Momentum distribution dynamics of a Tonks-Girardeau gas: Bragg reflections of a quantum many-body wavepacket

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(Dated: November 5, 2018)

The dynamics of the momentum distribution and the reduced single-particle density matrix (RSPDM) of a Tonks-Girardeau (TG) gas is studied in the context of Bragg-reflections of a many-body wavepacket. We find strong suppression of a Bragg-reflection peak for a dense TG wavepacket; our observation illustrates dependence of the momentum distribution on the interactions/wavefunction symmetry. The momentum distribution is calculated with a fast algorithm based on a formula expressing the RSPDM via a dynamically evolving single-particle basis.

PACS numbers: 03.75.-b,03.75.Kk

The possibility of constraining atomic gases to one-dimensional (1D) geometries \cite{1,2,3} has lead to experimental realizations of exactly solvable 1D models describing interacting bosons \cite{4,5}. At low temperatures, low linear densities, and strong repulsive effective interactions, these 1D atomic gases enter a Tonks-Girardeau (TG) regime \cite{6,7,8}, which is described by an exactly solvable model of 1D bosons with "impenetrable core" repulsive interactions \cite{4}. Two recent experiments achieved the TG regime and observed the properties of a TG gas \cite{9,10}. One particularly interesting aspect of these 1D systems is their nonequilibrium dynamics. A recent experiment studying nonequilibrium dynamics of a 1D interacting boson gas (including the TG regime) has shown that its momentum distribution does not need to relax to thermodynamic equilibrium even after numerous collisions \cite{9}. These experimental advances and the possibility of exactly solving the TG model \cite{1,4,10}, motivate us to study the momentum distribution of the dynamically evolving TG gas.

The TG model is exactly solvable via Fermi-Bose mapping, which relates the TG gas to a system of noninteracting spinless 1D fermions \cite{11,10}. Many properties of the two systems such as the the single-particle (SP) density \cite{4,5} or the thermodynamic properties \cite{11} are identical. However, quantum correlations contained within the reduced single-particle density matrix (RSPDM), or the momentum distribution of the TG gas \(n_B(k)\), considerably differ from those of the ideal Fermi gas \(n_F(k)\) \cite{12,13,14,15,16,17,18,19,20,21,22}. Although the exact many-body wavefunction describing TG gas can be written in compact form \cite{4,10}, the calculation of the RSPDM and the momentum distribution is a difficult task \cite{13,14,15,16,17,18,19,20,21,22}. In the stationary case, the RSPDM and \(n_B(k)\) were studied for a TG gas on the ring \cite{13,18} and in the harmonic confinement \cite{14,15,17,18}. In the homogeneous case, the momentum distribution has a singularity at \(k = 0\), \(n_B(k) \propto k^{-1/2}\) \cite{13}, and slowly decaying tails \(n_B(k) \propto k^{-4}\) \cite{15}. In both the homogeneous and the harmonic case, the occupation of the leading natural orbital (effective SP state) is \(\propto N^{1/2}\) for large \(N\) \cite{18}. An analytic approximation for momentum distribution of a TG gas in a box has been made by generalizing the Haldane’s harmonic-fluid approach \cite{10}.

In the time-dependent case, the RSPDM and momentum distribution of the TG gas was studied in a harmonic potential with the time-dependent frequency \cite{21}; dynamics was solved with a scaling transformation \cite{21}. Irregular motion, and the dynamics of the momentum distribution, was studied numerically for different interaction strengths (up to the TG limit) in Ref. \cite{19}; solutions for \(N = 6\) bosons were presented. Several recent studies have addressed the dynamics of hard-core bosons (HCB) on the lattice \cite{20,22}. Numerical studies of this model revealed a number of interesting results including fermionization of the momentum distribution during 1D free expansion \cite{20}, and the possibility of relaxation of this system to a steady state, which carries memory of the initial conditions \cite{22}. However, the behavior of the discrete HCB-lattice model is not equivalent to the TG bosons in a continuous potential \cite{23}. A feasible numerical study of the RSPDM and related observables during motion in a continuous potential \(V(x,t)\) demands an efficient method for the calculation of the RSPDM, independent of the external potential, the state of the system, and which would be operable for a larger number of particles.

