Finite Temperature Off-Diagonal Long-Range Order for Interacting Bosons

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Characterizing the scaling with the total particle number \(N\) of the largest eigenvalue of the one-body density matrix \(\lambda_0\), provides informations on the occurrence of the off-diagonal long-range order (ODLRO) according to the Penrose-Onsager criterion. Setting \(\lambda_0 \sim N^{C_0}\), then \(C_0 = 1\) corresponds to ODLRO. The intermediate case, \(0 < C_0 < 1\), corresponds for translational invariant systems to the power-law decaying of (non-connected) correlation functions and it can be seen as identifying quasi-long-range order. The goal of the present paper is to characterize the ODLRO properties encoded in \(C_0\) [and in the corresponding quantities \(C_{k \neq 0}\) for excited natural orbitals] exhibited by homogeneous interacting bosonic systems at finite temperature for different dimensions.

We show that \(C_{k \neq 0} = 0\) in the thermodynamic limit. In 1D it is \(C_0 = 0\) for non-vanishing temperature, while in 3D \(C_0 = 1\) \((C_0 = 0)\) for temperatures smaller (larger) than the Bose-Einstein critical temperature. We then focus our attention to \(D = 2\), studying the XY and the Villain models, and the weakly interacting Bose gas. The universal value of \(C_0\) near the Berezinskii–Kosterlitz–Thouless temperature \(T_{BKT}\) is \(7/8\). The dependence of \(C_0\) on temperatures between \(T = 0\) (at which \(C_0 = 1\)) and \(T_{BKT}\) is studied in the different models. An estimate for the (non-perturbative) parameter \(\xi\) entering the equation of state of the 2D Bose gases, is obtained using low temperature expansions and compared with the Monte Carlo result. We finally discuss a double jump behaviour for \(C_0\), and correspondingly of the anomalous dimension \(\eta\), right below \(T_{BKT}\) in the limit of vanishing interactions.

I. INTRODUCTION

Off-diagonal long-range order in the one–body density matrix of Bose particles signals the appearance of Bose-Einstein condensation (BEC) in quantum systems. This relation is established by the Penrose-Onsager criterion [1] which applies in all dimensions [1] for translational invariant systems with continuous symmetry, such as interacting bosons or \(O(N)\) spin models with \(N \geq 2\) – no long-range order can be found at finite temperature. Indeed, the theorem forbids the occurrence of spontaneous symmetry breaking for \(T > 0\) in low dimensional systems, where the symmetry of the Hamiltonian is always restored by the proliferation of low–wavelength fluctuations, often called Goldstone modes. For a Bose gas the Goldstone modes are represented by the phonons, which in \(D = 2\) destroy long-range order, leaving low temperature superfluidity intact. In such a case, due to the persistence of \(U(1)\) symmetry, the equilibrium finite-temperature average of the bosonic field operator \(\Psi\) vanishes, due to the lack of phase coherence [3]. It is worth noting that a similar effect occurs in a wide range of systems, even if the Mermin-Wagner theorem does not strictly apply, when the scaling dimension of the bosonic order parameter \(\Psi\) becomes zero [6,8].

A compact way to define off-diagonal long-range order (ODLRO) is to introduce the one–body density matrix (1BDM) [9]

\[
\rho(x, y) = \left\langle \Psi^\dagger(x) \Psi(y) \right\rangle , \tag{1}
\]

where the field operator \(\Psi(x)\) destroys a particle at the point identified by the \(D\)-dimensional vector \(x\). The 1BDM, as an Hermitian matrix, satisfies the eigenvalue equation

\[
\int \rho(x, y) \phi_i(y) dy = \lambda_i \phi_i(x) , \tag{2}
\]

with the eigenvalues \(\lambda_i\) being real. They denote the occupation number of the \(i\)-th natural orbital eigenfunction \(\phi_i\), with \(\sum_i \lambda_i = N\), where \(N\) is the total number of particles. The occurrence of ODLRO (and therefore of BEC) is characterized by a linear scaling of the largest eigenvalue \(\lambda_0\) with respect to the total number of particles \(N\) in the system [11] [10]:

\[
\lambda_0 \sim N^{C_0(T)} , \tag{3}
\]

the Mermin-Wagner theorem implies that \(C_0(T) < 1\) for \(T > 0\) and \(D \leq 2\), so there is no ODLRO at finite temperature. One can show as well that \(C_0(T = 0) = 1\) for \(D = 2\) and \(C_0(T = 0) < 1\) in \(D = 1\) (for the interacting case), see Ref. [11]. For a translational invariant system, the indices \(i\) in Eq. [2] are wavevectors, which are conventionally denoted by the vector \(\vec{k}\). Introducing the scaling formula

\[
\lambda_0 \sim N^{C_0(T)} , \tag{3}
\]

the Mermin-Wagner theorem implies that \(C_0(T) < 1\) for \(T > 0\) and \(D \leq 2\), so there is no ODLRO at finite temperature. One can show as well that \(C_0(T = 0) = 1\) for \(D = 2\) and \(C_0(T = 0) < 1\) in \(D = 1\) (for the interacting case), see Ref. [11]. For a translational invariant system, absence of ODLRO, or equivalently of BEC, in \(D = 2\) at finite temperature amounts to the following behaviour of the 1BDM at large distances:

\[
\left\langle \Psi^\dagger(x) \Psi(y) \right\rangle \xrightarrow{|x - y| \rightarrow \infty} 0 . \tag{4}
\]
The existence and regimes for BEC, \textit{i.e.} whether $C_0 = 1$ or not, in various physical systems has been the subject of a remarkable amount of work. It would be therefore desirable to complete such analysis with a systematic study of when $C_0$ is smaller than 1: In this case there is no ODLRO/BEC but nevertheless the condition $0 < C_0 < 1$ implies that, in translational invariant systems, the correlation function $\langle \Psi^\dagger(\vec{x})\Psi(\vec{y}) \rangle$ have a power-law decay. One may refer to this situation as \textit{quasi-long-range order}. A general classification of different behaviours of the correlation functions characterizing different types of order is discussed in Ref. \cite{12}. Here, we find convenient to identify the ODLRO properties in terms of the scaling with the particles number $N$ of the eigenvalues $\lambda_k$ of the 1BDM. Let’s stress that, for a system of interacting bosons, the index $C_0$ may also depend on the interaction strength and, moreover, one may expect that increasing the repulsion among the bosons, $C_0$ gets dampened with respect to the weak interacting case, as seen explicitly in the 1D case at zero temperature \cite{13}.

