intermediate states.

Ingredients (i) and (ii) are known from the Bethe ansatz exact solution. Matrix elements (iii) were computed in many exactly soluble models on the basis of the so-called determinant representation. Recent progress in computation of the matrix elements of operators in the basis of the Bethe ansatz wavefunctions makes it possible to advance in this direction. Decomposition of the initial states (iv) over the complete basis depends significantly on the concrete nature of the states. We were able to evaluate these overlaps for a 1D Bose gas at large interaction strength for initial conditions of two types: all particles in a zero-momentum state and all particles in the Gaussian wavefunction in real space. Currently we perform the summation over intermediate states numerically. This imposes certain restrictions on the number of particles in our system. We checked that in equilibrium this number is sufficient for saturating any correlators to their values in the

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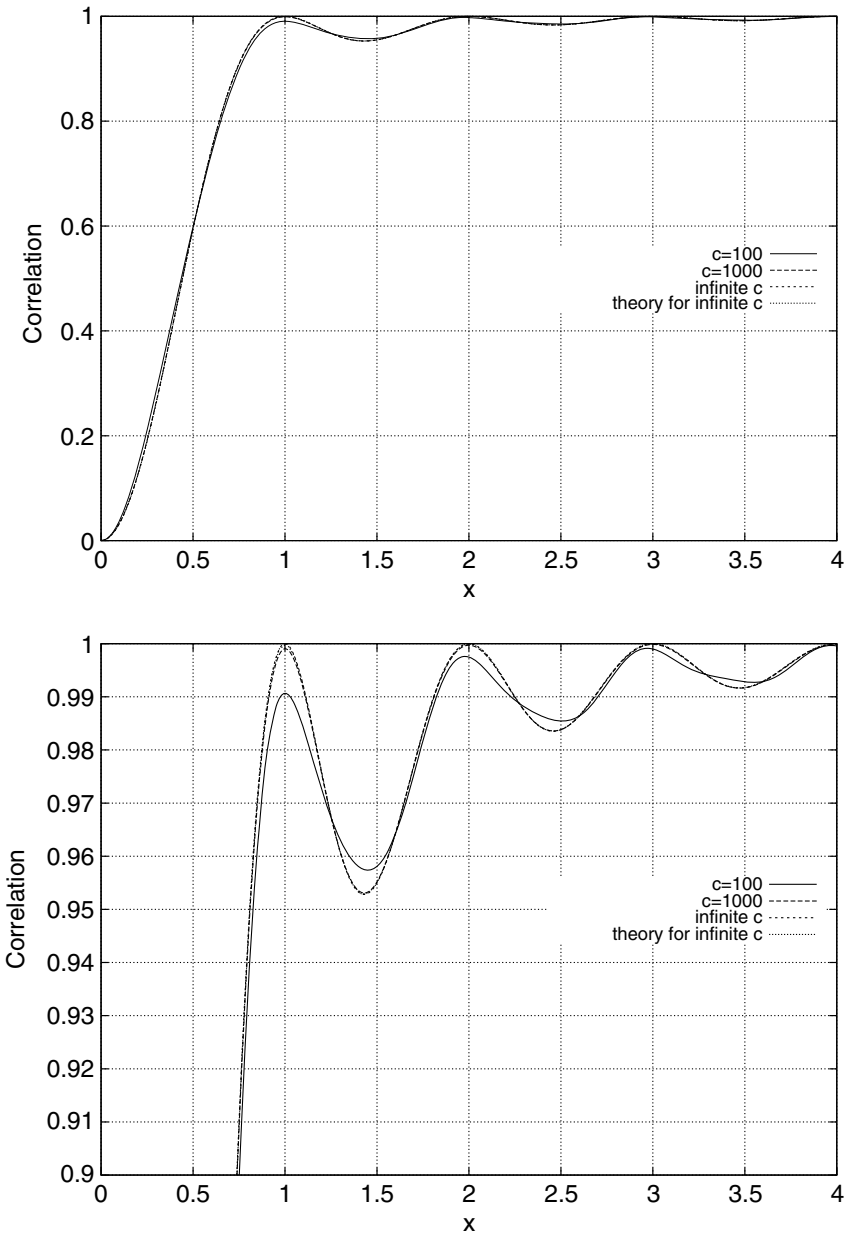

Figure 1. Upper panel: calculated and theoretical spatial correlation functions for a ground state for $c = 100$, $c = 1000$, and $c \to \infty$. Lower panel: zoom of the upper panel.

thermodynamic limit. To illustrate this observation we plot $g_2(x)$, computed in the ground state using our method, and compare it to the known analytic expression in figure 1.

Here we make general comments on the structure of the phase space of the form factors. For a system with a gap only a small number of states need to be taken into account. Contributions of many-particle states are suppressed by the gap. This is the case for the NLS system with attraction, which can be identified with the non-relativistic limit of the quantum sine–Gordon model for which the previous statement is also correct (see e.g. review [43] and references therein for direct comparison of different contributions

to the form-factor expansion of the correlation functions). Contributions coming from higher order terms grow in the limit of long time evolution, but should only generate subleading corrections. The situation is very different for gapless systems, such as the NLS system with repulsion. Many-particle contributions are suppressed at most as a power law. Hence ideally we need to take into account the entire phase space. This makes the problem of summation over intermediate states very difficult. In this paper we deal with the most difficult case of repulsively interacting Bose gas in the regime of strong interaction, when, in principle, the allowed phase space is huge and multi-particle states are in general not suppressed.

The form-factor approach has been successfully applied in the computation of equilibrium correlation functions in many models [58]. A review of the applications of this method to massive models is given in [59]. The gap in the spectrum leads to the rapid convergence of the form-factor expansion. It is enough to take contributions from a few particles to saturate any correlation function. This is not the case for massless models where contributions of multi-particle processes are essential. Recently this approach was applied to compute equilibrium correlation functions of the 1D Bose gas in [60, 61] (see also [62] for the attractive case[7]). Earlier studies reviewed in [4] allowed us to evaluate various asymptotics of the time-dependent correlation functions at equilibrium (for a concrete example with non-zero temperature see e.g. [63, 64]). Recently, a form-factor approach has been applied to the time evolution of a specific (domain wall) initial state in the XXZ model [65]. This specific choice of the initial state allows for successful analytical analysis of the time-evolved state. This is one of the rare examples where a work function and a Loschmidt echo, important quantities related to the properties of a stationary state [66], have been evaluated analytically.

One of the advantages of the direct application of the form-factor technique is the possibility of considering non-equilibrium dynamics of weakly non-integrable systems. In [67] the form-factor perturbation theory has been developed for a class of models which deviate weakly from an integrable 'fixed point'. This perturbation theory is unusual because its unperturbed states are highly correlated states of an interacting integrable theory. We expect that this formalism can be extended to treat non-equilibrium dynamics as well.

The form-factor approach supplemented by a procedure of decomposing the initial state into a complete set of many-body eigenstates is universal and can be applied to a large class of integrable models. This method allows several extensions and modifications. In the rest of this paper we focus on this method and demonstrate that it is a powerful tool for analyzing non-equilibrium evolution of correlation functions.

In section 3 we also show that one can use the intertwining operator to find a coefficient of overlap between interacting and non-interacting states. We do this explicitly in the strong coupling limit[8].

[7] Note that direct quantum-mechanical computations has been done in [17]; they agree with [62] up to a multiplicative factor.

[8] We also comment on some particular kinds of models where these and other overlaps can be found explicitly for various coupling constants. This is the case for some kinds of Gaudin models, e.g. Richardson models of mesoscopic BCS pairing and the central spin problems. In these models the BA states do not depend explicitly on the strength of the coupling constant, so one could use the Gaudin–Slavnov determinant formula for these overlaps.

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To conclude this section we note that other possible approaches to computation of the correlation functions for integrable systems out of equilibrium have been discussed in [68] and [69]. Recently, in [70] an approach to the time evolution of the wavefunction of the Lieb–Liniger model has been proposed. It can be applied to the initial states of the type (A.11) (see the appendix) which is characterized by the ordering of coordinates of the particles on a line. We believe that the method presented in [70] has an overlap with those presented here. Yet another approach, closely linked to the form-factor method in the *infinite volume*, allows for computation of the time evolution of the one-point function. This is based on the possibility of representing *certain* (integrable) initial states as a *boundary state* which is a coherent superposition of the eigenstates of the model [71, 72]. Recently, an interesting approach to equilibrium correlators in the Lieb–Liniger model has been developed in [73]. The idea of the latter approach is to consider first a relativistic *massive* model (the so-called sinh–Gordon model), which, in the specific non-relativistic limit, goes over into a Lieb–Liniger model. The form factors of the sinh–Gordon model are known and the rapid convergence of the form-factor expansion for the correlation functions in this model is due to the mass gap in the spectrum. In the special non-relativistic limit, all of the expressions for the field operators and correlators of the sinh–Gordon model go over into corresponding expressions for the LL model. Moreover, the non-relativistic limit profits from the rapid convergence of the form-factor expansions in its relativistic counterpart. One could hope that this interesting approach can be successfully applied to non-equilibrium dynamics as well.

3. The exact approach to non-equilibrium dynamics based on form factors

In this section we describe the application of the method of form factors to the computation of non-equilibrium correlation functions. This method is general for any integrable system. In this paper we focus on the 1D Bose gas. As discussed earlier, the treatment of the gapless system is more challenging because of the large number of contributions from intermediate states which need to be included. To overcome this difficulty we devised a special numerical procedure of summation over intermediate states. This procedure is described in section 3.1.