Here we study dynamics of the momentum distribution, the RSPDM, natural orbitals (NOs), their occupancies, and Shannon entropy for a TG gas in a continuous potential. Our calculation is based on a formula expressing the RSPDM via a dynamically evolving SP basis; the method does not depend on the external potential, the state of the system, and it is operative for a larger number of particles. The method is employed in studying Bragg reflections of a TG many-body wavepacket in periodic potentials. A comparison of the TG bosonic (\(n_B\)) and non-interacting fermionic (\(n_F\)) momentum distributions illustrates the influence of interactions/wavefunction symmetry on this observable. The momentum distribution of the ideal fermi gas displays a beating peak at the edge of the Brillouin zone. In contrast, such a Bragg-reflection peak is completely absent for a dense TG wavepacket. As the TG wavepacket reflects from the potential, it undergoes a rapid decrease of coherence, characterized by the increase of entropy and decrease of spatial correlations.

Bragg reflections of a quantum many-body wavepacket

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Here we study dynamics of the momentum distribution, the RSPDM, natural orbitals (NOs), their occupancies, and Shannon entropy for a TG gas in a continuous potential. Our calculation is based on a formula expressing the RSPDM via a dynamically evolving SP basis; the method does not depend on the external potential, the state of the system, and it is operative for a larger number of particles. The method is employed in studying Bragg reflections of a TG many-body wavepacket in periodic potentials. A comparison of the TG bosonic (\(n_B\)) and non-interacting fermionic (\(n_F\)) momentum distributions illustrates the influence of interactions/wavefunction symmetry on this observable. The momentum distribution of the ideal fermi gas displays a beating peak at the edge of the Brillouin zone. In contrast, such a Bragg-reflection peak is completely absent for a dense TG wavepacket. As the TG wavepacket reflects from the potential, it undergoes a rapid decrease of coherence, characterized by the increase of entropy and decrease of spatial correlations.
The model.- We consider dynamics of $N$ indistinguishable bosons in 1D configuration space, located in an external potential $V(x,t)$, and interacting via impenetrable pointlike interactions [4]. The bosonic many-body wavefunction $\psi_B(x_1,\ldots,x_N,t)$ describing the state of this system is related to a fermionic wavefunction $\psi_F(x_1,\ldots,x_N,t)$, which describes a system of $N$ noninteracting spinless 1D fermions: $\psi_B(x_1,\ldots,x_N,t) = A(x_1,\ldots,x_N)\psi_F(x_1,\ldots,x_N,t)$, where $A = \Pi_{1 \leq i < j \leq N} \text{sgn}(x_i - x_j)$ is a "unit antisymmetric function"; this is the famous Fermi-Bose mapping [4]. The dynamics of the fermionic wavefunction $\psi_F$ can be constructed from the Slater determinant $\psi_F(x_1,\ldots,x_N,t) = \sqrt{1/N!} \det|\psi_m(x_j,t)|$, where $\psi_m(x,t)$ denote $N$ orthonormal SP wavefunctions $\psi_m(x,t)$ obeying

$$\hbar \partial \psi_m \over \partial t = \left[ -h^2 \partial^2 \over 2m \partial x^2 + V(x,t) \right] \psi_m(x,t), \quad m = 1,\ldots,N. \quad (1)$$

