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Source / Izvornik: **Physical Review Letters, 2008, 100**

Journal article, Published version

Rad u časopisu, Objavljena verzija rada (izdavačev PDF)

<https://doi.org/10.1103/PhysRevLett.100.080406>

Permanent link / Trajna poveznica: <https://urn.nsk.hr/urn:nbn:hr:217:397408>

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Download date / Datum preuzimanja: **2025-03-09**



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Fermi-Bose Transformation for the Time-Dependent Lieb-Liniger Gas

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(Received 10 September 2007; revised manuscript received 5 December 2007; published 29 February 2008)

Exact solutions of the Schrödinger equation describing a freely expanding Lieb-Liniger gas of delta-interacting bosons in one spatial dimension are constructed. We demonstrate that for any interaction strength the system enters a strongly correlated regime during such expansion. The asymptotic form of the wave function is shown to have the form characteristic for “impenetrable-core” bosons. Exact solutions are obtained by transforming a fully antisymmetric (fermionic) time-dependent wave function that obeys the Schrödinger equation for a free gas. This transformation employs a differential Fermi-Bose mapping operator that depends on the strength of the interaction and the number of particles.

DOI: [10.1103/PhysRevLett.100.080406](https://doi.org/10.1103/PhysRevLett.100.080406)

PACS numbers: 05.30.-d, 03.75.Kk, 67.85.De

Nonequilibrium phenomena in quantum many-body systems are among the most fundamental and intriguing phenomena in physics. One-dimensional (1D) interacting Bose gases provide a unique opportunity to study such phenomena. In some cases, the models describing these systems [1–3] allow one to determine exact time-dependent solutions of the Schrödinger equation [4,5], providing insight beyond various approximations, which is particularly important in strongly correlated regimes. These 1D systems are experimentally realized with atoms tightly confined in effectively 1D waveguides [6–8], where nonequilibrium dynamics is considerably affected by the kinematic restrictions of the geometry [8], while quantum effects are enhanced [9–11]. Today, experiments have the possibility to explore 1D Bose gases for various interaction strengths, from the Lieb-Liniger (LL) gas with finite coupling [6,8] up to the so-called Tonks-Girardeau (TG) regime of “impenetrable-core” bosons [7,8]. However, most theoretical studies of the exact time dependence address the TG regime (see, e.g., Refs. [4,12–18]). In this limit, the complex many-body problem is considerably simplified due to the Fermi-Bose mapping property [4] where dynamics follows a set of uncoupled single-particle (SP) Schrödinger equations [4]. It is therefore desirable to employ an efficient method for calculating the time evolution of a LL gas with finite interaction strength.

In 1963, Lieb and Liniger [1] presented, on the basis of the Bethe ansatz, a solution for a homogeneous Bose gas with (repulsive) δ -function interactions, for arbitrary interaction strength c ; periodic boundary conditions were imposed. This system was analyzed by McGuire on an infinite line with attractive interactions [3]. The renewed interest in 1D Bose gases stimulated recent studies of static LL wave functions [19–21] including a LL gas in box confinement [21]. Besides the wave functions, the correlations of a LL system with finite coupling [22–31] provide a link to many observables and were analyzed by using various techniques, including the inverse scattering method [24,25,30,31], $1/c$ expansions [23] relying on the analytic

results in the TG regime [32], and numerical quantum Monte Carlo techniques [28]. Regarding dynamics, a full numerical study of the irregular dynamics in a mesoscopic LL system was presented in [33]. In Ref. [5], Girardeau has shown that phase imprinting by light pulses conserves the so-called cusp condition imposed by the interactions on the LL wave functions, and suggested to use time-evolving SP wave functions to analyze the subsequent dynamics. However, as pointed out in Ref. [5], the presented scheme does not obey the cusp condition during the evolution, which limits its validity. This situation can be remedied by using an ansatz that obeys the cusp condition at all times by construction [24,34].

Here we construct exact solutions for the freely expanding LL gas with localized initial density distribution. We demonstrate that for any interaction strength c , the LL system enters a strongly correlated regime during such expansion. Consequently, the asymptotic form of the wave function and single-particle density assume the form characteristic for that of a TG gas. Exact solutions are obtained by differentiating a fully antisymmetric (fermionic) time-dependent wave function, which obeys the Schrödinger equation for a free Fermi gas [34]. This method, outlined by Gaudin [34], employs a differential operator that depends on the interaction strength c and the number of particles.