3.1. Formulation of the problem

To fix notation we consider the nonlinear Schrödinger Hamiltonian on a finite interval $[0, L]$:

$$H = \int_0^L \mathrm{d}x \left[\partial_x \Psi^\dagger(x)\partial_x \Psi(x) + c\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)\right] \tag{26}$$

where the commutation relation between the bosonic field $\Psi(x)$ and its conjugated $\Psi^\dagger(x)$ as well as the pseudovacuum state $|0\rangle$ are defined as [4]

$$[\Psi(x), \Psi^\dagger(y)] = \delta(x-y), \qquad [\Psi(x), \Psi(y)] = [\Psi^\dagger(x), \Psi^\dagger(y)] = 0 \tag{27}$$

$$\Psi(x)|0\rangle = 0, \qquad \langle 0|\Psi^\dagger = 0, \qquad \langle 0|0\rangle = 1. \tag{28}$$

The total number of particles and the momentum operators are conserved quantities:

$$N = \int_0^L \Psi^\dagger(x)\Psi(x), \qquad P = -\frac{\mathrm{i}}{2}\int_0^L [\Psi^\dagger(x)\partial_x\Psi - (\partial\Psi^\dagger(x))\Psi(x)] \tag{29}$$

$$[H, N] = [H, P] = 0. \tag{30}$$

In each N-particle sector this system is equivalent to the 1D Bose gas with a contact interaction potential (the Lieb–Liniger model) [1]–[3], [5]. In connection with the previous section we note that the inverse scattering transform for this problem has been developed in many papers (see [35, 74, 32, 44] for extensive reviews).

The problem that we are considering here can be formulated as follows: suppose we prepared a system in a certain initial N-particle state $|\psi_0^{(N)}\rangle$ (e.g. the coherent state can be considered as a superposition of states with different values of N). This state evolves according to the Hamiltonian (26). The question is how to compute the correlation functions of the following type:

$$\langle\psi_0^{(N)}|\Psi^\dagger(x_1,t_1)\Psi(x_2,t_2)|\psi_0^{(N)}\rangle, \tag{31}$$

$$\langle\psi_0^{(N)}|\Psi^\dagger(x_1,t_1)\Psi(x_1,t_1)\Psi^\dagger(x_2,t_2)\Psi(x_2,t_2)|\psi_0^{(N)}\rangle, \tag{32}$$

$$\langle\psi_0^{(N)}|\exp(\alpha Q(x))|\psi_0^{(N)}\rangle, \tag{33}$$

where the last formula expresses a generation function for the density–density correlator,

$$Q(x,t) = \int_0^x \Psi^\dagger(y,t)\Psi(y,t)\,\mathrm{d}y. \tag{34}$$

The density is defined as

$$\rho(x,t) = \Psi^\dagger(x,t)\Psi(x,t). \tag{35}$$

Assuming that the initial state is normalized, one can insert a resolution of unity several times:

$$\mathbf{1} = \sum_{\{\lambda\}} \frac{|\{\lambda\}\rangle\langle\{\lambda\}|}{\langle\{\lambda\}|\{\lambda\}\rangle} \tag{36}$$

into the expression for the correlation functions. This suggests defining normalized correlation functions:

$$\begin{aligned}&\langle\psi_0^{(N)}|O(x_1,t_1)O(x_2,t_2)|\psi_0^{(N)}\rangle\\ &= \sum_{\{\lambda\}_N}\sum_{\{\mu\}_N}\sum_{\{\nu\}_N} \frac{\langle\psi_0^{(N)}|\{\lambda\}_N\rangle\langle\{\lambda\}_N|O(x_1,t_1)|\{\mu\}_N\rangle\langle\{\mu\}_N|O(x_2,t_2)|\{\nu\}_N\rangle\langle\{\nu\}_N|\psi_0^{(N)}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle\langle\{\mu\}|\{\mu\}\rangle\langle\{\nu\}|\{\nu\}\rangle}.\end{aligned} \tag{37}$$

In the following we concentrate on the density–density correlation function. According to our program we need matrix elements of the operators in the complete basis of states. In this basis, the time and space dependence are trivial: using the Galilei invariance (we

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implicitly assume periodic boundary conditions) the matrix elements which we need are given by the expressions

$$\langle\{\mu\}_N|Q(x,t)|\{\lambda\}_N\rangle = (\mathrm{e}^{\mathrm{i}x(P_\lambda^{(N)}-P_\mu^{(N)})}-1)\mathrm{e}^{\mathrm{i}t(E_\lambda^{(N)}-E_\mu^{(N)})}F_Q(\{\mu\};\{\lambda\}). \quad (38)$$

Here the energy and momentum are given by

$$E_\lambda^{(N)} = \sum_{j=1}^N \lambda_j^2, \qquad P_\lambda^{(N)} = \sum_{j=1}^N \lambda_j. \quad (39)$$

In the following it will be convenient to use more compact notation:

$$A_\lambda^{(0)} = \langle\psi_0^{(N)}|\{\lambda\}_N\rangle \quad (40)$$

$$F_Q(\{\mu\};\{\nu\}) = \langle\{\mu\}_N|Q(0,0)|\{\nu\}_N\rangle \quad (41)$$

$$||\{\lambda\}|| = \langle\{\lambda\}|\{\lambda\}\rangle. \quad (42)$$

We can write down an expression for the density–density correlator as

$$\begin{aligned}\langle\psi_0^{(N)}|\rho(x,t)\rho(0,0)|\psi_0^{(N)}\rangle &= \frac{\partial^2}{\partial x_1\partial x_2}\sum_{\{\lambda\}_N}\sum_{\{\mu\}_N}\sum_{\{\nu\}_N}\frac{A_\lambda^{(0)}(A_\nu^{(0)})^* F_Q(\{\lambda\};\{\mu\})(F_Q(\{\mu\};\{\nu\}))^*}{||\{\lambda\}||||\{\mu\}||||\{\nu\}||} \\ &\times (\mathrm{e}^{\mathrm{i}x_1(P_\mu^{(N)}-P_\lambda^{(N)})}-1)\mathrm{e}^{\mathrm{i}t_1(E_\mu^{(N)}-E_\lambda^{(N)})}(\mathrm{e}^{\mathrm{i}x_2(P_\nu^{(N)}-P_\mu^{(N)})}-1)\mathrm{e}^{\mathrm{i}t_2(E_\nu^{(N)}-E_\mu^{(N)})} \quad (43)\end{aligned}$$

where $*$ means complex conjugation.

3.2. Bethe ansatz ingredients for the 1D Bose gas

As discussed above in section 2.5 we need several ingredients: a set of exact eigenstates and eigenenergies of the model; an overlap of the initial state with the eigenstates; an explicit expression for the matrix elements of operators in the eigenbasis.

3.2.1. BA states. The BA states are described by a set of N real numbers λ which are given by the solution of the BA equations [1, 5, 4]

$$\lambda_j + \frac{1}{L}\sum_{l=1}^N 2\arctan\frac{\lambda_j-\lambda_l}{c} = \frac{2\pi}{L}\left(I_j - \frac{N+1}{2}\right), \qquad j = 1\cdots N. \quad (44)$$

Here the quantum numbers I_j are half odd integers for N even, and integers for N odd. For eigenfunctions the rapidities do not coincide, $\lambda_j \neq \lambda_k$ for $j \neq k$. The whole Fock space is obtained by choosing sets of ordered quantum numbers $I_j > I_k$, $j > k$, meaning that $\lambda_j > \lambda_k$, $j > k$.

From solution of these equations we immediately obtain energies and momenta via equation (39).

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3.2.2. Overlaps between BA states. The overlap between BA states is given by the Gaudin–Korepin formula [75, 76, 5, 4], [77]–[79], [81, 61]

$$\langle\{\lambda\}_N|\{\lambda\}_N\rangle = c^N \prod_{j>k=1}^{N} \frac{(\lambda_j-\lambda_k)^2+c^2}{(\lambda_j-\lambda_k)^2} \det_N \mathcal{G}(\{\lambda\}) \tag{45}$$

where

$$\mathcal{G}_{jk}(\{\lambda\}) = \delta_{jk}\left[L + \sum_{l=1}^{N} K(\lambda_j,\lambda_l)\right] - K(\lambda_j,\lambda_k) \tag{46}$$

$$K(\lambda_j,\lambda_k) = \frac{2c}{(\lambda_j-\lambda_k)^2+c^2}. \tag{47}$$

3.2.3. Matrix elements. The matrix elements (form factors) for the current operator are given by the following determinantal expression [80, 81, 61]:

$$F_Q(\{\mu\}_N;\{\lambda\}_N) = \frac{\mathrm{i}^N}{(V_N^+ - V_N^-)} \prod_{j,k=1}^{N}\left(\frac{\lambda_j-\lambda_k+\mathrm{i}c}{\mu_j-\lambda_k}\right) \times \det\left(\delta_{jk}\left(\frac{V_j^{(+)}-V_j^{(-)}}{\mathrm{i}}\right) + \frac{\prod_{a=1}^{N}(\mu_a-\lambda_j)}{\prod_{a\neq j}^{N}(\lambda_a-\lambda_j)}[K(\lambda_j-\lambda_k)-K(\lambda_N-\lambda_k)]\right) \tag{48}$$

where

$$V_j^{(\pm)} = \frac{\prod_{a=1}^{N}(\mu_a-\lambda_j\pm\mathrm{i}c)}{\prod_{a=1}^{N}(\lambda_a-\lambda_j\pm\mathrm{i}c)} \tag{49}$$

and where K is given by (47). The matrix inside det() has only real entries. This matrix has size $N\times N$. Real numbers $\{\lambda\},\{\mu\}$ are solutions of the BA equation (44).

3.3. Overlaps of the initial states with the Bethe ansatz basis

Here we study in detail two physically motivated examples of initial states. The first one has its origin in the condensate physics whereas the second one describes a Gaussian pulse created in special nonlinear media. Before going to these examples we make several general observations.

