Contact and static structure factor for bosonic and fermionic mixtures

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We study measurable quantities of bosonic and fermionic mixtures on a one-dimensional ring. These few-body ensembles consist of majority atoms obeying certain statistics (Fermi or Bose) and an impurity atom in a different hyperfine state. The repulsive interactions between majority-impurity and majority-majority are varied from weak to strong. We show that the majority-impurity repulsion is mainly responsible for the loss of coherence in the strongly interacting regime. The momentum distribution follows the $C/p^4$ universal behavior for the high-momentum tail, but the contact $C$ is strongly dependent on the strength of the majority-impurity and in a different way on the majority-majority interactions. The static structure factor of the majority atoms exposes a low-momentum peak for strong majority-impurity repulsion, which is attributed to an effective attraction not expected for purely repulsive forces.

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I. INTRODUCTION

Nonlocal measurable quantities of cold atom systems play a major role in the experimental probe of their properties. From the momentum distributions in the first realizations of Bose-Einstein condensates [1,2] and the time-of-flight images of phase transitions in optical lattices [3], to the probing of the Tonks-Girardeau (TG) gas (an infinitely repulsive one-dimensional (1D) bosonic ensemble with fermionic properties [4,5]), experimental techniques have given rise to an unprecedented degree of control, manipulation, and measurement of atomic systems [6–8]. For 1D systems, theoretical research has developed analytical and numerical methods to study properties of those quantities, like the universal $C/p^4$ asymptotic behavior of the momentum distribution [9–11], which is governed by the contact $C$. This is a notion that captures all universal properties of such systems even close to phase transitions [12] and has been recently measured in ultracold gases [13–15]. The structure factor, another important concept originated in solid-state physics to probe crystalline lattices, has recently been studied [16–18] and observed for 1D Bose gases via Bragg spectroscopy [19].

More recent advances in experiments deal with mixtures of Bose-Bose, Bose-Fermi, and Fermi-Fermi cold gases [20–23]. It also became possible to realize few-body ensembles of bosons [24,25] and fermions in different hyperfine states [26] and measure the effects of an impurity by increasing the number of fermions one by one [27]. For composite mixtures of bosons and fermions several local quantities have been studied and have exhibited various phases not present in pure ensembles [28–30], but some advances are still to be done on the side of nonlocal correlators [31].

In this work we investigate, using a Jastrow-type ansatz, some measurable nonlocal quantities for a few-body ensemble of bosons or fermions in a 1D ring in the presence of an impurity of the same mass but in a different hyperfine state.

In these systems, repulsive interactions between impurity-majority or, for the bosonic case, majority-majority pairs can be tuned via Feshbach resonances. For the integrable system constituted by an impurity in a Fermi sea, the ground state wave functions and energies have been exactly obtained in Ref. [32], and results for correlations are discussed in Ref. [33]. For a system of bosons, if all interaction strengths are equal, the Lieb-Liniger integrable model can be applied [34]. However, when the interaction strengths differ and the system becomes nonintegrable [35–37], we show that all measurable nonlocal correlation quantities exhibit a behavior substantially different from that of the integrable one. In particular, the reduced one-body density matrix of the majority atoms, a correlation function that shows the degree of coherence in its off-diagonal terms, is strongly dependent on the impurity-majority coupling strength. At the same time, the high-momentum tail of the momentum distribution obeys a $C/p^4$ universal behavior for all cases studied here. The numerical values for the contact $C$ depend not only on the impurity-majority and majorit-majority couplings, but also on the nature of the atom being considered. For different interactions, the static structure factor deviates from the integrable case, above and below the phononic behavior of the TG gas; most surprisingly, a pronounced peak arises for strong majority-impurity repulsion, which is an indicator of a quasicrystalline structure and of effective attractive correlations in a purely repulsively interacting ensemble. The results obtained here for the correlations via a simple Jastrow ansatz are compared with the exact solutions in the corresponding cases where those solutions exist, showing in general very good agreement.