In the present work, we are going to characterize ODLRO, and possible deviations from it, in translational invariant bosonic systems interacting via short-range potential in 1-, 2- and 3-dimensions at finite temperatures. With “possible deviations” we also mean a study of the behaviour of the index $C_k(T)$, defined as

$$\lambda_k \sim NC_k(T), \quad (5)$$

where $k \neq 0$. The study of $C_{k\neq 0}(T)$ gives an insight about the possible \textit{quasi-fragmentation} of the system, \textit{i.e.} how the particles occupy the other, $k \neq 0$, states. Notice that in literature usually one refers to fragmentation when more than one eigenvalue of the 1BDM scales with $N$. So, one can refer to the case in which at least two $C_k$ are larger than zero (and at least one is smaller than 1) as a quasi-fragmentation.

The power-law behaviour in Eq. (3) determines the leading scaling of the largest eigenvalue of the 1BDM and, according to the Penrose-Onsager criterion, there is a BEC/ODLRO, \textit{i.e.} a macroscopic occupation of the lowest energy state, if $C_0(T) = 1$. There will be instead a mesoscopic condensate (\textit{i.e.} quasi-long-range order), with a finite value for the condensate fraction $\frac{N \lambda_0}{N}$ for finite values of $N$, if $0 < C_0(T) < 1$. In this case the condensate fraction of course vanishes for $N \to \infty$ but, even though the system is not a true BEC, one would observe nevertheless a clear peak in the momentum distribution in an experiment with ultracold gases: The reason is that the number of particles which are typically used in these apparatus are of order $N \sim 10^3 - 10^5$, and therefore the condensate fraction $\frac{N \lambda_0}{N} \sim \frac{N \lambda_0(T)}{N}$ could be very close to the unity for $C_0(T)$ close to 1. For $C_0(T) = 0$ there will be no order at all, and the system behaves like a Fermi gas where for all the eigenvalues we have $\lambda_i = 1$, because of the Pauli principle.

The plan of the paper is the following. In Section \textbf{III} we discuss the relation between the 1BDM and the momentum distribution, setting the notation for the Sections which follow. The cases $D = 3$ and $D = 1$ are discussed respectively in Section \textbf{IV} and \textbf{V}; these two cases provide the reference frame and the warming up for the discussion of the finite temperature ODLRO properties of two-dimensional Bose gases in Section \textbf{VI}. In Section \textbf{VII} we also present a study of the ODLRO in the XY and the Villain Hamiltonians. Our conclusions are presented in Section \textbf{VIII}.

**II. MOMENTUM DISTRIBUTION OF HOMOGENEOUS SYSTEMS**

The advantage of studying how the largest eigenvalue scales with the number of particles, instead of the large distance behaviour of the 1BDM, becomes evident once we define another important quantity: the momentum distribution. To introduce this quantity, let’s initially consider the Fourier transform $\hat{\Psi}(\vec{k})$ of the field operator $\Psi(\vec{x})$:

$$\hat{\Psi}(\vec{k}) = \frac{1}{(2\pi)^D/2} \int d\vec{x} e^{i\vec{k} \cdot \vec{x}} \hat{\Psi}(\vec{x})$$

and the momentum distribution $n(k)$ given by

$$n(\vec{k}) = \langle \hat{\Psi}^\dagger(\vec{k})\hat{\Psi}(\vec{k}) \rangle, \quad (6)$$

$$= \frac{1}{(2\pi)^D} \int d\vec{x} \int d\vec{y} e^{i\vec{k} \cdot (\vec{x} - \vec{y})} \langle \hat{\Psi}^\dagger(\vec{x})\hat{\Psi}(\vec{y}) \rangle.$$  

For a homogeneous system, $\rho(x, y) = \langle \hat{\Psi}^\dagger(\vec{x})\hat{\Psi}(\vec{y}) \rangle$ depends only on the distance among two points, therefore writing the relative distance vector as $\vec{r} = \vec{x} - \vec{y}$, we can rewrite $\rho(\vec{x}, \vec{y}) = \rho(\vec{r})$ and assume $\rho(\vec{r}) = \rho(|\vec{r}|) \equiv \rho(r)$. Passing to center of mass and relative coordinates, since $\int d\vec{R} = L^D$ where $L$ denotes the size of the system (\textit{e.g.} $L$ is the circumference of a ring in one–dimensional geometry), Eq. (6) can be rewritten in an universal form as

$$n(\vec{k}) = (\frac{L}{2\pi})^D \int e^{i\vec{k} \cdot \vec{r}} \rho(r) dr.$$  

(7)

The integral in the right-hand-side depends of course on $D$. Notice that the momentum distribution peak is simply given by the integral of the 1BDM

$$n(\vec{k}) = 0 = (\frac{L}{2\pi})^D \int \rho(r) dr.$$  

(8)

and, as expected, the large distance asymptotic of the density matrix determines the small momenta behaviour of the momentum distribution.

For a homogeneous system the quantum number labeling the occupation of natural orbitals is clearly the wavevector $|\vec{k}| \equiv k$. In particular, the Galilean invariance tells us that the effective single–particles states $\phi_k(\vec{x})$ may be written as plane waves, \textit{i.e.} $\phi_k(\vec{x}) = \frac{1}{L^{D/2}} e^{i\vec{k} \cdot \vec{x}},$
After discussing the explicit expression for the homogeneous interacting Bose gases in different dimensions. Formulations for ODLRO at finite temperature for homogeneous systems have a one-to-one correspondence between the scaling of the eigenvalues of $\rho(r)$ and the scaling of the dimensionless momentum distribution:

$$\lambda_k \sim N^{C_k(T)} \sim \frac{n(k)}{L^D}.$$  \hspace{1cm} (9)

The advantage of characterizing the different types of order in terms of the exponent $C_0(T)$ instead of the large distance behaviour of the 1BDM is now clear and it stems from the fact that, in the experiments, it is easier to analyze the momentum distribution peak instead of looking at what happens to $\rho(\vec{x}, \vec{y})$ for very large (ideally infinite) distances $|\vec{x} - \vec{y}| \to \infty$, since one should discern with high precision if the 1BDM is zero or not at large distances.