3.3.1. General remarks. To compute the overlap with the initial state we consider the following (coordinate) representation for the Bethe ansatz states of the NSE:

$$|\Psi_N(\lambda_1,\dots\lambda_N)\rangle = \frac{1}{L^N\sqrt{N!}}\int \mathrm{d}^N z\, \chi_N(z_1,\dots,z_N|\lambda_1,\dots,\lambda_N)\Psi^\dagger(z_1)\cdots\Psi^\dagger(z_N)|0\rangle \tag{50}$$

where the function χ_N is given by

$$\chi_N(z_1,\ldots,z_N|\lambda_1,\ldots,\lambda_N) = \text{const}\prod_{N\geq j>k\geq 1}\left(\frac{\partial}{\partial z_j}-\frac{\partial}{\partial z_k}+c\right)\det[\exp(\mathrm{i}\lambda_j z_k)]$$
$$= \frac{1}{\sqrt{N!\prod_{j>k}[(\lambda_j-\lambda_k)^2+c^2]}}\sum_{\mathcal{P}}(-1)^{[\mathcal{P}]}$$
$$\times\ \exp\left[\mathrm{i}\sum_{n=1}^{N} z_n\lambda_{\mathcal{P}n}\right]\prod_{j>k}[\lambda_{\mathcal{P}j}-\lambda_{\mathcal{P}k}-\mathrm{i}c\epsilon(z_j-z_k)]. \tag{51}$$

It is convenient to define the basic wavefunction

$$|\Psi\rangle_0^{(N)} = \frac{1}{\sqrt{N!}}\Psi^\dagger(x_1)\cdots\Psi^\dagger(x_N)|0\rangle. \tag{52}$$

In principle, any quantum state can be expanded as

$$|\Psi^{(0)}\rangle = \sum_n a_n\int\frac{1}{\sqrt{n!}}f_n(x_1,\ldots,x_n)|\Psi\rangle_0^{(n)} \tag{53}$$

with

$$\sum_n|a_n|^2=1,\qquad \int|f_n(x_1,\ldots,x_n)|^2\,\mathrm{d}x_1\cdots\mathrm{d}x_n=1. \tag{54}$$

Intuitively one expects that the evolution of some *special* initial states can, under certain assumptions about these states and about the Hamiltonian, be relatively simple. This is indeed the case for the 1D Bose gas. Using the expansion (2) and contour integration it was shown in [32] that the state defined as

$$|\psi_N(t=0)\rangle_{\text{ord}} = \theta(x_1>x_2>\cdots>x_N)|\Psi^\dagger(x_1)\Psi^\dagger(x_2)\cdots\Psi^\dagger(x_N)|0\rangle \tag{55}$$

is equal to the state $R^\dagger(x_1)R^\dagger(x_2)\cdots R^\dagger(x_N)|0\rangle$ where $R(x)=\int(\mathrm{d}\xi/2\pi)\mathrm{e}^{\mathrm{i}x\xi}R(\xi)$ (see section 2.1 for definitions). The calculation of the evolution of this state is therefore straightforward.

3.3.2. The overlap with a delta function in momentum space. We first construct a Fourier transform of the basic state:

$$|\Psi(q_1),\ldots\Psi(q_N)\rangle = \frac{1}{\sqrt{N!L^N}}\left[\int_0^L\mathrm{e}^{\mathrm{i}q_1x_1}\Psi^\dagger(x_1)\,\mathrm{d}x_1\right],\ldots\left[\int_0^L\mathrm{e}^{\mathrm{i}q_Nx_N}\Psi^\dagger(x_N)\,\mathrm{d}x_N\right]|0\rangle. \tag{56}$$

At the end of all computations one could take all momenta to be equal, $q_1=q_2=\cdots q_N$, to obtain a condensate state

$$|\psi_0^{(N)}(q)\rangle_C = [\Psi^\dagger(q)]^N|0\rangle. \tag{57}$$

Let us consider the overlap of this state with the Tonks–Girardeau wavefunction corresponding to the large c limit. There are several reasons for focusing on this limit: (1) from our basic interest in the application to quantum optics with strongly correlated photons the TG case is the most interesting since the effects of fermionizations [82] should

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be most pronounced [20] in this limit; (2) equations for the overlap are relatively simple and amenable to analytical calculations; (3) one could use an expansion in powers of $1/c$ around TG limit to produce results for the correlation functions beyond the TG limit.

In the TG limit the wavefunction takes the following form [13, 83, 84]:

$$|\Psi_{\rm TG}\rangle = \frac{1}{\sqrt{N!}}\int_0^L {\rm d}x_1 \cdots \int_0^L {\rm d}x_N\, \chi_{\rm TG}^{(N)}(\{\lambda_i\}|\{x_i\})\Psi^\dagger(x_1)\cdots\Psi^\dagger(x_N)|0\rangle \tag{58}$$

such that $\langle\Psi_{\rm TG}|\Psi_{\rm TG}\rangle = 1$ and where

$$\chi_{\rm TG}^{(N)}(\{\lambda_i\}|\{x_i\}) = \frac{1}{\sqrt{N!L^N}}\prod_{1\le j<k\le N}\epsilon(x_j-x_k)\det_N({\rm e}^{{\rm i}x_m\lambda_n}). \tag{59}$$

Here

$$\lambda_i = \frac{2\pi}{L}n_i, \qquad \begin{cases} n_i \in \mathbf{Z}, & N \text{ odd};\\ n_i \in \mathbf{Z}+\frac{1}{2}, & N \text{ even}. \end{cases} \tag{60}$$

The overlap therefore is reduced to the following integral:

$${}_C\langle\psi_0^{(N)}(q)|\Psi_{\rm TG}\rangle = \frac{N!}{N!L^N}\int_0^L {\rm d}x_1\int_0^L {\rm d}x_2\cdots\int_0^L {\rm d}x_N \prod_{1\le j<k\le N}\epsilon(x_j-x_k)\det_N({\rm e}^{{\rm i}x_m(\lambda_n-q)}) \tag{61}$$

where the factor $N!$ comes from the overlap with the basic state and the denominator comes from the normalization.

The result for the overlap is given by

$${}_C\langle\psi_0^{(N)}(q)|\Psi_{\rm TG}\rangle = A_\lambda^{(0)} \tag{62}$$

$$= \frac{N!2^N\prod_{1\le j<k\le N}(\lambda_j-\lambda_k)}{L^N\prod_{i=1}^N(\lambda_i-q)\prod_{1\le i<j\le N}(\lambda_i+\lambda_j-2q)} \times \begin{cases} (-{\rm i})^{N/2}\left(\cos\left(\dfrac{Lq}{2}\right)\right)^{N/2}\left(\sin\left(\dfrac{Lq}{2}\right)\right)^{N/2}, & N \text{ even};\\ (-{\rm i})^{(N-1)/2}\left(\cos\left(\dfrac{Lq}{2}\right)\right)^{(N-1)/2}\left(-\sin\left(\dfrac{Lq}{2}\right)\right)^{(N+1)/2}, & N \text{ odd} \end{cases}$$

$$\times (-1)^{\sum_{i=1}^N n_i}\exp\left(\frac{{\rm i}L}{2}\sum_{j=1}^N\lambda_j\right)\exp\left(-{\rm i}NL\frac{q}{2}\right). \tag{63}$$

This formula can be simplified further—see section 4.3.2 below.

A straightforward generalization is a construction of a coherent state in k-space. One can take a superposition of $|\Psi^{(N)}(q)\rangle$ states with different N values for real or complex α:

$$|\alpha(q)\rangle = {\rm e}^{-(1/2)|\alpha|^2}\sum_{N=0}^\infty\frac{\alpha^N}{\sqrt{N!}}|\Psi^{(N)}(q)\rangle. \tag{64}$$

We will not consider this state here.

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3.3.3. The overlap with the Gaussian pulse. In the case of a pulse prepared at time $t = 0$ we consider a state

$$|\psi_0^{(N)}\rangle_{\rm G} = \int \prod_{i=1}^{N} {\rm d}x_i\, f(x_1, \dots x_N)\Psi^\dagger(x_1)\cdots\Psi^\dagger(x_N)|0\rangle \tag{65}$$

and choose a function $f(x_1 \cdots x_N)$ in the form of a product of Gaussians,

$$f(x_1, \dots x_N) = \prod_{i=1}^{N} \exp[-x_i^2/2\sigma_i^2]. \tag{66}$$

For simplicity, we take $\sigma_i = \sigma, \forall i$. The overlap with the TG state is given by

$$\langle\Psi_{\rm TG}|\psi_0^{(N)}\rangle_{\rm G} = \frac{1}{N!}\left(\frac{\pi}{2}\right)^{N/2}\sigma^N \exp\left(-\frac{\sigma^2}{2}\sum_i \lambda_i^2\right)\prod_i\left[{\rm erf}\left(\frac{L - {\rm i}\lambda_i\sigma^2}{\sqrt{2}\sigma}\right) + {\rm i}\,{\rm erfi}\left(\frac{\lambda_i\sigma}{\sqrt{2}}\right)\right]. \tag{67}$$

For all practical purposes the erf function can be replaced by the Gaussian.

3.4. The Tonks–Girardeau limit

From our understanding of the equilibrium structure factor of the 1D Bose gas [60] we expect the allowed phase space of the weakly interacting gas to be limited to the vicinity of the dispersion curve of Bogoliubov quasiparticles. On the other hand, we expect that in the opposite case of the TG limit the allowed phase space should be considerably larger. Hence the non-equilibrium dynamics should be more involved in this case as well. Here we thus focus on this interesting limit in more detail. Certain simplifications occur in the equations for the matrix elements, which are described below.

3.4.1. Reduction of the form factors. To compute the density–density function in the TG limit

$$\langle\psi_0^{(N)}|\rho(x_1,t_1)\rho(x_2,t_2)|\psi_0^{(N)}\rangle = \frac{1}{L^{2N}N!}\sum_{\lambda,\mu,\nu} F_N^{\rho *}(x_1,t_1,\lambda,\mu)F_N^{\rho}(x_2,t_2,\mu,\nu)A_\lambda A_\nu \tag{68}$$

we have to know the following form factor:

$$F_N^{\rho}(x,t,\{\lambda\},\{\mu\}) = {\rm e}^{{\rm i}t(E_\lambda - E_\mu)}\frac{N}{N!L^{2N}}\int_0^L {\rm d}x_1\cdots{\rm d}x_N \sum_{\mathcal{P},Q}(-1)^{[\mathcal{P}]+[\mathcal{Q}]}\exp[-{\rm i}x(\lambda_{\mathcal{P}} - \mu_{\mathcal{Q}})]$$
$$\times\ \exp\left[-{\rm i}\sum_{a=1}^{N-1} x_a(\lambda_{\mathcal{P}_a} - \mu_{\mathcal{Q}_a})\right]. \tag{69}$$

A limiting procedure for the form factors in this case has been developed earlier [85]–[87]. We use here the fact that the TG limit can be obtained as a double-scaling limit of the

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XX chain, using

$$\int_0^L \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}x(\lambda_a-\mu_b)} = \begin{cases} L, & \lambda_a = \mu_b \\ 0, & \lambda_a \neq \mu_b \end{cases} \tag{70}$$

where we use the boundary conditions $\mathrm{e}^{\mathrm{i}L\lambda_a} = \mathrm{e}^{\mathrm{i}L\mu_b} = (-1)^{N+1}$. Therefore

$$\begin{aligned} F_N^\rho(x,t,\{\lambda\},\{\mu\}) &= \begin{cases} L^N\rho_0, & \{\lambda\} = \{\mu\} \\ L^{N-1}\mathrm{e}^{-\mathrm{i}x(\lambda-\mu)}, & \lambda_1 = \mu_1, \dots \lambda_{N-1} = \mu_{N-1}, \quad \lambda \neq \mu \end{cases} \\ &= L^N\left(\rho_0\delta_{\lambda\mu} + \frac{\mathrm{e}^{-\mathrm{i}x(\lambda-\mu)}}{L}(1-\delta_{\lambda\mu})\right) \end{aligned} \tag{71}$$

and this is 0 otherwise.

