Off-diagonal correlations in a one-dimensional gas of dipolar bosons

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Abstract. We present a quantum Monte Carlo study of the one-body density matrix (OBDM) and the momentum distribution of one-dimensional (1D) dipolar bosons, with dipole moments polarized perpendicular to the direction of confinement. We observe that the long-range nature of the dipole interaction has dramatic effects on the off-diagonal correlations: although the dipoles never crystallize, the system goes from a quasi-condensate regime at low interactions to a regime in which quasi-condensation is discarded in favor of quasi-solidity. For all strengths of the dipolar interaction we considered, the OBDM shows an oscillatory behavior coexisting with an overall algebraic decay, while the momentum distribution shows sharp kinks at the wavevectors of the oscillations, \(Q = \pm 2\pi n\) (where \(n\) is the atom density), beyond which it is strongly suppressed. This momentum filtering effect introduces a characteristic scale in the momentum distribution, which can be arbitrarily squeezed by lowering the atom density. This shows that 1D dipolar Bose gases, realized e.g. by trapped dipolar molecules, show strong signatures of the dipolar interaction in time-of-flight measurements.

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1. Introduction

Trapped quantum degenerate gases currently offer the possibility of a thorough investigation of fundamental models of correlated quantum liquids, spanning a wide range of regimes from weak to strong interactions [1]. A particularly appealing aspect of cold atoms is indeed the tunability of the interparticle interactions. So far most of the experiments have been performed in a regime in which the interaction can be faithfully described as a contact s-wave interaction; tuning an applied magnetic field close to a Feshbach resonance allows us to control continuously the magnitude and sign of the associated s-wave scattering length [2]. The use of Feshbach resonances allows one, in particular, to suppress almost completely the contact interaction, leading to the observation of the effects of weaker magnetic dipole–dipole interactions for atoms that have a net magnetic moment, such as $^{52}$Cr [3]–[5]. On the other hand, the recent realization of a stable degenerate gas of heteronuclear molecules [6] appears to pave the way for the exploration of the physics of quantum fluids with strong (and variable) electric dipole–dipole interactions; in fact, the application of an electric field on the heteronuclear molecules, or the dressing of molecules with a microwave field, can induce a tunable electric dipole.

On the theoretical side, the presence of the dipolar interaction has been shown to lead to many intriguing effects when the system is confined to two spatial dimensions, such as roton-like excitations in the liquid regime (for a recent review, see [7]), spontaneous crystallization [8], and even supersolidity in the presence of an optical lattice [7]. In the case of dipolar bosons confined to one spatial dimension, in the absence of an optical lattice, the Mermin–Wagner–Hohenberg theorem forbids crystallization even at $T = 0$ due to unboundedly strong quantum fluctuations. Hence, the system can be described as a Luttinger liquid for all strengths of the dipolar interaction [9]–[12]. While it can develop arbitrarily strong diagonal correlations, resulting in a so-called super-Tonks behavior [13, 14], such correlations always decay as a power of the distance.

All the existing studies of the one-dimensional (1D) dipolar Bose gas have mainly focused on diagonal correlations and on the static structure factor [9, 10], [12]–[14]. Yet the most natural observables in cold atom experiments are off-diagonal correlations, namely the one-body density matrix (OBDM) and its Fourier transform, the momentum distribution, which is obtained from time-of-flight measurements. In this paper, we focus our attention on these...
quantities, which we compute numerically exactly by quantum Monte Carlo simulations. In particular, we show that off-diagonal correlations exhibit very strong signatures of dipolar physics. In fact, the OBDM has a characteristic oscillatory behavior at the ordering vector $Q$ of the Wigner crystal obtained in the classical limit. Such a behavior translates into a strong feature in the momentum distribution, namely a sharp kink at the $Q$ vector, and a strong suppression of the momentum population for larger wavevectors. This effect of momentum filtering in the range $[-Q, Q]$ is completely controlled by the density of the system, so that the momentum distribution can be arbitrarily squeezed in momentum space, although the system never attains condensation at finite density. A study of the two-body problem suggests that momentum filtering is a special feature of long-range interactions already at the few-body level, although its manifestation in the $N$-body problem is much more pronounced.

The paper is structured as follows. Section 2 describes the system Hamiltonian and the numerical method; section 3 presents a study of off-diagonal correlations in the two-body problem with dipolar interactions, contrasting it with the case of contact interactions; section 4 focuses on the OBDM as compared to predictions from the Luttinger liquid theory; and finally section 5 discusses the results concerning the momentum distribution.