Since a complete closed form for the density matrix is not in general available for all interaction strengths and temperatures, we cannot directly compute the eigenvalues of $\rho(\vec{x}, \vec{y})$ and then study their scaling with $N$. In order to obtain this information we will use the following procedure. From the large distance asymptotic behaviour of the 1BDM, whose expression for different configurations of the system is usually available in the literature, we first make it a periodic function of period $L$ by adding terms which have the same scaling behaviour of the density matrix in the range $r \in [0, \frac{L}{2})$, and which represent the reflected parts in the range $[\frac{L}{2}, L]$. In this way we construct a fully symmetric and circulant matrix, whose eigenvalues are known to be real, as required, since they represent the occupation numbers of the system. Finally, we perform the Fourier transform of this symmetrized density matrix and obtain in this way the behaviour of the momentum distribution. Writing $k = \frac{2\pi}{L} l$ with $l \in \mathbb{N}$, the scaling of the largest eigenvalue of the 1BDM can be identified just imposing $l = 0$ and tracking its $N$ dependence. In this way, we are able to explicitly compute the exponent $C_0(T)$ of the system. On the other hand, choosing $l \propto L$ the behaviour of the Fourier transform in the limit $N \to \infty$ at fixed density $n = N/L^D$ yields the expression for the exponents $C_{k \neq 0}(T)$ via Eq. (9).

In the following, we aim to characterize the deviations from ODLRO at finite temperature for homogeneous interacting Bose gases in different dimensions. After discussing the explicit expression for $C_0$, we will also discuss the finite non-zero momenta landscape, ruling out the possibility of having quasi-fragmentation in bosonic interacting systems with repulsive interactions. Our findings provide a counterpart to the corresponding results for fragmentation in macroscopically occupied states with eigenvalues scaling with $N$.

### III. THREE DIMENSIONS

Let’s begin with the case of a three–dimensional homogeneous Bose gas. It is well known that, below the critical temperature $T_C$, a BEC takes place and the lowest allowed state for the gas is then macroscopically occupied. This amounts to say that the momentum distribution of the system is constituted by two parts: a non-singular part, relative to the occupation of the single particle states according to the Bose-Einstein distribution, and a singular part $\propto N_0 \delta(\vec{k})$ which refers to the macroscopic occupation $N_0 \propto N$ of the lowest energy state, also called the condensate state. Therefore, at $T < T_C$ ODLRO are found and the exponent will be $C_0 = 1$ in the condensed phase. For temperatures above the critical $T_C$ there is no more condensation and the singular part of the momentum distribution, i.e. the Dirac delta peak, disappears together with the system ordering. From all of these facts one can conclude that

$$C_0(T) = \begin{cases} 1, & \text{for } T < T_C \\ 0, & \text{for } T > T_C \end{cases},$$ \hspace{1cm} (10)

as shown in Fig. 1.

In the weakly interacting Bose gas, one may use the Bogoliubov approximation to obtain the scaling of the momentum distribution at $\vec{k} \neq 0$. Indeed, at this approximation level, the non-singular part of the momentum distribution at $T < T_C$ reads:

$$n(\vec{k}) = \frac{1}{L^D} \left( \frac{1}{(2\pi)^3} e^{\varepsilon(\vec{k})/k_B T} - 1 \right),$$ \hspace{1cm} (11)

where $\varepsilon(\vec{k}) = \frac{\sqrt{n}}{m} k^2 k^2 + \left( \frac{\hbar^2 k}{2m} \right)^2$ is the Bogoliubov dispersion relation and $g = \frac{4\pi \hbar^2 a}{m}$ weights the interaction among particles in terms of the s-wave scattering length $a$. Therefore for $\varepsilon(\vec{k})/k_B T \gg 1$ we obtain:

$$n(\vec{k}) = \frac{1}{L^D} \sim \frac{1}{(2\pi)^3} e^{-\frac{k^2 a^2}{2m k_B T}} \propto e^{-(l/L)^2} \propto N^0,$$ \hspace{1cm} (12)

where in the second equality we used $k \propto l/L$, and in the last one we acknowledged that $l \propto L$ in order to
have a finite momentum \( k \) in the thermodynamic limit. A similar procedure may be used to prove the absence of fragmentation also for \( T > T_C \), yielding

\[
C_{k \neq 0}(T) = 0,
\]

at any temperature for the three-dimensional Bose gas. Notice that this result has been obtained using Bogoliubov theory and it may not be applicable to gases with non-weak interactions. However, since the exponents \( C \) are not expected to increase for larger interactions, one may reasonably conclude that this result is valid also for larger interactions.

IV. ONE DIMENSION

We now turn to the study of a one-dimensional homogeneous Bose gas, within the framework of the Lieb–Liniger model, where the interaction between particles is represented by a repulsive \( \delta \)-potential. The Lieb–Liniger Hamiltonian for \( N \) bosons of mass \( m \) then reads:

\[
H = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i<j} \delta(x_i - x_j),
\]

leading to the definition of the dimensionless coupling constant

\[
\gamma = \frac{2mc}{\hbar^2 n},
\]

where \( n = N/L \) is the density of the gas and \( L \) is the size of the system (with periodic boundary conditions this would be the circumference of the ring in which the system is enclosed). As it is well known, the Lieb–Liniger model is exactly solvable by the Bethe ansatz technique which provides an exact expression for the many-body eigenfunctions. Nevertheless a closed expression for the 1BDM for every coupling \( \gamma \) and particle number \( N \) is not known. One should then rely both on approximations and numerical approaches, which are suitable for working at large particle numbers.