We consider the dynamics of N indistinguishable δ -interacting bosons in a 1D geometry [1]. The Schrödinger equation for this system is

$$i \frac{\partial \psi_B}{\partial t} = - \sum_{i=1}^N \frac{\partial^2 \psi_B}{\partial x_i^2} + \sum_{1 \leq i < j \leq N} 2c \delta(x_i - x_j) \psi_B, \quad (1)$$

where $\psi_B(x_1, \dots, x_N, t)$ is the many-body wave function, and c quantifies the strength of the interaction (for connection to physical units see, e.g., [5]). The x space is infinite (we do not impose any boundary conditions), which corresponds to a number of interesting experimental situations where the gas is initially localized within a certain region

of space and then allowed to freely evolve. This is relevant for free expansion [13–16] or interference of two initially separated clouds during such expansion [12], etc. Because of the Bose symmetry, it is sufficient to express the wave function ψ_B in a single permutation sector of the configuration space, $R_1: x_1 < x_2 < \dots < x_N$. Within R_1 , ψ_B obeys

$$i\partial\psi_B/\partial t = -\sum_{i=1}^N \partial^2\psi_B/\partial x_i^2, \quad (2)$$

while interactions impose boundary conditions at the borders of R_1 [1]:

$$\left[1 - \frac{1}{c}\left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j}\right)\right]_{x_{j+1}=x_j} \psi_B = 0. \quad (3)$$

This constraint creates a cusp in the many-body wave function when two particles touch, which should be present at any time during the dynamics.

In the TG limit (i.e., when $c \rightarrow \infty$) the cusp condition is $\psi_B(x_1, \dots, x_j, x_{j+1}, \dots, x_N, t)|_{x_{j+1}=x_j} = 0$ [2,4], which is trivially satisfied by an antisymmetric fermionic wave function $\psi_F(x_1, \dots, x_N, t)$; thus $\psi_B = \psi_F$ within R_1 , which is the famous Fermi-Bose mapping [2,4]. In many physically interesting cases, ψ_F can be constructed as a Slater determinant

$$\psi_F(x_1, \dots, x_N, t) = (N!)^{-(1/2)} \det[\phi_m(x_j, t)]_{m,j=1}^N. \quad (4)$$

Since $\psi_B = \psi_F$ within R_1 , ψ_F must obey $i\partial\psi_F/\partial t = -\sum_{j=1}^N \partial^2\psi_F/\partial x_j^2$, which implies that the SP wave functions $\phi_m(x_j, t)$ evolve according to

$$i\partial\phi_m/\partial t = -\partial^2\phi_m/\partial x^2; \quad (5)$$

$m = 1, \dots, N$. Thus, in the TG limit, the complexity of the many-body dynamics is reduced to solving a simple set of uncoupled SP equations, while the interaction constraint (3) is satisfied by the Fermi-Bose construction.

The simplicity and success of this idea motivates us to choose an ansatz that automatically satisfies constraint (3) for any finite c [24,34]. It can be shown that the wave function

$$\psi_{B,c} = \mathcal{N}_c \hat{O}_c \psi_F(\text{inside } R_1), \quad (6)$$

where

$$\hat{O}_c = \prod_{1 \leq i < j \leq N} \left[1 + \frac{1}{c} \left(\frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_i}\right)\right] \quad (7)$$

is a differential operator and \mathcal{N}_c is a normalization constant, obeys the cusp condition (3) by construction [24,34]. In order to exactly describe the dynamics of LL gases, the wave function (6) should also obey Eq. (2) inside R_1 . From the commutators $[\partial^2/\partial x_j^2, \hat{O}_c] = 0$ and $[i\partial/\partial t, \hat{O}_c] = 0$ it follows that if ψ_F is given by Eq. (4) and the $\phi_m(x_j, t)$ obey Eq. (5), then $\psi_{B,c}$ obeys Eq. (2). Note that for $c \rightarrow \infty$, one recovers Girardeau's Fermi-Bose mapping [2,4], i.e., $\hat{O}_c = 1$.