2. Model and methods

We investigate a system of $N$ bosons confined to a 1D box of length $L$ with periodic boundary conditions. The system Hamiltonian reads

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{d^2}{dx_i^2} + \sum_{i<j} V(x_i - x_j).$$

(1)

In the following, unless otherwise specified, we will focus on the dipolar potential

$$V_{\text{dip}}(x - x') = \frac{V_d}{|x - x'|^3}.$$  

(2)

Introducing the particle density $n = N/L$, the rescaled length $\tilde{x}_i = nx_i$ and the effective Bohr radius $r_0 = m V_d/\hbar^2$ associated with the potential, the Hamiltonian with dipolar interactions can be rewritten in the convenient form

$$H(\text{Ryd}) = (nr_0)^2 \left[ -\frac{1}{2} \sum_{i=1}^{N} \frac{d^2}{dx_i^2} + (nr_0) \sum_{i<j} \frac{1}{|\tilde{x}_i - \tilde{x}_j|^3} \right].$$

(3)

Here the Hamiltonian is expressed in effective Rydberg units, $\text{Ryd} = \hbar^2/(mr_0^2)$.\footnote{Our definitions of $r_0$ and Ryd are slightly different from those of e.g. [9]–[12]. There $r_0 = 2m V_d^2/\hbar^2$ and Ryd = $\hbar^2/(2mr_0^2)$. Consequently the Hamiltonian, equation (3), differs by a factor of 1/2 in the kinetic term.} Hence $nr_0$ gives the dimensionless strength of the dipolar potential, and it contains a fundamental property of scale invariance, typical of power-law decaying potentials: rescaling the density $n \rightarrow n/\lambda$ and the effective length $r_0 \rightarrow \lambda r_0$, the physics of the system is unchanged (apart from a rescaling of the box length, $L \rightarrow \lambda L$, and, accordingly, of the positions, $x \rightarrow \lambda x$). In the following, we will compare the behavior of the dipolar system with that of the Lieb–Liniger gas, characterized by the $\delta$-potential

$$V_\delta(x - x') = g \delta(x - x'),$$

(4)
with repulsive nature, $g > 0$. The associated scattering length is given by $a = -2\hbar^2/(mg)$. The dimensionless strength of the potential can be measured by $(n|a|)^{-1}$.

We investigate the ground-state properties of the 1D gas of dipolar bosons by quantum Monte Carlo simulations, based on the continuous-space Worm Algorithm, which allows one to obtain the OBDM straightforwardly [15, 16]. While the method is strictly valid for finite temperatures only, the zero temperature behavior can be recovered for low enough temperatures. In addition to Monte Carlo simulations, we also use standard exact diagonalization to study the problem of two interacting bosons, whose results are presented in the next section.

3. The two-body problem

The study of the off-diagonal correlations of the two-body problem turns out to be quite insightful in the perspective of the $N$-body problem, as some fundamental traits of the latter are already exhibited by the former. We numerically evaluate the ground-state wavefunction $\phi(r)$ for the relative coordinate of the two-body problem on an $L = 2l$ ring (where $l$ is an arbitrary length unit), and the associated momentum distribution

$$n(k) = \frac{2}{L} \left| \int dr \, e^{ikr} \phi(r) \right|^2$$

(5)

defined on discrete momenta $k = 2\pi p/L$, $p \in \mathbb{Z}$.

We begin our analysis by investigating the Lieb–Liniger two-body problem, whose results are shown in figure 1. The evolution of the momentum distribution with increasing strength of the potential term (decreasing $n|a|$) shows a depletion of the $k = 0$ contribution, and an increase of all the finite-momentum components, compatible with a gradual squeezing of the two-body wavefunction $\phi(r)$ in real space. In particular, for all strengths of the interaction, the momentum

Figure 1. Left panel: occupation of the lowest momentum states as a function of the interaction strength for the ground state of two bosons interacting via a $\delta$-potential. We observe that the weight lost at $k = 0$ is distributed over all momenta. Right panel: momentum distribution for varying strength of the $\delta$ potential.
distribution shows a characteristic decay as $1/k^4$ for all finite momenta—a behavior that is consistent with that of the large-$k$ tail of $n(k)$ in the $N$-body problem [17]. This means that an increasing interaction strength is simply imposing a global rescaling factor to the momentum distribution at finite $k$.