II. SYSTEM HAMILTONIAN AND ANSATZ

We consider a system of three atoms on a 1D ring of length $L$ with contact interactions and periodic boundary conditions. The Hamiltonian reads

$$H = -\frac{1}{2} \sum_{j=1}^{3} \frac{\partial^2}{\partial x_j^2} + \sum_{i<j} g_{ij} \delta(x_i - x_j).$$ (1)
where the lengths are in units of $L$ and energies in units of $\hbar^2/mL^2$. The interaction strength $g_{ij}$ may be different for each pair of atoms $i,j$ and is controllable via Feshbach or confinement-induced resonances since $g = g_{1D}/(\hbar^2/mL)$ with $g_{1D} = \frac{2n_0\zeta}{mL^2} \left(1 - \frac{\pi L}{2a_s}\right)^{-1}$, where $m$ is the atom mass, $\zeta$ is the Riemann zeta function, $a_{1D}$ is the three-dimensional $s$-wave scattering length, and $a_s$ is the length of the transversal confinement [38]. The latest is assumed to be very small such that the system is effectively 1D. The composite system where the only difference between the atoms is the coupling strengths $g_{ij}$ with respect to each other can be realized experimentally by using atoms of the same species in different hyperfine states.

As shown in Fig. 1 we consider three atoms on a ring, with two of them being in the same hyperfine state and obeying fermionic or bosonic statistics, and the third (which we call the impurity) in a different hyperfine state. Therefore we have two important parameters, the coupling strength $g$ between impurity and majority atoms and the $g'$ for the bosonic case for the interaction between the majority atoms. In the case where the majority atoms are fermions, the $s$-wave scattering is forbidden due to the statistics, and the only parameter that remains is the impurity-majority coupling strength $g$.

### A. Underlying physics

In Fig. 1 we schematically depict the extreme cases that indicate the basic underlying physical scenarios that appear in this system. Figure 1(a) represents the integrable case where $g = g'$ and the atoms are strongly repulsive, so they tend to maximize the distance between them. In Fig. 1(b) only the majority atoms repel strongly each other (or obey the Pauli exclusion principle if they are fermions), and therefore they tend to localize on diametric positions on the ring. The impurity is delocalized all over as a single particle since the interaction $g$ with the others is vanishing. On the other hand, in Fig. 1(c) the interaction between the bosonic majority atoms $g'$ is vanishing or very weak, and the impurity strongly repels both. In this case the majority atoms tend to maximize the distance with the impurity, and this leads to an effectively “attractive” scenario, where they bunch together (this kind of effect has also been verified in harmonically trapped systems [39]). We will see that this indirect attraction of the majority atoms via the impurity induces various effects in the observable properties, the most striking being the peak in low momentum for the static structure factor. Let us stress here that at least these extreme situations are representative also for ensembles of many majority atoms, since the underlying physics are similar to those explained above.

### B. Ansatz

Extreme cases in bosonic systems like the one depicted in Fig. 1(a) also allow for exact solutions of the many-body Schrödinger equation that are obtained by means of Bose-Fermi bosons to free fermions. The Jastrow-type ansatz that we employ here is based on those solutions and also on the two-body integrable Lieb-Liniger case:

$$\psi_{ij} = \cos[k_j(|x_i - x_j| - 1/2)],$$

where $k_j$ (in units of $1/L$) is related to the interaction strength $g_{ij}$ by $k_j = 2\arctan(g_{ij}/2k_j)$, with $k_j \in [0,\pi]$. The Jastrow ansatz for our system of three bosons reads:

$$\psi = N \cos[k(|x_i - x_m1| - 1/2)] \cos[k(|x_i - x_m2| - 1/2)] \times \cos[k'(|x_m1 - x_m2| - 1/2)],$$

where $N$ is a normalization constant, $x_i$ denotes the position of the impurity atom, $x_m1$ and $x_m2$ the positions of the majority atoms, and $k,k'$ are related to $g$ and $g'$, respectively. Although here we conveniently write the ansatz for our particular system it is clear that it can be generalized for more atoms and different pairs. Indeed, for fermionic majority atoms, we modify the last term to $\sin[\pi(x_m1 - x_m2)]$, which respects the fermionic exchange property. Note that, contrary to the bosonic case, this term does not correspond to the exact ground state wave function for a pair of identical fermions (see Ref. [41] for details). However, as we will show next, this expression, besides of being simpler to handle, is able to reproduce the relative correlations for the cases that we study here.