Interestingly, for a single time-dependent noninteracting fermionic wave function ψ_F , transformation (6) generates a whole family of LL wave functions $\psi_{B,c}$ for different interaction strengths c . An important question is this: What is the difference in the structure of the LL wave functions and corresponding observables for different c , and what happens to these differences during evolution?

Let us assume that for $t < 0$ the LL gas is confined by an external potential $V(x)$ and is in its ground state, before at $t = 0$ the potential is suddenly switched off. In order to find the exact form of the ground state, we have to solve the static Schrödinger equation for the LL gas in the potential $V(x)$. By using the above formalism, we express the ground state as $\psi_{B0} = \mathcal{N}_c \hat{O}_c \psi_{F0}$, which should (within R_1) obey $\sum_j H_j \psi_{B0} = E_{B0} \psi_{B0}$ or, equivalently,

$$\hat{O}_c \sum_j H_j \psi_{F0} - \left[\hat{O}_c, \sum_j H_j\right] \psi_{F0} = \hat{O}_c E_{B0} \psi_{F0}. \quad (8)$$

Here, E_{B0} is the ground-state energy, and $H_j = -\partial^2/\partial x_j^2 + V(x_j)$ is the SP Hamiltonian. Equation (8) shows that, due to the nonvanishing commutator $[\hat{O}_c, \sum_j H_j] = [\hat{O}_c, \sum_j V(x_j)]$, operating with \hat{O}_c on the fermionic ground state in the trap does not give the bosonic ground state. However, for sufficiently strong interactions and/or weak and slowly varying potentials, we can approximate $[\hat{O}_c, \sum_j V(x_j)] \approx 0$. In the TG limit, the commutator vanishes identically. Thus, for sufficiently strong interactions, the ground state is approximated by $\psi_{B0} = \mathcal{N}_c \hat{O}_c \det[\phi_m(x_j, 0)]_{m,j=1}^N / \sqrt{N!}$, where $\phi_m(x_j, 0)$ is the m th eigenstate of the SP Hamiltonian.

In what follows we study free expansion from such an initial condition, $\psi_{B,c}(x_1, \dots, x_N, 0) = \mathcal{N}_c \hat{O}_c \det[\phi_m(x_j, 0)]_{m,j=1}^N / \sqrt{N!}$, which describes a LL gas with a localized density distribution. Even though this initial condition cannot be interpreted as the ground state of a LL gas in $V(x)$ for weak interactions, we emphasize that transformation (6) generates a family of exact time-dependent solutions $\psi_{B,c} = \mathcal{N}_c \hat{O}_c \det[\phi_m(x_j, t)]_{m,j=1}^N / \sqrt{N!}$ for all values of c . In what follows we assume that $V(x) = \nu^2 x^2/4$, with $\nu = 2$. The properties of the initial condition are illustrated in Fig. 1 (left column), which depicts the section $|\psi_{B,c}(0, x_2, x_3, 0)|^2$ of the probability density for $N = 3$ particles, and $c = 1, 3$, and 10. We observe that, as the interaction strength increases, the initial state becomes more correlated. Given that one particle is located at zero, for $c = 1$ there is a considerable probability that the other two particles are to the left or to the right of the first one; i.e., their positions are weakly correlated with that of the first particle. However, for larger c , if one particle is at zero, it is more likely that the other two particles are on opposite sides of the first one, and their distance grows with increasing interaction strength.