The behavior in the dipolar case is radically different, as shown in figure 2. First of all, in the limit $nr_0 \to 0$ the system maintains a finite occupation of nonzero momentum states, due to the fact that, in this limit, dipolar bosons reproduce the physics of the Tonks–Girardeau gas of impenetrable particles [10, 14] (see section 5 for further discussion). Moreover, upon increasing the potential strength $nr_0$ we observe not only a suppression of the $k = 0$ momentum component but also at finite momenta $|k| \geq Q = 2\pi n$, at least for moderate potential strength. Hence, the increase of finite momentum components, associated with the squeezing of the two-body wavefunction in real space, is highly inhomogeneous, and it only takes place within a momentum window $-Q < k < Q$, while the momentum components outside this window are strongly suppressed. This inhomogeneous redistribution of populations in momentum space, driven by increasing the interaction, results in a peculiar momentum filtering effect, which is present in an even more dramatic fashion in the $N$-body problem, as will be discussed in section 5.

4. The one-body density matrix

The OBDM

$$C(x - x') = \langle \psi^\dagger(x)\psi(x') \rangle$$

for a system of $N$-dipolar bosons in a box of length $L = Nl$ with periodic boundary conditions has been investigated via quantum Monte Carlo simulations, for interaction strengths ranging
Figure 3. OBDM for $N = 30$ dipolar bosons. The dashed lines are fits to the Luttinger liquid formula, equation (8), truncated to the $m = 2$ order.

between $nr_0 = 0.2$ and $nr_0 = 5$. The number of particles utilized for the results shown here is $N = 30$, but we performed calculations with $N = 15$ and $N = 60$ as well, in order to gauge the importance of finite-size effects. We generally find that simulations at a temperature $k_B T \lesssim 0.1 nr_0$ Ryd do not show any significant thermal effect, and all the results presented in the paper refer to this temperature range.

Figure 3 shows the OBDM for two representative values of the potential strength $nr_0$. Strong quantum fluctuations in one dimension strongly suppress correlations, so that the OBDM displays an algebraic decay. In addition to this behavior, we observe an oscillation with period $1/n$, revealing the strong role played by interactions. Indeed, as we will see later, interactions lead to arbitrarily strong diagonal correlations, which imply a crystalline structure of the particles at short range. This structure is reflected in the OBDM, which exhibits a modulation with an amplitude that decays spatially in the same way as the density correlations.

According to the general Luttinger liquid theory, density–density correlations in a boson liquid display a dominant decaying behavior at large distances in the form [18]

$$G(x - x') = \langle \rho(x) \rho(x') \rangle \sim \cos[Q(x - x')] d(x - x'|L)^{2K}, \quad (7)$$

where $K$ is the Luttinger liquid exponent; $Q = 2\pi n$ is the ordering vector of the classical Wigner crystal and $d(x|L) = L |\sin(\pi x/L)|/\pi$ is the cord function. On the other hand, the OBDM is predicted to exhibit the following (asymptotic) decay [18]:

$$C(r) \to r \to \infty \frac{1}{d(r|L)^{1/(2K)}} \left[ b_0 + b_1 \cos(Q r) \frac{d(r|L)^{2K}}{d(r|L)^{2m^2+K}} + \sum_{m=2}^{\infty} b_m \cos(mQ r) \right]. \quad (8)$$

Hence, besides the dominant decay of the type $|r|^{-1/(2K)}$, the OBDM may also show a modulation at wavevector $Q$ with an amplitude decaying as the density–density correlations, $|r|^{-2K}$, and modulations at higher harmonics $mQ$ with increasingly rapid decay. We can successfully fit our numerical results to equation (8), and we are able to resolve harmonics up to $m = 2$ within our numerical precision. In particular, for the coefficient $b_1$ of the lowest harmonic,
we obtain negative values ranging in the interval $b_1 \sim -(3/5) \times 10^{-2}$. The negativity of this coefficient has important consequences for the shape of the momentum distribution, as will be discussed in the next section.

In addition, fits to equation (8) allow us to extract the exponent $K$, which is plotted in figure 4 as a function of the interaction strength $n r_0$. $K$ has the fundamental property of governing the scaling of the peak in the momentum distribution and in the static structure factor with increasing system size. Introducing the momentum distribution