At \( T = 0 \), techniques coming from bosonization provide an expression for the large distance behaviour of the density matrix for any values of the interaction strengths. In this case, the density matrix is written in terms of the dimensionless parameter called the Luttinger parameter, which for Lieb–Liniger model reads \( K = v_F/s \), where \( v_F = \hbar n/m \) is the Fermi velocity and \( s \) is the sound velocity of the Lieb–Liniger gas, which depends on \( \gamma \) and can be obtained via Bethe ansatz. At leading order, the large distance asymptotic of the 1BDM reads:

\[
\rho(r) \sim \frac{B_0}{(nr)^{1/2K}},
\]

where \( B_0 \) is a numerical prefactor. Symmetrizing its expression in order to retrieve periodic boundary conditions, and then performing the integral between 0 and \( L \), we get access to the dimensionless momentum distribution peak scaling

\[
\frac{n(k=0)}{L} = \frac{n^{1-1/2K}}{2\pi} \left[ \int_0^{L/2} \frac{dr}{r^{1/2K}} + \int_{L/2}^{L} \frac{dr}{(L-r)^{1/2K}} \right] \propto N^{1-1/2K},
\]

which implies:

\[
C_0(T = 0, \gamma) = 1 - \frac{1}{2K(\gamma)},
\]

in agreement with Ref. We verified that Eq. also holds also if we symmetrize the density matrix according to the formula

\[
\rho(r) \sim \frac{n^{1-1/2K}}{2\pi} \left[ \frac{1}{2} \sin \left( \frac{\pi l}{L} \right) \right]^{1/2K}.
\]

Notice that \( C_0(T = 0, \gamma) \) depends only on \( \gamma \) through the Luttinger parameter, \( i.e. \) it depends on the ratio \( c/n \) and not on the interaction strength and the density separately. The power \( C_0(T = 0, \gamma) \) varies between 1 and the value 1/2 obtained for the Tonks–Girardeau gas. For very small values of the interaction parameter, say \( \gamma \approx 10^{-4} \), one gets \( C_0 \approx 0.99 \), which is very close to unity. Therefore the condensate fraction, \( \lambda_0/N \), for finite number of particles can be large and this could be seen in experiments with \( Rb \) atoms (when this occurs, one can say it is in presence of a mesoscopic condensate).

Since \( \lambda_0 \) scales less than linearly with \( N \) and at the same time we should have \( \sum_k \lambda_k = N \), in principle we could expect that at least for small values of \( k \) there may exist some \( C_{k \neq 0} \) different from zero. However, as we are going to show in the following, this is not the case in the thermodynamic limit. To obtain the behaviour of the momentum distribution at non-zero momenta, we have to perform the Fourier transform, for which we get:

\[
\frac{n(k)}{L} \propto \int_0^{L/2} \frac{e^{ikr}}{r^{1/2K}} dr + \int_{L/2}^{L} \frac{e^{ikr}}{(L-r)^{1/2K}} dr \propto L^{1-1/2K} \Gamma_F \left( \frac{1}{2} - \frac{1}{4K}; \frac{3}{2}, \frac{1}{2}; \frac{1}{4K} - \frac{\pi^2 r^2}{4} \right),
\]

where \( \Gamma_F(a; b_1, b_2; c) \) is the generalized hypergeometric function and we used the fact that \( kL = \pi l \) with \( l \in \mathbb{N} \). Expanding the hypergeometric function for large \( l \) and keeping only the leading term, we obtain

\[
\frac{n(k)}{L} \propto L^{1-1/2K} l^{-1+1/2K} \propto N^0,
\]

where in the last equality we used the fact that \( l \) needs to grow like \( L \) in the thermodynamic limit in order to have
a fixed finite momentum $k$. Therefore the power $C_{k \neq 0}$ for the one–dimensional gas at zero temperature and any interaction strength is simply vanishing

$$C_{k \neq 0} (T = 0, \gamma) = 0,$$  \hspace{1cm} (21)

and there is no fragmentation of the mesoscopic condensate. The same result can be found also using Eq. [19].

In Ref. [13] it was verified that the largest eigenvalue of the density matrix indeed scales with the exponent in Eq. [18] by directly computing $\rho(r)$ using an interpolation method, which allows to get a simple expression for the density matrix valid at any distance and interaction strengths. The power-law scaling shows very good agreement, confirming that the method sketched above to get access to the power $C$ is correct. We have then used the same interpolation scheme to get access to the $N$ dependence of the $k \neq 0$ eigenvalues of the 1BDM [30]. Apart from oscillations at small particle numbers arising from a competition between the growth of $l$ and $L$, for very large values of $N$ the eigenvalues $\lambda_{k \neq 0}$ saturates and the power $C_{k \neq 0}$ is indeed vanishing, confirming our theoretical prediction.

In the finite temperature ($T \neq 0$) case, several results are available for the asymptotic behaviour of the density matrix of the Lieb–Liniger gas [37–39]. In Ref. [39] an expression for the 1BDM as a sum of exponential functions is given in the form:

$$\rho(r) = n \sum_i \bar{B}_i e^{-\xi_{[\bar{v}_i]}},$$  \hspace{1cm} (22)

with $\bar{B}_i$ are distance independent amplitudes and $\xi_{[\bar{v}_i]}$ the correlation length (shown to be always positive), depending on the temperature-dependent functions $\bar{v}_i$ defined in Ref. [39], where it is also shown that the result in Eq. [(22) reduces to Eq. (16) in the $T = 0$ case, as it should. We may now take the Fourier transform of the symmetrized version of Eq. [22], and obtain

$$n(k) / L = \frac{1}{2\pi} \sum_i \bar{B}_i \left( \int_0^{L/2} e^{-r/\xi_{[\bar{v}_i]}} dr + \int_{L/2}^L e^{-r/\xi_{[\bar{v}_i]}} dr \right) \propto e^{-k/\xi_{[\bar{v}_i]}},$$

where the last proportionality is valid both at zero and non-zero momentum $k$. Since $L = N/n$, analyzing the $N$ leading dependence only, we have that for $N \to \infty$ the dimensionless momentum distribution is just a constant for any $k$, leading to the finite temperature result:

$$C_k (T \neq 0, \gamma) = 0,$$  \hspace{1cm} (23)

which indicates complete absence of ordering.

In Fig. 2 we summarize the behaviour of the exponent $C_0$ for a homogeneous one–dimensional Bose gas for different temperatures. An inset shows the relation between $C_0$ and the interaction parameter $\gamma$ in the zero temperature case, i.e. Eq. [18].