The exact many-body wavefunction of the TG system is

$$\psi_B = A(x_1,\ldots,x_N) \sqrt{1 \over N!} \det_{m=1}^N \left[ \psi_m(x_j,t) \right], \quad (2)$$

i.e., its evolution is constructed after solving Eq. (1). The RSPDM of the TG system, $\rho_B(x,y,t) = N \int dx_2 \ldots dx_N \psi_B(x,x_2,\ldots,x_N,t)^* \psi_B(y,x_2,\ldots,x_N,t)$, furnishes the expectation values of one-particle observables such as the position density $\rho_B(x,y,t)$, or momentum distribution $n_B(k,t) = (2\pi)^{-1} \int dy \, e^{ik(y-x)} \rho_B(x,y,t)$ [13]. The natural orbitals $\phi_i(x,t)$ (NOs) of the TG system, obtained as eigenfunctions of the RSPDM,

$$\int dy \, \rho_B(x,y,t) \phi_i(y,t) = \lambda_i(t) \phi_i(x,t), \quad i = 1,2,\ldots$$

represent effective SP states, while eigenvalues $\lambda_i(t)$ represent their occupancies [14]. The SP wavefunctions $\psi_m(x_j,t)$ are NOs of the fermionic system, with occupancy unity, because the fermionic RSPDM is $\rho_F(x,y,t) = \sum_{m=1}^N \psi_m^*(x,t) \psi_m(y,t)$ [14]. The momentum distributions can be expressed via the Fourier transform of the NOs, $n_F(k,t) = \sum_{m=1}^N |\psi_m(k,t)|^2$, and $n_B(k,t) = \sum_{i=1}^\infty \lambda_i(t) |\phi_i(k,t)|^2$. The method.- The RSPDM can be expressed in terms of the dynamically evolving SP basis:

$$\rho_B(x,y,t) = \sum_{ij} \psi_i^*(x,t) A_{ij}(x,y,t) \psi_j(y,t). \quad (3)$$

The $N \times N$ matrix $A(x,y,t) = \{A_{ij}(x,y,t)\}$ is

$$A(x,y,t) = \det \mathbf{P}(\mathbf{P}^{-1})^T, \quad (4)$$

where the entries of the matrix $\mathbf{P}$ are $P_{ij}(x,y,t) = \delta_{ij} - 2 \int_x^y dx' \psi_i^*(x',t) \psi_j(x',t)$; we have assumed $x < y$ without loss of generality.

Derivation of formula (4) as follows. Define permutations $(k_2\ldots k_N) = P (1\ldots i - 1 i 1\ldots N)$, $(l_2\ldots l_N) = Q (1\ldots j - 1 j 1\ldots N)$, and their signatures $\epsilon(P)$ and $\epsilon(Q)$. From the definition of the RSPDM and Eq. (3) it follows that

$$A_{ij} = \frac{(-1)^{i+j}}{(N-1)!} \int \prod_{n=2}^N dx_n \text{sgn}(x-x_n) \text{sgn}(y-x_n) \sum_P \epsilon(P) \psi_{k_2}^*(x_2)\ldots\psi_{k_N}^*(x_N) \sum_Q \epsilon(Q) \psi_{l_2}(x_2)\ldots\psi_{l_N}(x_N) \quad (5)$$

$$= \frac{(-1)^{i+j}}{(N-1)!} \int \prod_{P,Q} \epsilon(P) \epsilon(Q) \prod_{n=2}^N P_{k_n,l_n} \quad (6)$$

$$= (-1)^{i+j} \det\mathbf{P}_{ij}, \quad (7)$$

where $\mathbf{P}_{ij}$ is a minor of matrix $\mathbf{P}$ obtained by crossing its $i$th row and $j$th column. Equation (6) is obtained after rearranging the product factors of Eq. (5), and formally performing the integrations $P_{k_n,l_n} = \delta_{k_n,l_n} - 2 \int_x^y dx' \psi_{k_n}^*(x',t) \psi_{l_n}(x',t)$. Eq. (7) follows from the definition of a determinant [13]. Eq. (4) follows immediately from Eq. (7) and the formula for the matrix inverse via algebraic co-factors.