Note that this form factor is an antisymmetric function with respect to any interchange of momenta for both sets $\{\lambda\}$ and $\{\mu\}$. So when they are not ordered in the formula above, we have to assign a factor $(-1)^{[P]_\lambda+[P]_\mu}$, where $[P]$ is a permutation index.

3.4.2. Delta function subtraction. When we calculate the density–density correlator (68), we need to subtract a contribution of the particle to itself. This contribution comes from commutation relations for Bose operators:

$$\begin{aligned} \langle\lambda|\Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x_2)\Psi(x_1)|\nu\rangle &= \langle\lambda|\Psi^\dagger(x_1)\Psi(x_1)\Psi^\dagger(x_2)\Psi(x_2)|\nu\rangle \\ &\quad - \langle\lambda|\Psi^\dagger(x_1)\Psi(x_1)|\nu\rangle\delta(x_1-x_2) \end{aligned} \tag{72}$$

Considering the TG limit and using (71) we can calculate the corresponding δ-function contribution

$$-\langle\lambda|\Psi^\dagger(x_1)\Psi(x_1)|\nu\rangle\delta(x_1-x_2). \tag{73}$$

For the ground state in the continuous limit this contribution is given by

$$-\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}q\,\mathrm{e}^{\mathrm{i}q^2t-\mathrm{i}qx}, \tag{74}$$

where $x \equiv x_1 - x_2$ and $t \equiv t_2 - t_1$. In the general case (68) the delta function yields an additional term

$$-\left(\rho_0 + \frac{1}{L}\sum_{a,b:\lambda_a\neq\nu_b,\forall b}(-1)^{[P]_\lambda+[P]_\nu}A_\lambda A_\nu \mathrm{e}^{\mathrm{i}x_1(\lambda_a-\nu_b)-\mathrm{i}t_1(E_\lambda-E_\nu)}\right)\frac{1}{L}\sum_q \mathrm{e}^{\mathrm{i}xq-\mathrm{i}tE_q}. \tag{75}$$

Now we can combine all components together to calculate the density–density correlation function in the TG limit. For the ground state we have

$$g^{(2)}(\Delta x,\Delta t) = \rho^2 + \frac{1}{4\pi^2}\int_{|q_1|>\pi\rho}\int_{|q_2|<\pi\rho}\mathrm{e}^{\mathrm{i}t(q_1^2-q_2^2)}\cos[(q_1-q_2)x] - \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}q\,\mathrm{e}^{\mathrm{i}q^2t-\mathrm{i}qx}. \tag{76}$$

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In a general non-equilibrium case the correlation function can be written as

$$\begin{aligned}\langle\psi_0^{(N)}(q)|\rho(x_1,t_1)\rho(x_2,t_2)|\psi_0^{(N)}(q)\rangle &= \rho_0^2 + \frac{1}{L^2}\sum_{a,b:\lambda_a\neq\mu_b,\forall b}|A_\lambda|^2\,\mathrm{e}^{\mathrm{i}x(\lambda_a-\mu_b)+\mathrm{i}t(E_\mu-E_\lambda)}\\
&+\frac{1}{L^2}\sum_{a,b,c:\lambda_a\neq\mu_{b\neq\nu_c},\forall b,\forall c}(-1)^{[P]_\lambda+[P]_\nu+2[P]_\mu}A_\lambda A_\nu\\
&\times\mathrm{e}^{\mathrm{i}x_1(\lambda_a-\mu_b)+\mathrm{i}x_2(\mu_b-\nu_c)+\mathrm{i}t_1(E_\lambda-E_\mu)+\mathrm{i}t_2(E_\mu-E_\nu)}\\
&+\rho_0\frac{1}{L}\sum_{a,b:\lambda_a\neq\mu_b,\forall b}(-1)^{[P]_\lambda+[P]_\mu}A_\lambda A_\mu(\mathrm{e}^{\mathrm{i}x_1(\lambda_a-\mu_b)-\mathrm{i}t_1(E_\lambda-E_\mu)}\\
&+\mathrm{e}^{\mathrm{i}x_2(\lambda_a-\mu_b)-\mathrm{i}t_2(E_\lambda-E_\mu)})\\
&-\left(\rho_0+\frac{1}{L}\sum_{a,b:\lambda_a\neq\mu_b,\forall b}(-1)^{[P]_\lambda+[P]_\mu}A_\lambda A_\mu\mathrm{e}^{\mathrm{i}x_1(\lambda_a-\mu_b)-\mathrm{i}t_1(E_\lambda-E_\mu)}\right)\\
&\times\frac{1}{L}\sum_q\mathrm{e}^{\mathrm{i}xq-\mathrm{i}tE_q},\end{aligned}\tag{77}$$

where the first term represents δ–δ contribution, the second one corresponds to $\lambda=\nu$ (the diagonal part), the third and fourth terms come from the nondiagonal ($\lambda\neq\mu\neq\nu$) part, and the last term is a delta contribution discussed above. Here everywhere λ differs from μ by one filling number only, and μ differs from ν by one filling number as well.

Here, the δ–δ part as well as diagonal parts are symmetric with respect to interchange of momenta since these are the products of two antisymmetric functions. On the other hand, in off-diagonal terms we inserted the sign factors in order to ensure that proper symmetry is preserved: since each F is antisymmetric, the *nondiagonal* part will be antisymmetric as well provided that functions A_λ and A_ν are symmetric.

The second term (diagonal part) can be simplified further using the following relation:

$$\sum_{\lambda_a\neq\mu_1\cdots\mu_N}f(\lambda_a)=\sum_{a=1}^{N}f(\lambda_a)-\sum_{b=1}^{N}f(\mu_b)\tag{78}$$

for arbitrary function f. Then

$$\begin{aligned}&\frac{1}{L^2}\sum_{a,b:\lambda_a\neq\mu_b,\forall b}|A_\lambda|^2\mathrm{e}^{\mathrm{i}x(\lambda_a-\mu_b)+\mathrm{i}t(E_\mu-E_\lambda)}\\
&\quad=-\frac{1}{L^2}\left|\sum_{a=1}^{N}A_\lambda\mathrm{e}^{\mathrm{i}x\lambda_a-\mathrm{i}tE_\lambda}\right|^2+\frac{1}{L^2}\sum_{a=1}^{N}\sum_{b=1}^{N}|A_\lambda|^2\mathrm{e}^{\mathrm{i}x\lambda_a-\mathrm{i}tE_\lambda}\mathrm{e}^{-\mathrm{i}x\mu_b+\mathrm{i}tE_\mu}.\end{aligned}\tag{79}$$

This identity can also be used to simplify the nondiagonal part.

3.4.3. Deviation from the TG limit. The main difficulty of our approach is computing overlaps with the initial state in a compact, analytical form for arbitrary interaction strength. At present we do not have a complete solution of this problem for an arbitrary state. For particular kinds of states the problem can be attacked using one of the formalisms of section 2. Thus, in particular, if the initial state can be expressed in second-quantized notation via creation–annihilation operators acting in momentum space,

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then the second-quantized version of the intertwining operator can be used. If the initial state has a simple form in coordinate space, the coordinate version of the intertwining operator might be useful. One form of this operator in real space, mostly useful for the $1/c$ expansion around the TG limit, has the form of a differential operator acting on the TG wavefunction [5, 88]. It relates the TG wavefunction (which is almost fermionic) to the finite c Bethe state:

$$|BA\rangle_c = \frac{1}{\sqrt{N!}} \prod_{1\le i<j\le N} \left[1 + \frac{1}{c}\left(\frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_i}\right)\right] |\det(\mathrm{e}^{\mathrm{i}\lambda_n x_n})|. \tag{80}$$

Manipulations using intertwining operators will be discussed in more detail in the future in connection with concrete physical problems. Here we note that expanding the intertwining operator up to order $1/c$ one observes[9] that a correction to the overlap coefficients up to the order $1/c$ (neglecting the boundary effects) for the condensate initial state has the following form:

$$\tilde{A}^{(0)}_\lambda = A^{(0)}_\lambda \left(1 + \frac{\mathrm{i}(N-1)}{c} P^{(N)}_\lambda\right) + o(1/c^2). \tag{81}$$

Note also that deviations from the TG limit include other ingredients. One of them is an expansion of rapidities in powers of $1/c$,

$$\lambda_j = (2j - N - 1)\frac{\pi}{L}\left[1 - 2\frac{\rho}{c} + 4\left(\frac{\rho}{c}\right)^2 - 8\left(\frac{\rho}{c}\right)^3 + \frac{4\pi^2}{3} N(2j^2 + (N+1)(N-2j))\left(\frac{1}{cL}\right)^3\right]. \tag{82}$$

Using this expression one can get a systematic expansion of the form factors. We do not need these $1/c$ corrections since our procedure uses numerical expressions of the form factors.

We finally note that a computation of the overlap of the arbitrary BA state $\langle 0|C(\lambda_1)\cdots C(\lambda_n)$ with the initial state of a special form $\Psi(x_1)\cdots\Psi(x_n)|0\rangle$ can be considered as a particular case of the evaluation of the multiple-point form factor if we regard the pseudovacuum state as the BA state. The problem of the computation of such a multi-point form factors can be solved using the formalism of multi-site generalization of the NLS problem. This problem was addressed in [69]. Another way to go beyond the TG limit is to use different formalisms described in section 2.