In Fig. 2 we compare the results for correlations using the Jastrow ansatz to the exact ones given by the Bethe ansatz in the integrable cases. We particularly focus on basic quantities such as the one-body correlation function,

$$\rho(x,x') = \int dx_2 \cdots dx_N \psi(x,x_2,\ldots,x_N)\psi^*(x',x_2,\ldots,x_N).$$

![FIG. 1. (Color online) Schematic depiction of the physical system for representative cases: (a) strongly repulsive integrable case, in which the separation between the three atoms is at maximum. (b) The interaction between the majority pair is strong, but the impurity-majority interaction is weak; therefore the impurity atom appears “delocalized” across the ring. (c) The impurity strongly repels the majority pair but the majority-majority interaction is weak, so these atoms tend to bunch together on the other side of the ring.](Image 78x626 to 266x726)
have been studied in Refs. [44, 45].

correlations for the two-component trapped fermionic system
in a harmonic trap has been discussed in Ref. [43], while
state that even without a variational approach, this ansatz
and reliable approximation of this solution. Therefore, we can
deviations for intermediate interaction strengths. Here
is calculated for an impurity-majority pair, so
function with respect to the relative distance
r = x1 − x2 as shown in Fig. 2(b). As expected, in the extreme cases of vanishing and infinite repulsion (TG gas) the agreement is at best since the Jastrow ansatz coincides with the exact solution [42]. For the case of two majority fermions with an impurity, we compare the results of the Jastrow ansatz with the exact solution [32, 33] in Figs. 2(c) and 2(d). Again we find that the agreement is very good in the weak and strong interaction limits, with slight deviations for intermediate interaction strengths. Here ρ(x, x′) refers to the impurity fermion, and the pair correlation function is calculated for an impurity-majority pair, so x1 = x and x2 = xmp1. For the homogeneous cases discussed here where an exact solution exists, the Jastrow ansatz provides a simple and reliable approximation of this solution. Therefore, we can state that even without a variational approach, this ansatz captures the basic physics of the systems that we discuss here. We mention that an approach to correlations for bosons in a harmonic trap has been discussed in Ref. [43], while correlations for the two-component trapped fermionic system have been studied in Refs. [44, 45].

III. MEASURABLE QUANTITIES

A. One-body correlation function

In our system we can find either the correlation function for the impurity or the majority atoms by integrating out the coordinates of the other pair of atoms in each case. The one-body correlation function, and in particular its off-diagonal terms, characterizes the degree of coherence of a given atom of the system. As we observe for the integrable case in Fig. 3(a) when the interactions are weak or intermediate (k = π/2 corresponds to g = π) there is coherence in the ensemble since diagonal and off-diagonal terms are almost equal. This behavior resembles that of the Bose-Einstein condensate, which is a coherent ensemble of many bosonic atoms. On the other hand, when the repulsive interaction becomes very strong as in Fig. 3(b) (k = 9π/10 corresponds to g ≈ 35.7) the atoms tend to localize and lose coherence. The diagonal r = x1 peak (and due to the periodic boundary conditions and symmetry the peak at distance L) becomes much more pronounced than the off-diagonal area around distance L/2. This is typical for few body 1D ensembles at strong interactions which are no longer represented by a single coherent wave function but are occupying higher single-particle states (orbits), an effect known as depletion of the condensate or fragmentation [46–49]. We have a similar effect for the impurity atom when the impurity-majority interaction is strong and also for the majority atoms when the interaction between them is strong. The most interesting nonintegrable case is depicted in Figs. 3(c) and 3(d) where we see the loss of coherence for the majority atoms solely due to the increase of the strength of the interaction with the impurity. Since the direct interaction term between the majority atoms is small (k = π/10, g ≈ 0.1) one would expect that they remain coherent, but it is shown that if the impurity repels them strongly, then they get localized [see also schematic Fig. 1(c)]. Since the one-body density matrix is always symmetric with respect to the diagonal [as we see in Figs. 3(a)–3(d)] we can depict the whole behavior as a function of r = x − x′ (as done in Fig. 2) and of the interaction. Therefore we show in Figs. 3(e)–3(i) the whole behavior of the correlation function as a function of k. The localization around r = 0 again shows that the loss of coherence appears gradually for high k. Very similar behavior is obtained for the impurity atom as shown in Fig. 3(f) due to the impurity-majority strong interaction. In Fig. 3(g) the bosonic majority atom is shown to lose coherence at large impurity-majority interactions even if majority-majority coupling is rather low. A comparison between the fermionic majority atoms and bosonic majority atoms with infinite repulsion (k2 = π) shows that the fermionic atoms have more pronounced localization. In other words, the infinitely repulsive bosonic atoms are resembling fermions in their nonlocal correlation also as a function of the repulsive strength with the impurity, but they never get as radically localised as the majority fermions.