Dynamics in the periodic potential.- The richness of the dynamics of ultracold Bose gases in optical lattices [24] motivate us to numerically (exactly) study the evolution of a quantum many-body wavepacket in a continuous periodic potential $V_p(x) = V_p(x + D)$ (also referred to as the lattice); periodic boundary conditions are assumed, i.e., dynamics occurs on a ring of length $L = n_s D$. The gas (wavepacket) is initially localized within a region significantly smaller than $L$, and it is given a certain amount of momentum. During dynamics, the many-body wavepacket will disperse on the ring. The dynamics of the TG momentum distribution $n_B$ is affected by the exchange of the momentum between the lattice and the gas, the many-body interactions, and the bosonic symmetry of the wavefunction. On the other side, the related fermionic momentum distribution $n_F$ is affected by the lattice and the Pauli exclusion principle. We find it illustrative to compare time-evolution of the two momentum distributions, as it illustrates the influence of the interactions/wavefunction symmetry on this observable.

In our numerical simulations we consider motion of $^{87}\text{Rb}$ atoms in the potential $V_p(x) = V_0 \cos^2(\pi x/D)$, where $D = 391.5 \text{ \mu m}$, and $V_0 = 11.9 \text{ eV}$ unless specified otherwise; $n_s = 52$. For concreteness, we assume that the SP wavefunctions describing the wavepacket at $t = 0$ are $\psi_m(x,0) = u_m(x)e^{ik_m x}$, $m = 1,\ldots,N$, where
$u_m$ is the $m$th SP eigenstate of the harmonic potential $V_h(x) = m \omega^2/2$, $\omega = 2\pi 316$ Hz; such a many-body wavepacket corresponds to a ground state of the gas in harmonic confinement, with a momentum $k'$ per particle imparted to the wavepacket. The initial expectation value of the SP momentum $k' = \langle k n p(k,0) \rangle dk$ is chosen to be exactly at the edge of the Brillouin zone $k' = \pi/D$. Although such an excitation is non-trivial to prepare, current high level of experimental techniques strongly suggests that it is more than just a theoretical curiosity.

It should be emphasized that the expectation value of the SP momentum is identical (at all times) for TG bosons and noninteracting fermions, $\langle k \rangle_B = \int dk k n p(k,t) = \int dk k n F(k,t) = \langle k \rangle_F$. Nevertheless, their momentum distributions show remarkable differences. Figure 1(a) shows $n_F$ in the initial stage of the evolution, and after long-time propagation (when the gas is already well-dispersed over the ring). A sharp peak beating up-down at the edge of the 1st Brillouin zone $k = -\pi/D$ arises from Bragg reflections. The fermionic momentum distribution is $n_F(k,t) = \sum_{m=1}^{N} |\tilde{\psi}_m(k,t)|^2$; a few of the SP spectra $|\tilde{\psi}_m(k,t)|^2$ are initially overlapping the edge of the Brillouin zone at $\pi/D$; as the dynamics of $\tilde{\psi}_m(k,t)$ are uncoupled, the spectra $|\tilde{\psi}_m(k,t)|^2$ of those NOs display a beating Bragg-reflection peak at $-\pi/D$ [see dot-dashed curve in Fig. 1(b) up], which is reflected onto $n_F(k,t)$.