$$n(k) = \frac{1}{L} \int_0^L dr \ C(r) e^{ikr}$$  \hspace{1cm} (9)$$

and the static structure factor

$$S(k) = \frac{1}{L} \int_0^L dr \ G(r) e^{ikr},$$  \hspace{1cm} (10)$$

one obtains that $n(k = 0) \sim L^{1-1/(2K)}$, while $S(k = Q) \sim L^{1-2K}$. According to the general definitions, the system exhibits quasi-condensation when the peak in the momentum distribution diverges with system size ($K > 1/2$); and it exhibits quasi-solidity when the peak in the structure factor diverges ($K < 1/2$). As shown in figure 4, increasing dipolar interactions allow us to continuously vary the $K$ exponent from $K = 1$ in the weakly interacting regime (characterized by fermionization [10, 14]), to $K \rightarrow 0$ in the strongly interacting regime. In particular, we find that for $nr_0 \approx 1.3$, the Luttinger exponent crosses the value $K = 1/2$, corresponding to a transition from quasi-condensation to quasi-solidity. Hence, dipolar interactions allow us to continuously tune the role of correlations, driving the system from a regime of dominant off-diagonal correlations to a regime of dominant diagonal ones. Our estimate of the $K$ exponent stemming from the OBDM is in good agreement with the semi-analytic formula given in [10], extracted from a fit to quantum Monte Carlo results for the ground-state energy.
Figure 5. Momentum distribution as a function of the interaction strength $nr_0$ for a system with fixed density $n = 1/l$. The dashed lines mark the momenta $Q = \pm 2\pi n$. The right panel shows the distribution in logarithmic scale, to evidence the sharp suppression for momenta $|k| > Q$.

Figure 6. Momentum distribution as a function of the interaction strength $nr_0$ for a system with fixed dipoles, namely a constant $r_0$. Here the number of particles is fixed at $N = 30$, and the system size changes when changing $nr_0$, and it goes from $L = 150l$ for $nr_0 = 0.2$ to $L = 6l$ for $nr_0 = 5$.

5. Momentum distribution

The evolution of the momentum distribution, equation (9), upon changing the interaction strength $nr_0$ is shown in figures 5 and 6. As discussed in the previous section, the OBDM exhibits a modulation term at wavevector $Q$ with a negative prefactor. This means that the corresponding feature in the momentum distribution is to be expected as a dip at the same wavevector. Indeed, the momentum distribution shows a sharp kink at $k = Q$, but it also shows...
a strong suppression of the momentum population at all momenta $|k| > Q$, observed for all the investigated values of $nr_0$. Hence, we observe that the dipolar interaction introduces a characteristic scale $Q$ in the momentum distribution, and a momentum filtering effect outside of the interval $[-Q, Q]$. This is to be contrasted with the case of contact interactions: indeed the Lieb–Liniger model has a momentum distribution with power-law wings, $n(k) \sim k^{-4}$ [17], and hence it does not contain any special momentum scale. The momentum filtering effect has the characteristic feature that, upon increasing the interaction strength $nr_0$, the weight lost in the $k = 0$ peak is redistributed almost exclusively over the $[-Q, Q]$ interval, similarly to what we have observed in the case of the two-body problem. As a result, the strongly peaked distribution at low $nr_0$ evolves into an almost triangular distribution for stronger $nr_0$. For extremely large values of $nr_0$, one might expect that the weight lost at $k = 0$ will eventually start redistributing over a broader interval than $[-Q, Q]$. Nonetheless the persistence of Luttinger liquid behavior in the system for arbitrary large values of $nr_0$ leads us to conclude that the characteristic periodic modulation of the OBDM, responsible for the suppression of the momentum distribution around $q = Q$, will also persist to much larger values of $nr_0$ than the ones considered here, so that the momentum distribution will maintain a strong signature of dipolar physics around that momentum value.

Momentum filtering can be probed experimentally in two different set-ups. Working at constant density $n$, $nr_0$ can be controlled by increasingly polarizing the dipoles and hence increasing $r_0$. This leads to the observations of figure 5, in which the momentum distribution is always defined on the same support and it changes shape from strongly peaked to triangular. A second type of experiment can be carried out at fixed dipole polarization, by changing the dipole density $n$, e.g. by varying the trapping potential that holds the system. Figure 6 illustrates such a protocol, which allows us to shrink arbitrarily the support $[-Q, Q]$ of the momentum distribution by lowering the trapping frequency and hence to concentrate all the atoms to an arbitrarily small volume in momentum space. Yet paradoxically the system never condenses; in contrast, as discussed in [10] and [14], it fermionizes in the limit $nr_0 \rightarrow 0$, reproducing the behavior of a Tonks–Girardeau gas.