B. Momentum distribution and contact

An observable directly connected to the one-body correlation function is the momentum distribution:

\[ n(p) = \int d x \, d x' \rho(x, x') e^{-i p (x - x')}, \]

(6)
FIG. 3. (Color online) One-body correlation function for representative cases interactions in the integrable, majority, and impurity cases. Loss of coherence [depletion of the off-diagonal terms of $\rho(x,x')$] from (a) weak to (b) strong interaction in the integrable case, and from (c) weak to (d) strong repulsion from the impurity for the majority bosonic atoms. Behavior of $\rho(|x-x'|)$ as a function of the interaction parameter $k$ in the cases of (e) integrable system, (f) impurity atom for strong majority interactions, majority atoms for (g) weak and (h) strong interactions, and (i) majority fermions.

where $p = 2\pi s$ and $s$ is an integer. We show in the Appendix that this is equivalent to calculating first the many-body wave function in momentum space for one atom,

$$\phi(p,x_1,\ldots,x_N) = \int dx_1 e^{-ipx_1} \psi(x_1,x_2,\ldots,x_N),$$

and then integrating out the rest of the coordinates from its square modulus.

It is known that the asymptotic behavior (the large $p$ tail) of the momentum distribution obeys an universal power law [11,31]:

$$n(p) \sim \frac{C}{p^4}, \text{ for } p \to \infty. \quad (7)$$

An expression for $C$ depending on the two-body correlation function is given in Ref. [50]:

$$C = \frac{4(N-1)\rho_2(0,0)}{a_{1D}^2}, \quad (8)$$

where $a_{1D}$ is the 1D scattering length, defined as $a_{1D} = -2/mg$, and $\rho_2(0,0)$ is the normalized two-body correlation function at vanishing distance between the atoms (an analytical expression for $\rho_2$ in the case of three atoms is given in Ref. [37], while thermodynamic limit formulas for weak and strong interactions are found in Ref. [51]). The proportionality constant $C$ is called contact and is determined by the strength of the interaction. The contact characterizes all the universal properties of such systems that are independent of the details of the interaction. For a fixed interaction, it is proportional to the probability that two atoms can be found at a short distance from each other (in this case at zero separation). In