The bosonic momentum distribution $n_B$ at $t = 0$ is shown in Fig. 1(b). The sharp peak of $n_B(k,0)$ is located exactly at the edge of the Brillouin zone, and it is much sharper than the peak of $n_F(k,0)$. From this one may erroneously conclude that there would be a sharp beating peak originating from Bragg reflections at $-\pi/D$. However, this signature of Bragg reflections is absent. This is illustrated in Fig. 1(c), which shows a contour plot of the bosonic momentum distribution $n_B(k,t)$ for $N = 25$ bosons propagating in the potential $V_p$. The signature is absent both at the beginning of the motion, when the wavepacket is still localized, and after it spreads over the ring. In the long-time propagation $n_B$ collectively oscillates due to the momentum-exchange with the lattice $\langle \langle k \rangle_B = \langle k \rangle_F \rangle$, but the changes in its shape are small. Our simulation clearly depicts that when the momentum is being transferred by the lattice to the TG gas, it redistributes among bosons; this leads to a smooth distribution without a beating Bragg-reflection peak. Unlike the fermionic NOs, the low-order bosonic NOs do not display Bragg-reflection peaks due to strong (nonlinear) coupling arising from interactions [see dot-dashed curve in Fig. 1(b) down].

However, Bragg-reflection peaks can be obtained for a smaller density of the TG gas. This is illustrated in Figure 1(d) showing an identical numerical simulation but with $N = 3$ bosons. In this case, as bosons disperse on the ring, their density is sufficiently low, leading to the fermionization of the bosonic momentum distribution discussed in Ref. [20]; consequently one observes a
beating peak at \( k = -\pi/D \).

Further insight into Bragg reflections of the TG many-body wavepacket follows from the behavior of the bosonic NOs \( \phi_i \) and their occupancies \( \lambda_i \). Initially (\( t = 0 \)), a few of the leading NO occupancies are fairly large [see Fig. 2(a)], which is characteristic for a cold Bose gas. However, when the evolution begins, the low order \( \lambda_i \) rapidly decrease, while the number of NOs with non-negligible occupations increase [Fig. 2(a)]. Figure 2(b) illustrates the time-evolution of the Shannon entropy \( S(t) = -\sum \rho_i \log \rho_i \), where \( \rho_i(t) = \lambda_i(t)/\lambda \), for different lattice depths \( \lambda \); the entropy \( S \) increases faster, and saturates at a higher value for a deeper lattice. Figure 2(c) shows bosonic (fermionic) quantum correlations 
\[
\rho_B(x,x',t)/\rho_B(x,x,t)\rho_B(x',x',t),
\]
respectively at \( t = 0 \) and \( t = 34.5 \) ms; in contrast to \( \mu_B \), the correlations of noninteracting fermions are not considerably changed during evolution. Figures 2(a)-(c) clearly illustrate the dynamical loss of coherence of the TG wavepacket, which is more rapid for a deeper lattice. This results from the interplay of the many-body interactions and scattering from the lattice. Namely, interactions couple bosonic NOs thereby providing a mechanism for the time-change of their occupancies. For a deeper lattice, the initial wavepacket effectively excites a larger number of system’s eigenstates; this is illustrated in Fig. 2(d) which shows the diagonal of the RSPDM represented in the Bloch-wave basis (extended Brillouin-zone scheme) for two different lattice depths. For a deeper lattice, the dynamics effectively involves a larger number of frequencies (i.e., energies), and it is more irregular.

Before closing, we note that the dynamics of the TG gas is related to the paraxial propagation of partially-incoherent light (PIL) beams in linear 1D photonic structures. Furthermore, the behavior of partially-condensed weakly-interacting Bose gases is similar to PIL in noninstantaneous nonlinear media. These facts motivate us to explore the recently observed phenomena with incoherent light in photonic lattices, within the context of quantum-dynamics of interacting bosons.

In conclusion, we have studied dynamics of the momentum distribution, RSPDM correlations, natural orbitals and their occupancies, and the entropy of the TG gas out of equilibrium. We analyzed Bragg reflections of the TG many-body wavepacket and found that their signature (observed as a beating resonant peak in the momentum distribution of the corresponding noninteracting fermionic gas) may be considerably suppressed by the TG many-body interactions. We have employed a fast numerical method, applicable for versatile continuous potentials, and operative for larger number of particles. Our results open the way for further studies of the RSPDM and related observables of the TG gas, both in the static and time-dependent cases.

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