V. TWO DIMENSIONS

Properties of two–dimensional systems stand on their own and are between those of 1D – where $C_0$ vanishes at finite temperature – and of 3D models – where $C_0 = 1$ below the BEC critical temperature. As discussed in the introduction, no ordinary phase transition takes place in 2D, due to the lack of ODLRO. However, 2D systems often feature the BKT topological phase transition named after Berezinskii, Kosterlitz and Thouless who first discussed it in the two–dimensional XY model [40–42]. This transition is related to the presence of vortex and anti-vortex spin configurations at finite temperatures. At low $T$, below the BKT temperature $T_{BKT}$, vortex and anti-vortex pairs with vanishing total winding numbers (neutrality condition) are present in the system and the correlation function between two distant spins decay as power-law, indicating a phase with quasi-long-range order, also called BKT phase.

A simple estimate of $T_{BKT}$ in the XY model is the Peierls value $T_{BKT} = 2 \pi J / \overline{\phi} [43]$, where $J$ is the interaction strength among the spins. In the low-temperature BKT regime the only relevant configurations are the spin waves and the spin-wave approximation shall describe the system properly. As the temperature increases, the presence of free vortices with non-vanishing winding numbers becomes energetically favoured, and, therefore, vortices and anti-vortices may unbind from each other. For temperatures above $T_{BKT}$, the presence of such topological excitations destroy the quasi-long-range order and the correlation functions become exponentially decaying [43–45]. An important statistical model used to approximatively describe the two–dimensional XY model is the one proposed by Villain [43–46]. While in the XY model the spin waves interact with the vortices, in the Villain model the spin waves are decoupled from the vortices.
of freedom, making its Hamiltonian simply quadratic. Both models have the same topological characteristics and they belong to the same universality class, as one can see from the critical behaviour of the anomalous dimension $\eta$ of the two systems. The Villain model well describes the low temperature phase of the XY model, since the Hamiltonian is essentially constituted by two decoupled harmonic oscillators terms, one for the spin waves and one for the vortices. Notice that the Villain model can be used both as a model per se and also as a convenient way to approximate the XY model \[47\].

Let pause here to comment on the qualitative similarity of the low dimensional ($D = 1$ and $D = 2$) systems studied in this work. In the thermodynamic limit at low temperatures, both for the one– and two–dimensional cases, the systems can be described by field theoretical models with Hamiltonians made up of two decoupled harmonic oscillators terms. These quadratic Hamiltonians are the Luttinger liquid and the Villain Hamiltonian for the one– and two–dimensional cases respectively. Therefore bosonization in $D = 1$ systems plays to a certain extent a similar role as the spin wave approximation in $D = 2$ systems, both of them describing systems with quasi-long-range order in the low temperature phase and absence of order above their critical temperatures (which is vanishing in $D = 1$). Nevertheless, the phase transitions that characterize the models are for short-range models intrinsically different in the one– and two–dimensional cases. In $D = 2$ this phase transition is related to the formation of single independent topological excitations, which cannot happen in $D = 1$ geometries. Moreover in one dimension there is no phase transition at all at finite $T$, since the quasi-long-range order is limited to the zero temperature limit.

Let us analyze the BKT phase transition in terms of the exponent $\xi_0$. At the BKT critical point the two–points correlation function scales as \[48\].

\[\rho(r) \sim \frac{1}{r^{D-2+\eta}}, \quad (24)\]

where $\eta$ is the anomalous dimension critical exponent, that depends on the system under consideration. What is universal is the value at $T = 0$, for which $\eta(T = 0) = 0$, and that at $T = T_{BKT}$, which is given by: $\eta(T = T_{BKT}) = 1/4$ \[49\]. The behaviour of $\eta$ between 0 and $T_{BKT}$ is not universal.

From the knowledge of the behaviour of the anomalous dimension – that will be discussed below – one can find an expression for the power $\xi_0$ with which the dimensionless momentum distribution peak scales. One has

\[\frac{n(k=0)}{L^2} = \frac{1}{2\pi} \lim_{L \to \infty} \left[ \int_{0}^{L/2} \frac{dr}{r^{\eta-1}} + \int_{L/2}^{L} \frac{dr}{(L-r)^{\eta-1}} \right] \sim L^{2-\eta}, \quad (25)\]

where we symmetrized the density matrix in Eq. (24) in the radial coordinate variable $r$, passing to polar coordinates and performing the trivial integration over the azimuth angle. Since fixing the density $n = \frac{N}{L^2}$ in the large particle number limit implies that $L \propto \sqrt{N}$, then we can extract the power $\xi_0(T/T_{BKT})$ with which the largest eigenvalue of the 1BDM scales, and it reads:

\[\xi_0 = 1 - \frac{\eta}{2}. \quad (26)\]

Notice that for the XY and Villain models the condensate fraction $\frac{\xi_0}{N}$ is the magnetization density of the spin system and therefore Penrose-Onsager ODLRO manifests in a complete magnetization of the system, while having $\xi_0 = 0$ is equivalent to say that there exist no correlation and order between the spin variables.

Since the value of the anomalous dimension for such systems at the critical temperature is equal to 1/4, one has

\[\xi_0(T = T_{BKT}) = \frac{7}{8}, \quad (27)\]

and $\xi_0$ jumps to zero for $T > T_{BKT}$, reflecting the universal jump for the superfluid stiffness \[49\]. A study of small corrections (found to be $\approx 0.02\%$) to the Nelson-Kosterlitz jump of the superfluid stiffness is in Refs. \[50, 51\]. Using spin wave approximation, one finds that at $T = 0$ there is ODLRO and therefore $\xi_0(0) = 1$. Notice that at $T = 0$ ODLRO is allowed because there is no entropy contribution to the free energy of the system and the Mermin-Wagner theorem does not apply.