$$n(p) \to \frac{\rho_2(0,0)}{p^4}, \text{ for } p \to \infty. \quad (9)$$

where we identify the prefactor as the contact. The index $j$ is inserted to account for different interactions between particle $x_1$ and the other particles of the ensemble. For our particular case of three particles, the interaction between the impurity and the remaining pair is the same (so $a_{1D}^{12} = a_{1D}^{13}$, and the difference from the integrable contact will be carried only Fig. 4(a) we verify the $C/p^4$ asymptotic behavior, not only for the integrable but also for all cases considered here. We
in the wave function. For the contact of the majority atoms, the scattering length will be different for each pair \(a_{21} \neq a_{23}\). For all nonintegrable cases this formula predicts very well the behavior of the momentum distribution at large large momentum for our data points as is shown for exemplary cases in Fig. 4(a). By using Eq. (9) we can then calculate the contact for all different interaction strengths, for impurity and majority atoms; the results for the contact as a function of the interaction parameters are presented in Figs. 4(b) and 4(c). In general the value of the contact increases with the interaction strength, but the main observation here is that the contact for the majority atoms is symmetrically dependent on \(k\) and \(k^t\) while for the impurity the major change comes, as expected, from the increase of the interaction with the majority atoms \(k\).
The structure factor is a property that defines how an ensemble of atoms scatters incident radiation. Experimentally, it is usually measured by two-photon Bragg scattering, in which the atom sample is subject to two detuned laser beams. The stimulated emission of light by the atoms gives rise to interference patterns that can be measured and contain information about the structure of the sample. For different wave vectors $p$ and frequencies $\omega$ of the beams, it is possible to measure the dynamic structure factor $S(p,\omega)$ of the system. Its integral over all frequencies provides the static structure factor, defined for 1D homogeneous systems as [16]

$$S(p) = 1 + \int dx_j \int dx_i e^{-ip(x_i-x_j)} [g(x_i,x_j) - 1].$$

where $p$ is again quantized as $2\pi s$ and the pair correlation $g(x_i,x_j)$ is renormalized to $N(N-1)/N^2$ for convenience. For our system, the pair correlation function can refer to an impurity-majority pair ($x_i = s_i$ and $x_j = x_{m1}$) or a majority-majority pair ($x_i = x_{m1}$ and $x_j = x_{m2}$), and $N(N-1)/N^2 = 6/9$.

In the low-momentum region and infinitely repulsive regime, hydrodynamic theory [53] predicts that the static structure factor should behave linearly with $p$. Particularly, for the TG limit this behavior is described by $S(p) = |p|/2\pi n$, where $n = N/L$ is the particle density. This result is characteristic of phonon excitations in many-body systems, but we confirm it also in our few-body system in the integrable case as shown in Fig. 5(a). For high momentum the structure factor always converges to 1 (a high-speed probe would not be scattered by the cold atom ensemble). For low momentum the behavior of the nonintegrable cases deviates much from that of the integrable, the first peak being below the TG phononic behavior or above it.

Most importantly, for the majority bosons $S$ can also be over 1, an effect that indicates a quasicrystalline structure and is not present in the integrable case. It results specifically from the fact that the repulsion with the impurity is inducing an effective attraction between the majority atoms as depicted in Fig. 1(c). This is also a characteristic of the so-called Super-Tonks gas, which is an excited state on the attractive side of the Feshbach resonance that also exhibits a peak above 1 in the structure factor at low momentum as shown in Ref. [54]. We focus in Figs. 5(b) and 5(c) on the behavior of the structure factor at low momentum $p = 1$. In (c) we observe again this peak arising smoothly for the majority atoms and being very pronounced at low $k'$ and high $k$. For the impurity-majority pair, $S \gg 1$, as is shown in Fig. 5(c), and the main change comes from impurity-majority repulsion. An important issue regarding the experimental determination of the structure factor is the possibility of measuring this quantity separately for impurity-majority and majority-majority pairs. This could be achieved, for instance, by having the beams polarized, in such a way that the photons could couple differently to the spin (or pseudospin) components in the system [55]. Another way to obtain this difference in the coupling involves a specific detuning of the laser beams, leading to separate measures in the components of the total structure factor, as argued in Ref. [56].

IV. CONCLUSIONS AND OUTLOOK

We have studied the nonlocal correlation functions of few-body bosonic and fermionic mixtures in a 1D ring in the presence of an impurity in a different hyperfine state. The interaction strengths between impurity-majority and majority-majority pairs may differ, which renders the system nonintegrable. The strength of this difference is responsible for pronounced effects in observable quantities. Most of the effects that we study on the one-body correlation function,
agreement with the existing exact solutions for certain cases, we are able to provide results for several observable quantities in the nonintegrable regime.