6. Experimental realization

The momentum distribution is notoriously the most accessible quantity in trapped gas experiments, simply obtained by time-of-flight measurements [1]. More challenging is the realization of a quantum degenerate gas with dominantly dipolar interactions [7]. Quantum degeneracy has been achieved in $^{52}$Cr [3]–[5], for which s-wave interactions can be suppressed by a Feshbach resonance in favor of residual magnetic dipolar interactions. In this system one has $V_d = \mu_0 \mu_m^2 / (4 \pi)$, where $\mu_m = 6 \mu_B$ (the Bohr magneton) is the magnetic moment of $^{52}$Cr, and consequently $r_0 = 2.7 \times 10^{-9}$ m. For characteristic condensate densities of $10^{13}$ cm$^{-3}$, we obtain linear densities $n \approx 2 \times 10^9$ m$^{-1}$, and an effective potential strength $nr_0 \approx 0.5 \times 10^{-2}$, which does not allow us to explore the transition from quasi-condensation to quasi-soldiety described in this paper, but it might be already sufficient to observe the effects of momentum filtering. Polar molecules, on the other hand, can potentially feature dipolar interactions with characteristic lengths $r_0$ that are three orders of magnitude higher than those for $^{52}$Cr [7], and they would hence allow us to fully span the regime of interactions described in this paper.
Another potentially challenging issue is the confinement of dipolar gases in 1D traps. Indeed confining the gas in an array of tubes created by a two-dimensional (2D) optical lattice leads to quasi-1D systems, with sizable residual inter-tube coupling due to the long-range nature of dipolar interactions. A possible solution is the use of largely spaced tubes, obtained via 2D optical lattices created by crossing lasers at an angle far smaller than \( \pi \). Another solution is trapping in single mode tight atom waveguides created e.g. by atom chips [19].

7. Conclusions

In this paper we have investigated the effect of dipolar interactions on the off-diagonal correlations of a 1D Bose gas. We have shown that the long-range nature of dipolar interactions changes radically the momentum distribution with respect to the case of contact interactions, introducing a characteristic momentum scale beyond which the momentum distribution is strongly suppressed. The effect of momentum filtering is fully controlled by the gas density, and it allows us to squeeze the momentum distribution to an arbitrarily small portion of momentum space. The momentum distribution can also reveal the interaction-induced transition from quasi-condensation to quasi-solidity, via the loss of scaling of the zero-momentum peak with system size. All the phenomena discussed in this paper can be observed via time-of-flight measurements on polar molecules trapped in largely spaced 2D optical lattices, or in tight atom waveguides.

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References

[1] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[2] Chin C, Grimm R, Julienne P and Tiesinga E 2009 arXiv:0812.1496
[3] Lahaye T, Koch T, Fröhlich B, Fattori M, Metz J, Griesmaier A, Giovanazzi S and Pfau T 2007 Nature 448 672
[4] Koch T, Lahaye T, Metz J, Fröhlich B, Griesmaier A and Pfau T 2008 Nat. Phys. 4 218
[5] Lahaye T, Metz J, Fröhlich B, Koch T, Meister M, Griesmaier A, Pfau T, Saito H, Kawaguchi Y and Ueda M 2008 Phys. Rev. Lett. 101 080401
[6] Ni K K, Ospelkaus S, de Miranda M H G, Pe’er A, Neyenhuis B, Zirbel J J, Kotochigova S, Julienne P S, Jin D S and Ye J 2008 Science 322 231
[7] Lahaye T, Menotti C, Santos L, Lewenstein M and Pfau T 2009 Rep. Prog. Phys. 72 126401
[8] Büchler H P, Demler E, Lukin M, Michel A, Prokof’ev N, Pupillo G and Zoller P 2007 Phys. Rev. Lett. 98 060404
[9] Citro R, Orignac E, De Palo S and Chiofalo M L 2007 Phys. Rev. A 75 051602
[10] Citro R, De Palo S, Orignac E, Pedri P and Chiofalo M L 2008 New J. Phys. 10 045011

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[11] Pedri P, De Palo S, Orignac E, Citro R and Chiofalo M L 2008 Phys. Rev. A 77 015601
[12] De Palo S, Orignac E, Citro R and Chiofalo M L 2008 Phys. Rev. B 77 212101
[13] Arkhipov A S, Astrakharchik G E, Belikov A V and Lozovik Y E 2005 JETP Lett. 82 39
[14] Astrakharchik G E and Lozovik Y E 2008 Phys. Rev. A 77 013404
[15] Boninsegni M, Prokof’ev N V and Svistunov B V 2006 Phys. Rev. Lett. 96 070601
[16] Boninsegni M, Prokof’ev N V and Svistunov B V 2006 Phys. Rev. E 74 036701
[17] Olshanii M and Dunjko V 2003 Phys. Rev. Lett. 91 090401
[18] Cazalilla M 2004 J. Phys. B: At. Mol. Opt. Phys. 37 S1–47
[19] Thywissen J H, Olshanii M, Zabow G, Drndić M, Johnson K S, Westervelt R M and Prentiss M 1999 Eur. Phys. J. D 7 361