\section{Villain model}

In the case of the square lattice planar Villain model, one expects that the anomalous dimension should be of the form $\eta_V \approx \frac{k_BT}{2\pi A}$ at low temperatures, since the theory is quadratic and the spin wave approximation shall apply everywhere, in particular very close to the critical point, where vortex configurations become relevant. The value for $A$ will be provided in the following. Villain \[46\] proposed a correction term to account for vortex contributions to the anomalous dimension close to the critical point. Assuming that the interaction between the vortices can be neglected, this correction yields \[46\]:

\[\eta_V = \frac{k_BT}{2\pi A} + \frac{\pi^2 k_BT}{\pi A - 2k_BT} e^{-\pi^2 A/k_BT}. \quad (28)\]

According to the renormalization group, the value for the critical temperature of the Villain models is found to be \[52\]

\[\frac{k_BT_{BKT}}{A} = \frac{1}{0.74} \approx 1.351, \quad (29)\]

which coincides with the result obtained from the high precision Monte Carlo simulation performed in Ref. \[52\] up to $L = 512$ lattice sites. Substituting Eq. (29) into Eq. (28), we have an estimate for the behaviour of the
anomalous dimension of the square lattice Villain model in terms of the dimensionless ratio $T/T_{BKT}$, which reads:

$$\eta_V(T/T_{BKT}) = A \frac{T}{T_{BKT}} + \frac{\pi^2}{2} \frac{e^{-B T_{BKT}}}{(-1 + D T_{BKT})},$$

(30)

where $A \approx 0.215$, $B \approx 7.304$ and $D \approx 1.162$.

Introducing Eq. (30) into Eq. (26), one obtains the results plotted as the red intermediate solid line in Fig. 3. Notice that according to the approximation in Eq. (28), one has $\eta_V(T = T_{BKT}) \approx 0.236$, i.e., $C_0^V(1) = 0.882$, with “V” referring to the Villain model. This result differs from the one coming from Monte Carlo simulations [52], $\eta_V = 0.2495 \pm 0.0006$, for about 5%. Low temperature predictions for the exponent $C_0^V(T)$ may be formulated in two ways:

1. Disregarding the second term in the right-hand-side of Eq. (28), which may be safely neglected in the low temperature regime at $T \ll T_{BKT}$ [40], which yields, via Eq. (26),

$$C_0^V(T/T_{BKT}) \approx 1 - \frac{1}{2} \left( \frac{T}{2 \pi T_{BKT}} \right) \cdot \frac{1}{0.74},$$

(31)

with $T_{BKT}$ obtained by Monte Carlo simulations [see Eq. (29)].

2. Using the Peierls argument $\frac{k_B T_{BKT}}{A} = \frac{\pi}{2}$, one has:

$$C_0^V(T/T_{BKT}) \approx 1 - \frac{1}{2} \left( \frac{T}{T_{BKT}} \right) \cdot \frac{1}{4}.$$

(32)

These two behaviours are reported as black solid and dashed lines, respectively, in Fig. 3. Notice from the plot that the low-$T$ behaviour of Eq. (31) is good even in region close to $T_{BKT}$, where the corrective term introduced by Villain starts to play a role. The predictions of (32), which at variance do not take into account the effect of vortices, do not match with the same accuracy with the expected results already from $T \approx 0.5 T_{BKT}$.

**B. XY model**

For the two-dimensional classical XY model, the critical temperature has been evaluated using Monte Carlo techniques obtaining [53,54]:

$$k_B T_{BKT} / J = 0.893 \pm 0.001,$$

(33)

while recent approximate, semi-analytical functional renormalization group (FRG) results give $k_B T_{BKT} = (0.94 \pm 0.02) J$ [57]. The anomalous dimension is found to be equal to

$$\eta_{XY} = \frac{k_B T}{2 \pi J_s(T)},$$

where $J_s(T)$ is the superfluid (or spin) stiffness of the model, and has been recently calculated for the XY model in a square lattice in Ref. [58] using simulations up to 256 lattice sites.

Therefore we may now compute the $k = 0$ Fourier transform of the spin–spin correlation function as in Eq. (25). Similarly to Eq. (26), one has

$$C_0^{XY}(T) = 1 - \frac{\eta_{XY}}{2}.$$

(34)

Using the Villain approximation we can obtain an expression for the behaviour of the anomalous dimension for the XY model. The Villain approximation, indeed, is based on the fact that there exist a (non-exact) map between the interaction parameter $A$ and the spin–spin interaction parameter $J$, which relates the Villain Hamiltonian to the XY model [46]. This mapping reads

$$A \frac{1}{k_B T} = -\frac{1}{2} \left\{ \ln \frac{I_1 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right\}^{-1},$$

(35)

where $I_n(x)$ are the modified Bessel functions of the first kind of degree $n$. We may therefore substitute this expression into the approximation given in Eq. (28). We find:

$$\eta_{XY} = -\frac{1}{\pi} \ln \left[ \frac{I_1 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right] + \frac{\pi^2}{2} \left\{ \ln \frac{I_1 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right\}^{-1} \left\{ -1 + \frac{\pi}{4} \ln \left[ \frac{I_1 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right] - 4 \ln \left[ \frac{I_0 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right] \right\}.$$}

(36)

Using the mapping of Eq. (35), the Monte Carlo results of Ref. [52] for the critical temperature of the Villain model, i.e., Eq. (29), translates into

$$k_B T_{BKT} / J = 0.842,$$

(37)
The Villain prediction in Eq. (38) remains reliable up to the second term in the right-hand-side of Eq. (36). Using a low temperature prediction can be made by neglecting Refs. [53–56] reported in Eq. (33). The equation which comes from the Villain prediction Eq. (36). Finally the black solid and dashed lines represent the low temperature predictions of Eqs. (37) and (38) respectively.

which is pretty close to the Monte Carlo results of Refs. [53–56] reported in Eq. (33). The equation which relates $A$ to $J$ seems then to be reliable within a ≈ 6% accuracy even very close to the critical point.