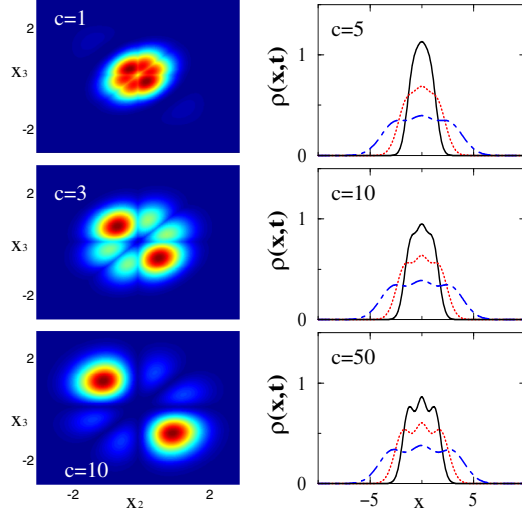


FIG. 1 (color online). The correlation properties of the initial state and the evolution of the SP density for various interaction strengths, for $N = 3$ particles. (Left column) The probability density $|\psi_{B,c}(0, x_2, x_3, 0)|^2$ for $c = 1, 3, 10$. (Right column) The SP density at $t = 0$ (black solid line), $t = 0.5$ (red dotted line), and $t = 1$ (blue dot-dashed line), for $c = 5, 10, 50$.

When the harmonic potential is turned off, the evolution of the SP states $\phi_m(x, t)$ is known exactly (see, e.g., Ref. [15]): $\phi_m(x, t) = \phi_m(x/b(t), 0) \exp[ix^2 b'(t)/(4b(t)) -$

$$\psi_{B,c} = \mathcal{N}(c, \nu, N) b(t)^{-(N/2)} e^{-i(N^2 \nu/2)\tau(t)} \hat{O}_c e^{-(\nu - i\nu^2 t)/4 \sum_{j=1}^N [x_j/b(t)]^2} \prod_{1 \leq i < j \leq N} (x_j - x_i), \quad (9)$$

where $\mathcal{N}(c, \nu, N)$ is a normalization constant, evaluating to $\mathcal{N} = 1$ for $c \rightarrow \infty$. The action of the operator \hat{O}_c yields lengthy expressions already for a few particles, and particular examples will be given elsewhere. Although Eq. (9) provides a family of exact wave functions for the time-dependent LL gas, it is desirable to calculate the evolution of observables such as the SP density $\rho_c(x, t) = N \int dx_2 \dots dx_N |\psi_{B,c}(x, x_2, \dots, x_N, t)|^2$. This task is complicated by the many-fold integral. However, we can find the evolution of $\rho_c(x, t)$ numerically for small numbers of particles. Figure 1 (right column) displays the evolution of the SP density for three different values of c . For larger c , the initial SP density exhibits typical TG-fermionic properties, characterized by N small separated humps [4,12]. For all values of c , the SP density acquires such humps during free expansion indicating that the system becomes strongly correlated in time. This is further illustrated in Figs. 2(a)–2(c), which show the section of the probability $|\psi_{B,c}(0, x_2, x_3, t)|^2$ for $c = 0.1$, at times $t = 0, 0.8$, and 2. By comparing Figs. 2(a)–2(c) with the left column of Fig. 1, we clearly see that with the increase of

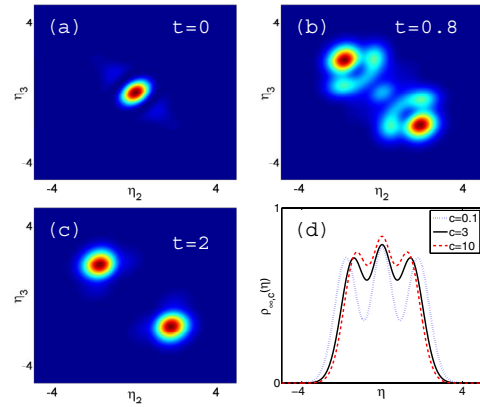


FIG. 2 (color online). The evolution of correlation properties during free expansion. (a)–(c) Contours of the probability density $|\psi_{B,c}(0, x_2, x_3, t)|^2$ for $c = 0.1$, at times $t = 0, 0.8$, and 2; the labels are $\eta_i = x_i/b(t)$. (d) The asymptotic form of the SP density $\rho_{\infty,c}(\eta)$ for $c = 0.1, 3$, and 10.

$iE_m \tau(t)]/\sqrt{b(t)}$, where E_m is the energy of the m th SP eigenstate $\phi_m(x, 0)$, $b(t) = \sqrt{1 + t^2 \nu^2}$, and $\tau(t) = \arctan(\nu t)/\nu$. We can make use of the expression for the ground state of a TG gas in harmonic confinement [35] to calculate ψ_{F0} . Employing Eq. (6), the evolution of $\psi_{B,c}$ can be formally expressed (within R_1) as

time the system qualitatively behaves as if the interaction strength increases.