4. Numerical treatment

4.1. Introduction

In this part we present results of numerical computations of correlation functions for various non-equilibrium initial states and their time evolution. In order to do that, we needed to sum expression (43) over all initial λ, intermediate μ, and final ν states.

[9] We note that $\int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{N-1}} \prod_{p=1}^N \mathrm{e}^{-\mathrm{i}qx_p} \sum_{n=1}^N n(\partial/\partial x_n) \det(\mathrm{e}^{\mathrm{i}k_n x_m})\, \mathrm{d}x_N \cdots \mathrm{d}x_1 \overset{q\to 0}{=} Ni(\prod_{1\le i<j\le N}(k_i - k_j) \sum_{n=1}^N k_n / \prod_{n=1}^N k_n \prod_{1\le i<j\le N}(k_i + k_j))$ which is equal then to $\mathrm{i}N\sum_{i=1}^N k_i A^{(0)}_\lambda$, where $A^0_\lambda = \int_0^\infty \int_0^{x_1} \cdots \int_0^{x_{N-1}} \prod_{p=1}^N \mathrm{e}^{-\mathrm{i}qx_p} \det(\mathrm{e}^{\mathrm{i}k_n x_m})\, \mathrm{d}x_N \cdots \mathrm{d}x_1 \overset{q\to 0}{=} (\prod_{1\le i<j\le N}(k_i - k_j) / \prod_{n=1}^N k_n \prod_{1\le i<j\le N}(k_i + k_j))$.

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Although we are interested in the thermodynamic limit $L \to \infty$, $N \to \infty$, numerically one can compute correlation functions for finite size systems only. In order to infer the thermodynamic limit from our finite size results we can set the size of the problem (N and L) to be sufficiently large that numerically computed correlation functions would be sufficiently close to the ones for an infinite system. One of the criteria for such sufficiency could be comparison of the numerical results to analytic results for the system for which a thermodynamic solution for the correlation functions is exactly known. For example, we already know the exact expression for a correlation function in the ground state (76). So we can use it to check the accuracy of our numerical procedures.

Let us estimate the cost of a brute force approach to the summation (43) for a reasonably large system size. Because we are interested in non-equilibrium states, states in λ, μ, and ν are filled way above the 'Fermi momentum'. We can estimate the number of terms in the sum (43) by taking $N \sim 100$ and a momentum cutoff of $\sim 10N$. Then the number of terms in the sum is $\sim \binom{10N}{N}^3 \sim 10^{420}$. Obviously, the sum cannot be taken in a straightforward fashion.

Now we would like to look for possible simplifications of the problem. The first hint comes from [60], where the authors claim that when one considers a summation of the form

$$\sum_{\mu} |\langle GS|F|\mu\rangle|^2, \tag{83}$$

where GS is a ground state, then the sum has a very limited number of major contributions, most of which are one-particle ones. Note that this statement is not directly applicable in our case because we are not working with a ground state and also because we have a double summation, which might have different major contributions due to the larger phase space, or not have such major contributions at all.

A second simplification might come from the fact that we are interested in a large interaction constant c case. For our purposes we can consider the case of large c. As we found in section 3, relevant quantities become much simpler. The most prominent feature of the TG limit is that the only non-zero matrix elements $\langle\lambda|F|\mu\rangle$ come from zero- and one-particle processes (71). This means that in this limit for a given λ we need to do a two-particle summation in (68) with a one-particle transition $\lambda \to \mu$ and a one-particle transition $\mu \to \nu$. This observation also tells us that for large, but finite c, processes with small numbers of transitions should dominate.

Finally, the structure of the overlap factors A_λ for different initial states might provide some clues on how to simplify our task. In particular for the initial states that we are going to investigate, overlap factors can be simplified analytically so we do not need to perform the summation (51) over all permutations.

4.2. Implementation

Now we would like to discuss the ideas behind the concrete implementation of our calculations. Almost everywhere we consider the limit of large c, though we can do numeric calculations for arbitrary c at a cost of substantially higher cpu time.

For a ground state we do several large c calculations to check what values of c can be treated as 'infinite' and to investigate multi-particle contributions. For large, but finite

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c, it is possible to further simplify expressions (45)–(49) by doing a $1/c$ expansion, as explained in section 3. We implemented both direct and simplified versions of matrix elements and overlap calculations and did not find any visible discrepancy in the results, though the performance improvement was substantial.

After we sum the expression

$$\sum_{\lambda,\mu,\nu} A_\lambda A_\nu \langle\lambda|F|\mu\rangle\langle\mu|F|\nu\rangle \tag{84}$$

over intermediate states μ and final states ν for a given initial state λ, we are left with a problem of summation over λ. But the phase space is huge; therefore we cannot use a direct summation. We use Monte Carlo summation instead [89].

Namely, we sample the set of states $\{\lambda'\}$ from the set of all possible initial states $\{\lambda\}$ with the probability of the state λ' being selected being P_λ. Then we can replace summation in (84) over λ with summation over λ' to get

$$I^{\mathrm{MC}} = \frac{\sum_{\lambda',\mu,\nu} A_{\lambda'} A_\nu \langle\lambda'|F|\mu\rangle\langle\mu|F|\nu\rangle/P_{\lambda'}}{\sum_{\lambda',\mu,\nu} A_{\lambda'} A_\nu/P_{\lambda'}}. \tag{85}$$

As we increase the size of sample $\{\lambda'\}$, the value of this sum converges to the true value of (84) for any probability distribution P_λ. Depending on the selection of the probability distribution function, the convergence times can be very different. For instance if we take a uniform distribution over the entire set $\{\lambda\}$, than we can see from equation (67) that weights A_λ can be very different. As a result, many contributions to (85) will be negligibly small. On the other hand if we are picking λ such that $|A_\lambda|$ is around its maximum, all the contribution to the sum will be substantial.

Indeed, it is known [89] that the sum optimally converges to the true value if the distribution function is proportional to the expression that we sum. In our case this would (roughly speaking) mean $P_\lambda \propto A_\lambda \sum_\nu A_\nu$, where ν differs from λ by a process involving at most two particles. As a reasonable approximation, we use $P_\lambda \propto A_\lambda^2$.

The next question is how to sample such states λ'. We cannot sample states from the distribution directly, but we can use Gibbs sampling [90] to do that approximately. Note that any overlap factor can be expressed as a function of state λ and the parameters of the problem. λ itself is a function of a vector of quantum numbers $\vec{I}$ (44). We can fix all the components of $\vec{I}$ except one (I_j). By varying this component and resolving the equation (44) relative to λ, we can find conditional probabilities $P(I_j|I_1\cdots I_{j-1}I_{j+1}\cdots I_n) \propto A^2_{\lambda|I_j}$, where $\lambda|I_j$ is a solution for λ given quantum number I_j (and the rest of quantum numbers, which stay the same). In this way we can sample I_j from the P_λ distribution given that all other quantum numbers $I_{i\neq j}$ are fixed. Then we iterate the procedure with index j running from 1 to N several times. Using this algorithm we obtain a set of statistically independent states pooled with a probability $\propto A_\lambda^2$ [90].

In theory one can do Monte Carlo summation not only over λ states, but also over μ and ν. Nevertheless, we found such an approach impractical because of a much slower convergence stemming from the very poor cancelation of various harmonics.

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4.3. Results

4.3.1. The ground state. First we would like to focus on correlation functions for the ground state. We have several reasons for this. First, an exact analytical solution for such correlation functions is known (76), and hence we can at least partially verify the validity of our approach. Second, we do not have to sum over λ and ν, so computations are very fast and precise. Therefore we can use this case to investigate the effects of our approximations—what finite values of interaction constant c can be considered as infinite, how one-particle approximation affects results, and what the finite size effects of our calculations are.

First we looked at a spatial correlator, calculated at $L = 51$, $N = 51$. For the ground state it is translationally invariant both in space and time. In figure 1 we show a theoretical correlator along with ones calculated at $c = 100$, 1000, and ∞ for one-particle processes only. We see that for $c = 1000$ the correlator is almost indistinguishable from the theoretical $c \to \infty$ limit, though $c = 100$ slightly deviates from that limit. Hence all our further $c \to \infty$ results apply to the $c \gtrsim 1000$ case as well. Also note that the theoretical correlation function perfectly overlaps with one calculated for $c = \infty$; hence our choice of system size can be considered as a thermodynamic limit.

We calculated the same correlators in a separate run for the same finite values of c while taking into account all two-particle contributions and major three-particle contributions in addition to the original one-particle ones. We found that these contributions are negligible. We conclude that it is safe to ignore them in the large c limit.

On figure 2 we show a temporal correlation function for a ground state for $c \to \infty$ as well as a theoretical value given by (76). We see that they overlap perfectly except for the tiny region around $x = 0$ because of the momentum cutoff in our numerical calculations.

4.3.2. The delta function in momentum space. We consider the case where before interactions are switched on all particles are initially in the same state with a given momentum p. Such a state can be prepared experimentally from the condensate at rest using a Bragg pulse.

Before we proceed with calculations, we would like to take a closer look at overlap factors A_λ for this state (63). We are starting with the equation for the projection of our state onto eigenfunctions (TG) of the Hamiltonian $\langle \Psi^{(N)}(q)|\Psi_{\mathrm{TG}}\rangle$. Ignoring coefficients independent of the TG state and non-singular at $q = 0$, we have for odd[10] N

$$\langle \Psi^{(N)}(q)|\Psi_{\mathrm{TG}}\rangle \propto \frac{\prod_{1\le j<k\le N}(\lambda_j - \lambda_k)}{\prod_{i=1}^{N}(\lambda_i - q)\prod_{1\le j<k\le N}(\lambda_j + \lambda_k - 2q)} \left(\sin\left(\frac{Lq}{2}\right)\right)^{(N+1)/2}. \tag{86}$$

Note that our system is discretely translationally invariant in k space: we can shift all λ_i and q by the same constant $(2\pi/L)n$ for arbitrary n, change quantum numbers I_j by n, and all the equations (44)–(63) will hold.

Neglecting finite size effects (resulting in discretization), we can choose n such that $q = (2\pi/L)n$. Then we shift all λ_i by q, and consider the overlap (86) factor in the $q \to 0$ limit.