Similarly to what we have done for the Villain model, a low temperature prediction can be made by neglecting the second term in the right-hand-side of Eq. (36). Using Eq. (34) we get:

$$C_0^{XY}(T) \approx 1 + \frac{1}{2\pi} \ln \left[ \frac{I_1 \left( \frac{J}{k_B T} \right)}{I_0 \left( \frac{J}{k_B T} \right)} \right].$$

(37)

On the other hand, one can also employ the low-temperature expansion results: $\frac{J(T)}{J} \approx 1 - \frac{k_B T}{4J}$, which is known to be consistent with several approaches, such as self-consistent harmonic approximation [59], Monte Carlo simulations [60] and FRG [57]. This procedure leads to the expression:

$$C_0^{XY}(T/T_{BKT}) \approx 1 - \frac{T/T_{BKT}}{\frac{4J}{k_B T_{BKT}} + \frac{T}{T_{BKT}}}.$$  

(38)

In Fig. 4 we report as blue points the behaviour of Eq. (34) for $\eta_{XY} = \frac{k_B T}{\pi J_{\chi}(T)}$ with respect to the dimensionless quantity $T/T_{BKT}$ obtained using the results of Ref. [53]. The bottom red solid line represents the Villain prediction given in Eq. (36) with $T_{BKT}$ given by Eq. (33), while the black solid and dashed lines represent the low temperature behaviours in Eqs. (37) and (38) respectively. Fig. 4 confirms the validity of the low temperature expansion in Eq. (38) in the range $T \in [0, 0.8T_{BKT}]$, while the Villain prediction in Eq. (38) remains reliable up to $T_{BKT}$.

![FIG. 4: $C_0^{XY}(T/T_{BKT})$ vs $T/T_{BKT}$. Blue points are the numerical values of $C$ obtained from Eq. (34) with anomalous dimension $\eta_{XY} = \frac{J/T}{\pi J_{\chi}(T)}$ and using the superfluid stiffness results of Ref. [53]. The universal jump from $C_0(T_{BKT}) = \frac{2}{7}$ to $C_0(T > T_{BKT}) = 0$ is evident. The bottom red solid line comes from the Villain prediction Eq. (36). Finally the black solid and dashed lines represent the low temperature predictions of Eqs. (37) and (38) respectively.](image)

C. Bose gas

Under certain conditions a two–dimensional Bose gas can be mapped onto the XY model and from this mapping one can derive the decay of correlation functions and the ordering type of the bosonic system [61, 64]. Indeed, when density fluctuations are strongly suppressed the effective low–energy Hamiltonian of a two–dimensional Bose gas is equivalent to the continuous version of the Hamiltonian of the XY model on the lattice. The BKT phase of the XY model corresponds then to the superfluid state of the Bose gas and quasi-long-range order is present. Above the critical temperature the normal state appears and superfluidity breaks down. This abrupt change of phase is characterized by a universal jump of the superfluid density (stiffness), which switches between its low temperature value $\rho_s = \frac{2m^2k_B T}{\pi\hbar^2}$ to $\rho_s = 0$ for $T > T_{BKT}$ [49, 50].

In Refs. [63, 66] it has been shown that the asymptotic behaviour of the 1BDM of a two–dimensional weakly interacting Bose gas at finite temperatures scales as

$$\rho(r) \sim \frac{1}{\rho_s \ln \left( \frac{\hbar^2}{m U} \right)}.$$  

(39)

where $\rho_s$ is the superfluid density of the gas. The superfluid density of the system assumes the form [62]:

$$\rho_s = \frac{2m^2k_B T}{\pi\hbar^2} f(X),$$  

(40)

where $X = \frac{\hbar^2}{m k_B T U}$ measures the distance from the critical point, with $\mu$ the chemical potential and the critical value $\mu_c$ given by:

$$\mu_c = \frac{m k_B T U}{\hbar^2} \ln \left( \frac{\hbar^2}{m U} \right).$$  

(41)

The function $f(X)$ in Eq. (40) is a dimensionless universal function, which has been numerically determined in Ref. [62]. The variable $U$ appearing in $X$ is the interparticle interaction strength, so that $\frac{U}{\hbar^2} \ll 1$ and $X \gg 1$ correspond to the weakly interacting limit. While, the constant $\xi_\mu$ appearing in Eq. (41) is given by $\xi_\mu = 13.2 \pm 0.2$ [62].

Applying the same procedure used for the Villain and the XY models, we obtain the following exponent $C_0$ for the scaling of the dimensionless momentum distribution function $f(X)$ with respect to the number of particle of the two–dimensional Bose gas:

$$C_0^{Bose}(X) = 1 - \frac{1}{8f(X)}.$$  

(42)

The jump of the superfluid stiffness $\rho_s$ at criticality implies that $f(X)$ will jump from 0 to 1 at $X = 0$, i.e. at the critical point. Therefore, the exponent $C_0$ will jump from the universal value $\frac{2}{7}$ to 0 at the critical BKT temperature. The relation between the exponent $C_0$ and the ratio $T/T_{BKT}$ is constructed from the expression [62]:

$$C_0^{Bose}(X) = 1 - \frac{1}{8f(X)}.$$  

(42)
\[
\frac{T}{T_{BKT}}(X) = \frac{1}{1 + 2\pi \lambda(X)/\ln(h^2\xi/mU)},
\]
where \(\lambda(X) = [X + \theta(X) - \theta_0]/2\) with \(\theta(X)\) found via numerical simulations for system sizes up to 512 in Ref. [62]. The (non-perturbative) constant \(\xi\) in Eq. (43) is given by [62]:
\[
\xi = 380 \pm 3,
\]
and \(\theta_0 = \frac{1}{\pi} \ln \left( \frac{\xi}{\mu} \right)\) is then found to be \(\theta = 1.07 \pm 0.01\).

Knowing the relation between \(T/T_{BKT}\) and \(X\) and the relation between \(C_0^{\text{Bose}}\) and \(X\), we can then track down the dependence of the exponent \(C_0\) with which the dimensionless momentum distribution peak scales with the number of particles \(N\) for different temperatures. We report its behaviour in Fig. 5 for different values of the interaction \(U\).

An important comment about Fig. 5 is that in the limit of the dimensionless interaction parameter \(mU/\pi\) → 0, the exponent \(C_0\) tends to be closer (with respect to higher values of \(U\)) to the unity up to temperatures closer to \(T_{BKT}\). In other words, the smaller is \(U\), the closer to 1 is \(C_0\) at fixed \(T/T_{BKT} < 1\). Going further close to \(T_{BKT}\), from below, the decrease to the value \(\frac{1}{2}\) happens abruptly for \(mU/\pi\) ≈ 0 at \(T \cong T_{BKT}\). Since \(C_0\) has to be 7/8 at \(T = T_{BKT}\), this is to associate to a kind of double jump occurring for \(T \to T_{BKT}^−\) for \(U \to 0\), since in this limit \(C_0\) reaches a value different from (and larger than) 7/8, and then jumps from this value to 7/8 and then jumps to 7/8 to 0. More comments on the double jump occurrence are below.