The experimental verification of the quantities we study is possible since recent advances in ultracold atoms techniques allowed for measurements in few-body systems. Many of our results also hold qualitatively for a larger number of majority atoms. Our approach can be extended to other cases which are relevant for experiments, like differently mixed systems and larger ensembles.

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APPENDIX

The momentum distribution is usually obtained by performing the Fourier transform of the one-body correlation function $\rho(x,x')$ (assuming a normalized wave function):

$$n(p) = \int dx \int dx' \rho(x,x') e^{-ip(x-x')}.$$  \hspace{1cm} (A1)

We consider now $\rho(x,x')$ as given in Eq. (4). By replacing it in Eq. (A1), we get

$$n(p) = \int dx_2 dx_3 dx dx' \psi(x,x_2,x_3)\psi^*(x',x_2,x_3) e^{-ip(x-x')}.$$  \hspace{1cm} (A2)

which can be rewritten as

$$n(p) = \int dx_2 dx_3 dx dx' \psi(x,x_2,x_3)\psi^*(x',x_2,x_3) e^{-ipx} \times dx dx' \psi^*(x',x_2,x_3) e^{ipx}.$$  \hspace{1cm} (A3)

From Eq. (7), $\int dx \psi(x,x_2,x_3) e^{-ipx} = \phi(p,x_2,x_3)$, so Eq. (A3) results in

$$n(p) = \int dx_2 dx_3 |\phi(p,x_2,x_3)|^2.$$  \hspace{1cm} (A4)

on the contact and on the static structure factor refer to a weakly interacting majority pair which is strongly repelled by an impurity atom. In particular, this gives rise to effective attractive interactions and a pronounced peak in the structure factor. By means of our Jastrow ansatz, which is in very good

FIG. 5. (Color online) (a) Low momentum region of the static structure factor for several integrable and nonintegrable bosonic cases, as well the fermionic majority-majority case ($p$ is in units of $2\pi$). (b) Static structure factor as a function of $k$ and $k'$, obtained by using the majority-majority pair correlation function for bosons, with $p$ fixed as $2\pi$. (c) Same as in (b), but for an impurity-majority pair.
The normalization of the wave function for the fermionic system is given by
\[
\mathcal{N}_F \varphi(p,x_2,x_3) = \frac{-i e^{ip(x_2 + x_3)} p \cos[k(-1 + x_2 + x_3)] - 2ik \sin[k(-1 + x_2 + x_3)]}{2 - 4e^{i(1+x_2+x_3)}k^2 - 2i e^{ip(x_2+x_3)}(4k^2 + p^2) + e^{i(1+x_2+x_3)}(4k^2 + p^2)}
\]
if \( x_2 < x_3 \), (A5)

where \( \mathcal{N}_F \) is the normalization for the bosonic wave function [37]. For the fermionic wave function, we obtain
\[
\mathcal{N}_F \varphi(p,x_2,x_3) = \frac{1 + e^{ip}}{1 - 4e^{i(1+x_2+x_3)}k^2 + 2i e^{ip(x_2+x_3)}(4k^2 + p^2) - e^{i(1+x_2+x_3)}(4k^2 + p^2)}
\]
\[
\times \cos[k(-1 + x_2 + x_3)] - 1 \quad \text{if} \quad x_2 < x_3
\]

The normalization of the wave function for the fermionic system is given by
\[
\mathcal{N}_F = \frac{2k^6 - 2k^2 \pi^2 - 4k^4 \pi^2 + \pi^4 + 2k^2 \pi^4 + 2k^2 \pi^4 \cos(2k) - \pi^4 \cos(2k) + 4k^5 \sin(k) - 8k^3 \pi^2 \sin(k) + 4k^4 \pi^4 \sin(k)}{16k^2(-k + \pi)^2(k + \pi)^2}.
\]
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