[10] These calculations can be easily repeated for even N, resulting in the same conclusion.

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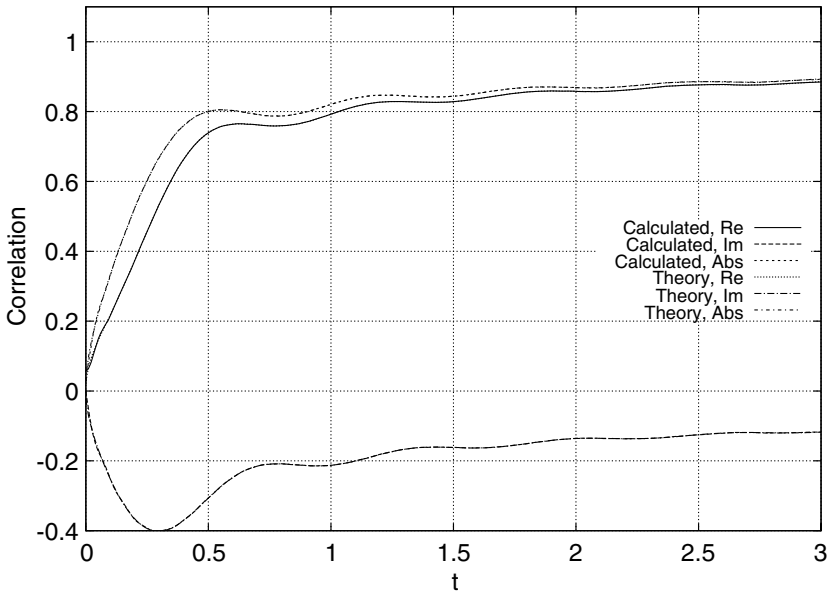

Figure 2. Theoretical and calculated temporal correlators for a ground state in the $c \to \infty$ limit. Real and imaginary parts, and absolute values are shown. Only three curves are visible because the theoretical and calculated plots overlap perfectly.

The sine in the expression (86) results in a $(N+1)/2$-order zero in the numerator in $q \to \infty$ limit. Zeros of the denominator at $q = 0$ are given by one of the $\lambda_i = 0$ in the first product, and all the pairs $(i, j), i < j$, such that $\lambda_i = -\lambda_j$ in the second product. The maximum order of zero that we can achieve in the denominator is when we have one zero λ_i, and for each of the rest of the lambdas we have one exactly opposite to it. For such configuration the zero order of the denominator is also $(N+1)/2$. In this case they cancel, resulting in a non-zero contribution. Any other configurations will result in a lower order of zero of the denominator, and hence zero overlap. We conclude that all of the states with non-zero overlap are symmetric. One can easily repeat this calculation for even N and show that states in this case are symmetric as well.

We can draw an immediate conclusion about the structure of the sum (85) that we use to calculate the correlation function. Remember that for an infinite c, $\langle\lambda|F|\mu\rangle$ has non-zero elements only if states λ and μ differ by at most one quantum number (71). Therefore in the summation (85), λ is symmetric, μ has one quantum number changed relative to λ, and ν, being symmetric, has one quantum number changed relative to μ. But this is possible only if either $|\lambda\rangle = |\nu\rangle$, or if the changed quantum number in $|\lambda\rangle \to |\mu\rangle$ is symmetric with respect to the corresponding change for $|\mu\rangle \to |\nu\rangle$; i.e. if first we change $I_i \to I_i'$, than later we should change either $I_i' \to I_i$ or $-I_i = I_j \to I_j' = -I_i'$. As a result, for a given $|\lambda\rangle$ the selection of $|\mu\rangle$ allows only two possible states for $|\nu\rangle$, strongly reducing the phase space that we need to consider.

Using the symmetry we can also simplify the expression for the overlap factors (63). Because in the sum (85) the normalization of A_λ does not matter, we drop all the constant terms and can consider (86) instead. Let us define $n = (N-1)/2$ (N is odd), and have

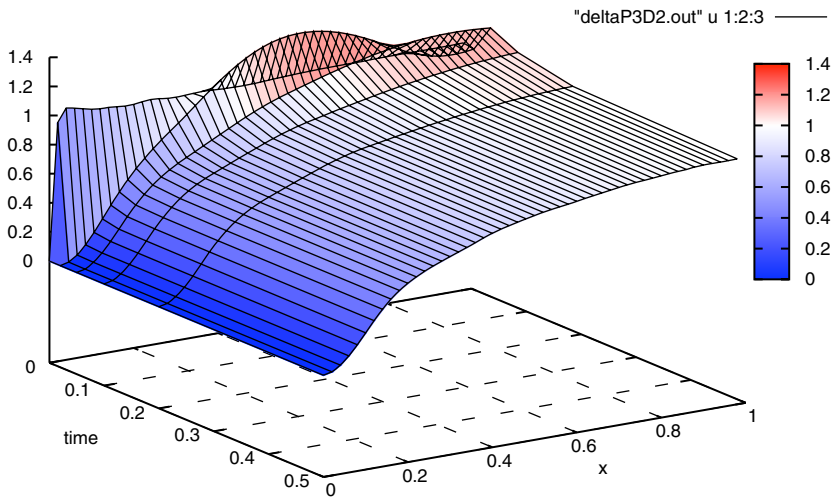

Figure 3. Three-dimensional image (coordinate, time and intensity) of the correlation function for the initial state corresponding to the delta peak in momentum space.

the indexes run from $-n$ to n. Then we can rewrite the numerator as

$$\prod_{0<j<k\leq n}(\lambda_j-\lambda_k)^2(\lambda_j+\lambda_k)^2\prod_{0<j\leq n}-2\lambda_j^3 \tag{87}$$

and the denominator as

$$(-q)^{(N+1)/2}2^{(N-1)/2}\prod_{0<j<k\leq n}(\lambda_j-\lambda_k)^2(\lambda_j+\lambda_k)^2\prod_{0<j\leq n}\lambda_j^4. \tag{88}$$

Then (63) simplifies to

$$A_\lambda \propto \frac{1}{\prod_{\lambda_j>0}\lambda_j}. \tag{89}$$

In the case of interest one can easily restore the constant coefficient and also prove that this expression is valid for even N as well.

Using the conclusions drawn above as regards the relative structure of λ, μ, and ν states, and using expression (89) for overlap factors, we perform a Monte Carlo summation over states for $N = 101$, $L = 101$. In figure 4 we show a spatial correlation $\langle\rho(x_0,t_0)\rho(x_0+x,t_0)\rangle$ as a function of x for $x_0 = 0$ and different values of t_0. Basically the plot represents time evolution of the x correlator starting from the moment that we momentarily switch on a very strong interaction. We can see that at the moment $t_0 = 0$ the entire correlation function is not distorted except for $x = 0$. This is because when we immediately switch on the interaction, particles stay where they are. They just do not have any time to move anywhere; hence the original non-interacting correlation function, which is flat, is preserved (small distortions around $x = 0$ are artifacts of our calculations; if we take into account their errors, they are indistinguishable from 1). But as the time goes by, the repelling interaction generates a wave, which transfers the matter away from the particle sitting at $x = 0$. In the figure we observe the evolution of this wave. When

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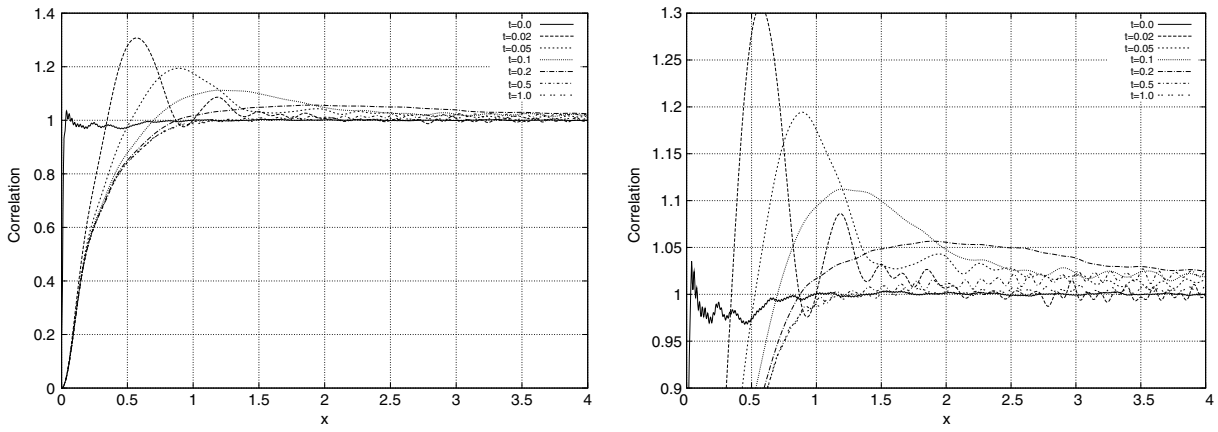

Figure 4. Left: spatial correlator for the initial state corresponding to the delta function in momentum space for different t_0 values. Right: zoom of the left panel.

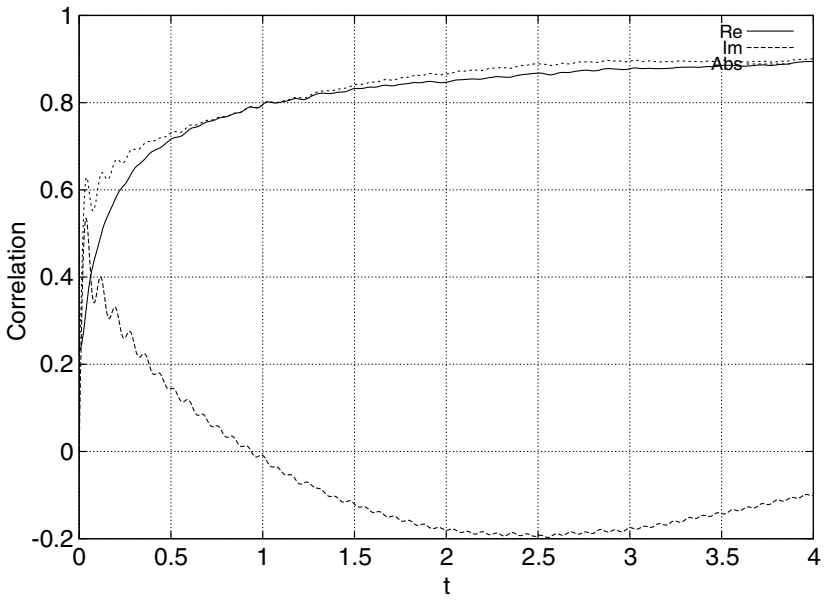

Figure 5. Real and imaginary parts of a temporal correlator for the initial state corresponding to the delta function in momentum space.

the time becomes sufficiently large ($t \gtrsim 1$), the correlation function stabilizes and does not evolve any further.