In order to gain deeper insight into this transformation of the system towards a strongly correlated regime during free expansion, it is instructive to study the exact form of the wave functions and the particle densities for large t . This is also motivated by the fact that the state of the system in experiments is often studied by measuring the density of the atomic cloud after free expansion. The spatial extent of the wave functions presented in Eq. (9) scales as $b(t)$ with time [$b(t) \sim \nu t$ for $t \gg \nu^{-1}$]. Hence, we are interested in the behavior of $\psi_{B,c}(\eta_1 b(t), \dots, \eta_N b(t), t)$ for large times, where $\eta_i = x_i/b(t)$ are the new rescaled spatial coordinates. From the fact that the operator \hat{O}_c is invariant under the transformation $x_i \rightarrow \eta_i$, $c \rightarrow b(t)c$, we immediately see that expansion of the system implies an increase of the effective interaction strength, which is in accordance with the result of Ref. [1] on the static LL gas. By using this fact, after some algebra it can be demonstrated that the leading term of $\psi_{B,c}(\eta_1 b(t), \dots, \eta_N b(t), t)$ for large times is (in any region R_n)

$$\psi_{B,c}(\eta_1 b(t), \dots, \eta_N b(t), t) \propto b(t)^{-(N/2)} e^{-i(N^2 \nu/2)\tau(t)} e^{-(\nu - i\nu^2 t)/4 \sum_{j=1}^N \eta_j^2} \prod_{1 \leq i < j \leq N} g(\eta_j - \eta_i) + \mathcal{O}\left(\frac{1}{t}\right), \quad (10)$$

where $g(\eta) = |\eta| + i\nu \eta^2/2c$. Equation (10) readily yields a comparison of the wave functions for different c . At any c ,

the wave function (10) has TG structure; i.e., it is zero for $\eta_i = \eta_j$, $i \neq j$. As a consequence of that, the asymptotic SP density $\rho_{\infty,c}(\eta) = \lim_{t \rightarrow \infty} b(t) \rho_c(\eta b(t), t)$ has a TG multihumped structure at any c [see Fig. 2(d) for $N = 3$]. It is interesting to note that for weaker interactions c , the asymptotic SP density has deeper valleys between the humps. This follows from the fact that as two particles approach the amplitude of the wave function Eq. (10) decreases faster for smaller c ; in the TG limit the amplitude behavior is dominated by $g(\eta_i - \eta_j) \sim |\eta_i - \eta_j|$, whereas for small c the term $g(\eta_i - \eta_j) \sim (\eta_i - \eta_j)^2/c$ dominates.

It should be emphasized that the Fermi-Bose transformation employed here differs from the fermion-boson duality discussed in Ref. [36] (see also [37]), because it transforms a *noninteracting* fermionic wave function into a family of wave functions describing LL gas. Using Ref. [36] it can be shown that the approach used here can also be applied to construct wave functions for a time-dependent Fermi gas with finite-strength interactions.

In conclusion, we have constructed exact solutions for the freely expanding LL gas with a localized initial density distribution. We have demonstrated that the system enters a strongly correlated regime during such expansion. The asymptotic form of the wave function is shown to have the form characteristic for that of a TG gas. Wave functions are obtained by differentiating a fully antisymmetric (fermionic) time-dependent wave function, which obeys the Schrödinger equation for a free Fermi gas. For a number of physically interesting situations, by using the operator \hat{O} , the state of the system can be derived from N SP time-dependent states, as anticipated in Ref. [5]. The construction of LL wave functions for various external potentials $V(x)$, and the derivation of correlation functions within the employed formalism is the subject of ongoing work.

The authors are grateful to M. Girardeau for pointing out to them that the formulation of the Bethe ansatz as in Eq. (6) was previously stated in Refs. [24,34]. H. B. and R. P. acknowledge support by the Croatian Ministry of Science (MZOS) (Grant No. 119-0000000-1015). T. G. acknowledges support by the Deutsche Forschungsgemeinschaft. This work is also supported by the Croatian-German scientific collaboration funded by DAAD and MZOS.

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