We also calculate a temporal correlator $\langle \rho(x_0, t_0)\rho(x_0, t_0 + t)\rangle$. Figure 5 shows real and imaginary parts of the correlator. Because the state is translationally invariant, the correlator does not depend on x_0. Interestingly, it also almost does not depend on t_0. All the plots for different t_0 overlapped, and the difference was invisible. On this plot we also observe two 'effects', which are artifacts of our calculation scheme because of the momentum cutoffs introduced: oscillations in the imaginary part and real part not going exactly to zero at $t = 0$.

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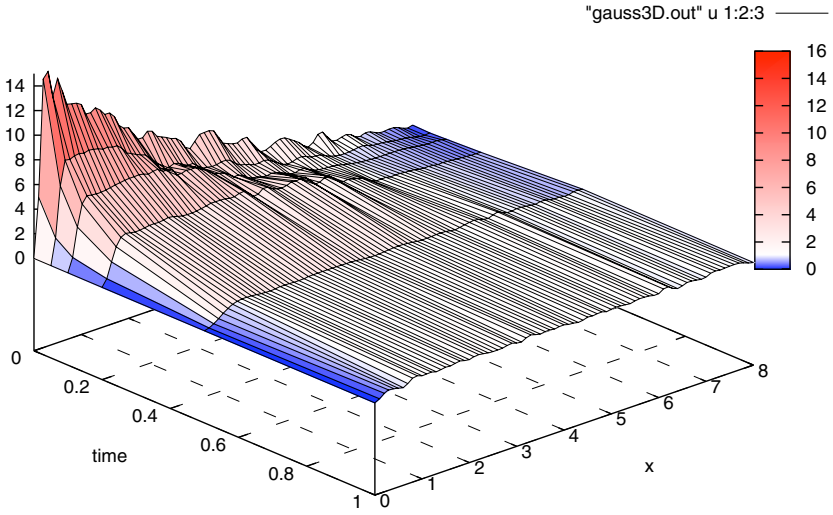

Figure 6. Evolution of the correlation function for the initial state corresponding to the Gaussian in the real space.

4.3.3. The Gaussian pulse. Now we proceed with the initial state—a Gaussian pulse in space, and hence in momentum space. Overlap factors for such a state are given by the expression (67). We neglect finite size effects by considering the limit $L \gg \sigma$, for which expression (67), up to a constant factor, can be written as

$$A_\lambda \propto \exp\left(-\frac{\sigma^2}{2}\sum_i \lambda_i^2\right). \tag{90}$$

In this case we do not have the nice symmetry that we had in section 4.2, so we have to sum over all one-particle μ states and two-particle ν states using expression (85). Summation over all two-particle processes substantially increases the computational time, so in order to partially compensate for this we used smaller values for problem parameters $L = 21$ and $N = 21$. For a packet width parameter we use the value $\sigma = 15/(2\pi)$.

In figure 7 we present the time evolution of the spatial correlator $\langle\rho(x_0, t_0)\rho(x_0+x, t_0)\rangle$ for $x_0 = 0$ and different fixed times t_0. We also show the errors of our calculations to distinguish true correlation function features from noise.

We would like to emphasize several features visible in these plots. First, for $t_0 = 0$, as expected, we see a dip at $x = 0$. Interestingly, the width of this dip is finite and is not determined by the momentum cutoff. From the computational point of view we can explain this by the fact that the overlap factor (90) for the Gaussian state strongly inhibits high harmonics; therefore we do not have momenta high enough to make this dip infinitesimally narrow. This is a finite size effect because of a small number of particles. As parameters L, N, and σ increase proportionally, the width of the dip goes to zero. Second, oscillations of the correlator at $t_0 = 0$ around the dip $x_0 = 0$ are not determined by the cutoff and much bigger than the error of our calculations. This is again the effect of a finite size system. Third, as we have already seen in the previous section, for times $t_0 \gtrsim 1$ the correlation function stabilizes. But the process of stabilization is quite remarkable. We do not have a widening of a Gaussian peak. Instead it looks like the peak has the same

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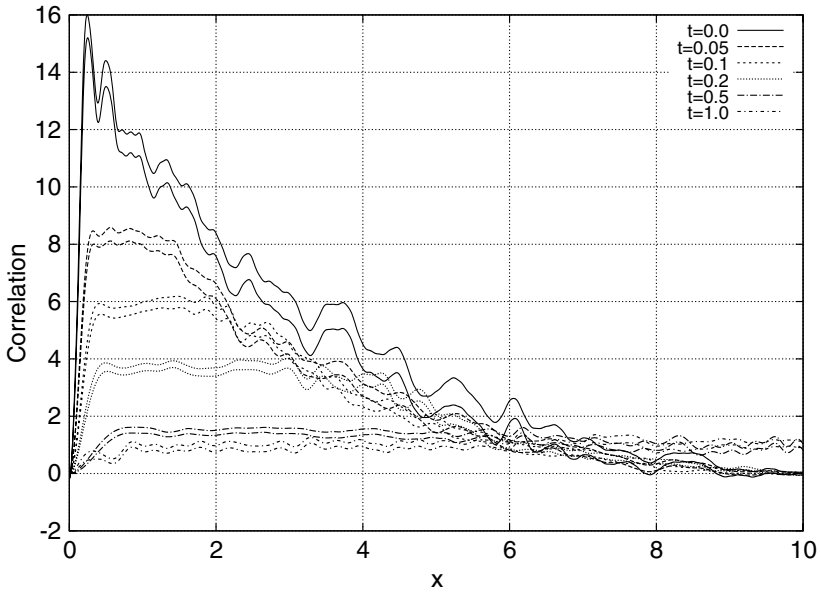

Figure 7. Spatial correlator for different t_0 values for a Gaussian initial state and its error. Two lines for each value of t_0 lie one standard deviation above and below, relative to the average value.

width, but its height decreases with time. Probably, the qualitative explanation lies in the fact that high density regions have high interaction energies; hence in these regions we have fast particles which quickly leave the region, i.e. we have a ballistic scenario, which differs from the diffusion scenario for which we would expect a widening of a Gaussian peak with time.

Unfortunately, due to some peculiarities of the computations that we had to conduct, we were unable to produce reliable results for a temporal correlator. The results, though reproducing an overall shape of the correlator, were very noisy because of beats attributed to the non-exact cancelation of various harmonics. We do not provide a plot for these results.

5. Discussion and summary

In this paper we addressed a problem of the non-equilibrium time evolution of one-dimensional Bose gas with a contact interaction from the general perspective of the dynamics of integrable systems. Several approaches have been proposed recently for analyzing the time evolution of integrable many-body models, including the quantum inverse scattering method, and using the formalism of the intertwining operator, and extended conformal symmetry. After critically reviewing these approaches we concentrated on conceptually the simplest method, based on using the Bethe ansatz to decompose initial states into precise eigenstates of the interacting Hamiltonian using the intertwining operator and then using form-factor expansion to calculate the time evolution of correlation functions. The main difficulty of this method is that it requires summation over a large number of intermediate states. In this paper we focused on the regime of strong repulsive interactions between bosons and developed an efficient numerical procedure for

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performing the summation over intermediate states. We analyzed two kinds of initial states: all particles having zero momentum and all particles in a Gaussian wavepacket in real space. In both cases we find a non-trivial time evolution of the second-order coherence $g_2(x_1, x_2, t) = \langle \rho(x_1, t), \rho(x_2, t) \rangle$, which reflects the intrinsic dichotomy between initial states and the Hamiltonian. Initial condensate states exhibit bunching at short distances, whereas strong repulsion in the Hamiltonian introduces strong antibunching. We note that the dynamics of more complicated initial states still awaits study. We hope that our treatment here will motivate others to go further into this subject.

For the initial state which has all particles in a state with zero momentum, results for g_2 are summarized in figure 3. Antibunching at the shortest distances is present at all times, reflecting repulsion between particles. A more striking feature is the appearance of bunching and oscillations in $g_2(x_1 - x_2, t)$ at intermediate scales of time and length. At transient times, g_2 has Friedel-like oscillations as a function of $x_1 - x_2$, which disappear at longer times. Crystallization of the TG gas in the process of non-equilibrium time evolution was also discussed in [20]. At longer times the form of g_2 is qualitatively similar to what one finds for the equilibrium Lieb–Liniger model with intermediate interactions at high temperatures [92]. Figure 3 also provides some support to the idea of light cone formation discussed in [91]. Some of these features are similar to those of the quench dynamics in other integrable systems [30, 93].

For the initial state which has all particles in a Gaussian wavepacket in real space, the time evolution of g_2 is shown in figures 6 and 7. As in the previous case we observe antibunching at the shortest distances. For intermediate timescales it is followed by a pronounced peak in g_2 reflecting dynamic bunching. This system would be naturally characterized by the time-dependent *short range correlation length*, which increases with time, reflecting expansion of the system in real space. Oscillations in g_2 which we observe in this case are small and are most likely related to the finite number of particles used in the analysis. Hence transient states of this system would be more naturally characterized as liquid rather than crystal.

It should be possible to test the predictions made in our paper for the behavior of g_2, in experiments with ultracold atoms and photons in a strongly nonlinear medium.

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Appendix: The inverse scattering transform and the algebraic Bethe ansatz—basic concepts

The nonlinear Schrödinger Hamiltonian represents the simplest example of a system solvable by using the algebraic Bethe ansatz [35, 74]. For a review and many details see [4]. Here we overview the basic construction with the connection to the inverse scattering transform in order to fix notation and for the sake of self-consistency.

The Zakharov–Shabat method starts from transforming the field $\Psi(x, t = 0)$ of the nonlinear Hamiltonian (1) at time $t = 0$ into a set of 'scattering data' given by the

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following linear problem:

$$\mathrm{i}\frac{\partial}{\partial x}\Phi(x,\xi) = Q(x,\xi)\Phi(x,\xi) \tag{A.1}$$

where

$$Q(x,\xi) = \begin{pmatrix} -\frac{\xi}{2} & -\sqrt{c}\Psi(x) \\ \sqrt{c}\Psi^\dagger(x) & \frac{\xi}{2} \end{pmatrix}. \tag{A.2}$$

The solution $\Phi(x,\xi)$ of this equation is defined by the condition $|\Psi(x)| \to 0$ as $x \to \pm\infty$ and by the properties of Jost solutions:

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \mathrm{e}^{\mathrm{i}\xi x/2} \underset{x\to-\infty}{\longleftarrow} \begin{pmatrix} \phi_1(x,\xi) \\ \phi_2(x,\xi) \end{pmatrix} \underset{x\to\infty}{\longrightarrow} \begin{pmatrix} A(\xi)\mathrm{e}^{\mathrm{i}\xi x/2} \\ B(\xi)\mathrm{e}^{-\mathrm{i}\xi x/2} \end{pmatrix}, \tag{A.3}$$

$$\begin{pmatrix} -B^\dagger(\xi)\mathrm{e}^{\mathrm{i}\xi x/2} \\ A(\xi)\mathrm{e}^{\mathrm{i}\xi x/2} \end{pmatrix} \underset{x\to-\infty}{\longleftarrow} \begin{pmatrix} \chi_1(x,\xi) \\ \chi_2(x,\xi) \end{pmatrix} \underset{x\to\infty}{\longrightarrow} \begin{pmatrix} 0\mathrm{e}^{\mathrm{i}\xi x/2} \\ 1\mathrm{e}^{-\mathrm{i}\xi x/2} \end{pmatrix} \mathrm{e}^{-\mathrm{i}\xi x/2}. \tag{A.4}$$

Rewriting the linear equation above with the boundary conditions as an integral equation gives the Gelfand–Levitan–Marchenko equation

$$\xi_1(x,\xi)\mathrm{e}^{\mathrm{i}x\xi/2} = -\sqrt{c}\int_{-\infty}^{\infty}\mathrm{d}y\,\theta(y-x)\mathrm{e}^{\mathrm{i}\xi y}\Psi^\dagger(y)\chi_2(y,\xi)\mathrm{e}^{-\mathrm{i}y\xi/2}, \tag{A.5}$$

$$\xi_2(x,\xi)\mathrm{e}^{-\mathrm{i}x\xi/2} = 1 + \mathrm{i}\sqrt{c}\int_{-\infty}^{\infty}\mathrm{d}y\,\theta(y-x)\mathrm{e}^{-\mathrm{i}\xi y}\chi_1(y,\xi)\Psi(y)\mathrm{e}^{\mathrm{i}y\xi/2} \tag{A.6}$$

which can be solved iteratively in powers of $\sqrt{c}$:

$$\begin{aligned}\chi_1(x,\xi)\mathrm{e}^{\mathrm{i}x\xi/2} = -\mathrm{i}\sqrt{c}\sum_{n=0}^{\infty}c^n\prod_{i=0}^{n}\int\mathrm{d}x_i\prod_{j=1}^{n}\mathrm{d}y_j\,\theta(x_0>y_1>\cdots y_n>x_n>x)\\ \times\ \mathrm{e}^{\mathrm{i}\xi(\sum_{i=0}^{n}x_i-\sum_{j=1}^{n}y_j)}\\ \times\ \Psi^\dagger(x_0)\cdots\Psi^\dagger(x_n)\Psi(y_n)\cdots\Psi(y_1),\end{aligned} \tag{A.7}$$

$$\begin{aligned}\chi_2(x,\xi)\mathrm{e}^{-\mathrm{i}x\xi/2} = 1+\sum_{n=0}^{\infty}c^n\prod_{i=0}^{n-1}\int\mathrm{d}x_i\prod_{j=1}^{n}\mathrm{d}y_j\,\theta(x_0>y_1>\cdots x_{n-1}>y_n>x)\\ \times\ \mathrm{e}^{\mathrm{i}\xi(\sum_{i=0}^{n-1}x_i-\sum_{j=1}^{n}y_j)}\\ \times\ \Psi^\dagger(x_0)\cdots\Psi^\dagger(x_{n-1})\Psi(y_n)\cdots\Psi(y_1)\end{aligned} \tag{A.8}$$

where $\theta(x_1>x_2>\cdots>x_n) = \theta(x_1-x_2)\theta(x_2-x_3)\cdots\theta(x_{n-1}-x_n)$. This solution can be written as a solution for the scattering data, $A(\xi)$ and $B(\xi)$. Finally, defining the reflection operator as

$$R(\xi) = \mathrm{i}[A(\xi)]^{-1}B(\xi) \tag{A.9}$$

one obtains the expansion (2). Operators $R(\xi)$ satisfy the Zamolodchikov–Faddeev algebra (6). In this formalism, the Bethe ansatz states are constructed by application

of Zamolodchikov–Faddeev operators to the pseudovacuum state $|0\rangle$,

$$|\psi_N\rangle_{BA} = R^\dagger(\xi_1)\cdots R^\dagger(\xi_N)|0\rangle. \tag{A.10}$$

These states are complete for the case of repulsion. Using the expansion (2) one can show [32] that the *special* ordered initial state of the form

$$|\psi_N\rangle_{\rm ord} = \theta(x_1 > x_2 > \cdots > x_N)|\Psi^\dagger(x_1)\Psi^\dagger(x_2)\cdots\Psi^\dagger(x_N)|0\rangle \tag{A.11}$$

is equal to the following state:

$$R^\dagger(x_1)R^\dagger(x_2)\cdots R^\dagger(x_N)|0\rangle \tag{A.12}$$

where

$$R(x) = \int \frac{d\xi}{2\pi} \mathrm{e}^{\mathrm{i}x\xi} R(\xi). \tag{A.13}$$

We note that the evolution of this state can be obtained explicitly, as discussed in section 2. The case of attraction is discussed in the appendix.

The transfer matrix is a central ingredient of the construction of the inverse scattering transform on the finite interval on the lattice (one performs a space discretization procedure for the LL model first). It can be represented as a matrix

$$T(\xi) = \begin{pmatrix} A(\xi) & B(\xi) \\ C(\xi) & D(\xi) \end{pmatrix}. \tag{A.14}$$

The transfer matrix is constructed as a product of monodromy matrices $L_j(\xi)$ for each site j, $T(\xi) = \prod_j L_j(\xi)$, which in the case of the NS problem has the form of matrix Q which is one of the matrices forming the Lax pair. Traces of the transfer matrix commute for different ξ values and are generators of the integrals of motion. The integrability condition is expressed by the special property

$$R(\xi - \xi')(T(\xi) \otimes T(\xi')) = (T(\xi') \otimes T(\xi))R(\xi - \xi') \tag{A.15}$$

where the matrix $R(\xi, \xi')$ is a solution of the Yang–Baxter equation, which for the case of the NS problem belongs to the class of six-vertex models:

$$R_{12}(\xi)R_{13}(\xi + \mu)R_{23}(\mu) = R_{23}(\mu)R_{13}(\xi + \mu)R_{12}(\xi) \tag{A.16}$$

$$R_{ab} = \beta I_{ab} + \alpha P_{ab}, \qquad \alpha = \frac{\xi_a - \xi_b}{\xi_a - \xi_b - \mathrm{i}c}, \qquad \beta = \frac{-\mathrm{i}c}{\xi_a - \xi_b - \mathrm{i}c} \tag{A.17}$$

where I_{ab} and P_{ab} are identity and permutation operators acting on the tensor product of two single-particle spaces indexed by a and b. In the finite size lattice formalism the diagonal entries of the matrix (more precisely its trace $\tau(\xi) = \mathrm{Tr}\, T(\xi) = A(\xi) + D(\xi)$) generate conserved quantities of the model whereas the off-diagonal elements $B(\xi)$ and $C(\xi)$ act as creation and annihilation operators for pseudoparticles. The n-particle Bethe ansatz eigenvectors are constructed using these off-diagonal elements of the transfer matrix as

$$|\Psi_n(\{\lambda_n\})\rangle = B(\lambda_1)B(\lambda_2)\cdots B(\lambda_n)|0\rangle \tag{A.18}$$

whereas the bra vectors are constructed as

$$\langle\Psi_n(\{\lambda_n\})| = \langle 0|C(\lambda_1)C(\lambda_2)\cdots C(\lambda_n). \tag{A.19}$$

The algebraic Bethe ansatz deals with diagonalization of the trace $\tau(\xi)$ of the transfer matrix, thus solving the eigenvalue equation $\tau(\lambda)|BA\rangle = \Lambda(\lambda,\{\lambda_a\})|BA\rangle$. This can be done using the commutation relations between operators $A(\lambda), B(\lambda), C(\lambda), D(\lambda)$ which can be deduced from the Yang–Baxter algebra. This procedure leads to expressions for the $\Lambda(\lambda,\{\lambda_a\}) = \alpha(\lambda)\prod_{a=1}^{n} f(\lambda-\lambda_a) + \beta(\lambda)\prod_{a=1}^{n} f(\lambda_a-\lambda)$ which can be further related to the energy and to the consistency relation, known as a Bethe ansatz equations for the momenta λ_a of the pseudoparticles:

$$\frac{\alpha(\lambda_a)}{\beta(\lambda_a)} = \prod_{b\neq a}\frac{\lambda_b-\lambda_a}{\lambda_a-\lambda_b}, \tag{A.20}$$

where the function $f(\lambda)$ is determined by the elements of the R-matrix. The connection with the continuum version of the NLS model is established by a limiting procedure of lattice size going to zero while keeping the density constant on a finite interval.

Due to the work of Sklyanin [94] it is possible to formulate an even more general NS problem which includes the boundaries. The boundary problems can be divided into two categories, soliton-preserving and soliton-non-preserving. For recent progress in the solution of the boundary NS model see [95].

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