Finally, it is worth noting that the values for \(mU/\pi = 1\), reported in Fig. 5, are out of the validity range for the weak interacting gas. Then, the mean field arguments of Ref. [62] cannot be applied anymore, and one should take into account quantum fluctuations.

Low temperature predictions may also be formulated, similarly to what we did for the Villain and XY models, but with some subtleties to be worked out. In the low \(T\) regime (i.e. far from the critical point), it is \(X \to \infty\) and the function \(\theta(X)\) satisfies [62]:
\[
\theta(X) - \frac{1}{\pi} \ln \theta(X) = X + \frac{1}{\pi} \ln(2\xi\mu),
\]
which is a transcendent equation admitting two values for \(\theta\) for a single value of \(X\). These two solutions can be distinguished in terms of the behaviour of \(\theta(X)\) for \(X \to \infty\). The first set is the one having a vanishing value of \(\theta(X \to \infty)\) and it is given by:
\[
\theta(X \to \infty) = \frac{e^{-\pi X}}{2\xi\mu},
\]
which is the solution of \(-\frac{1}{\pi} \ln \theta(X) = X + \frac{1}{\pi} \ln(2\xi\mu)\) and as well as a solution of Eq. (45) for \(X \to \infty\). This first set is not interesting for us and we look for a function \(\theta(X)\) which diverges for large \(X\). This represents the second set of solutions and one has
\[
\theta^{(0)}(X \to \infty) = X + \frac{1}{\pi} \ln(2\xi\mu),
\]
which is the zero-th order solution of Eq. (45), without the logarithmic term in the left hand side. In the low \(T\) regime one may also write [62]
\[
f^{(0)}(X \to \infty) = \frac{\pi}{2} \theta^{(0)}(X) - \frac{1}{4} = \frac{2\pi X + 2 \ln(2\xi\mu)}{4} - 1,
\]
where the last identity follows from Eq. (47). Reminding that \(\lambda(X) = [X + \theta(X) - \theta_0]/2\) and using Eq. (47), one has an expression also for the \(\lambda(X)\) function in the low temperature regime at the zero-th order of approximation:
\[
\lambda^{(0)}(X \to \infty) = X + \frac{1}{2\pi} \ln \left[ \frac{2(\xi\mu)^2}{\xi} \right].
\]

Therefore, substituting into Eq. (43), one can write an expression for \(X\) (at the zero-th order in terms of the variable \(T/T_{BKT}\)) reading:
\[
X^{(0)} = -\frac{1}{2\pi} \ln \left[ \frac{2(\xi\mu)^2}{\xi} \right] + \frac{1}{2\pi} \ln \left( \frac{h^2\xi}{mU} \right) \left( \frac{T_{BKT}}{T} - 1 \right).
\]
Finally, inserting Eq. (50) in Eq. (48), we may substitute the equation for \(f^{(0)}(X \to \infty)\) into Eq. (42) to obtain an analytical expression for the exponent \(C_0^{\text{Bose}}\) at low temperatures:
\[
C_0^{\text{Bose}}(T/T_{BKT}) \simeq 1 + \frac{1}{2} \left[ 1 - \ln(2\xi) - \ln \left( \frac{h^2\xi}{mU} \right) \left( \frac{T_{BKT}}{T} - 1 \right) \right]^{-1}
\]
where the superscript \(^{(0)}\) denotes we are at the lowest order in the considered approximation. One can obtain higher order solutions by substituting the expression in Eq. \((17)\) in the logarithmic term of the equation Eq. \((45)\) and solve for \(\theta(X)\), which will now be the solution at the first order of approximation, \(i.e.\) it reads:

\[
\theta^{(1)}(X) = X + \frac{1}{\pi} \ln(2\xi_m) + \frac{1}{\pi} \ln \theta^{(0)}(X) .
\]  

(52)

Following the same procedure sketched above for the zero-th order case, we obtained the following analytical form for \(C_0^{\text{Bose}}\) at low temperatures at first order approximation:

\[
C_0^{\text{Bose}}(1)\left( \frac{T}{T_{BKT}} \right) \approx 1 + \frac{1}{2} \left\{ 1 - 2 \ln \left[ \frac{2mU}{\hbar^2} \right] \right\}^{1/2} + \frac{mU}{\hbar^2} \left[ \left( \frac{2mU}{\hbar^2} \right)^{T_{BKT}/T} \right] + W \left\{ \left[ \frac{2mU}{\hbar^2} \right]^{T_{BKT}/T} \right\}^{-1},
\]  

(53)

where \(W(z)\) is the Lambert or product logarithm function. Higher order solutions may be obtained following the same recipe, but from the second order case is not possible to write an analytical expression for \(X\) in terms of \(T/T_{BKT}\). Therefore, one can work out only the numerics in order to obtain the low temperature behaviour of the exponent \(C_0^{\text{Bose}}(\geq 2)\left( T/T_{BKT} \right)\). In the present work the third order approximation has been also investigated, but we envisage no particular difficulty in going beyond.

In Fig. 6 we report the comparison between the low temperature expansions with the values for \(C_0^{\text{Bose}}\) obtained from the numerical Monte Carlo results of Ref. \([62]\) in the very small interaction limit \(mU/\hbar^2 = 10^{-12}\), and for the intermediate interaction case \(mU/\hbar^2 = 0.25\). The agreement is good up to 3% even for \(T \approx T_{BKT}\), where

\[
C_0^{\text{Bose}}(3) \approx 0.912, \tag{54}
\]

independently of the interaction parameter. It is important to notice that for smaller values of \(U\) the low temperature predictions for the exponent \(C_0^{\text{Bose}}\) are valid for a larger range of temperatures, since for very weak interactions the variable \(X\) is very large even at \(T \approx T_{BKT}\). So, decreasing \(U\) the range of validity of the low temperature predictions increase up to a value which becomes increasingly close to \(T_{BKT}\). Indeed, for \(mU/\hbar^2 = 10^{-12}\) the low \(T\) prediction remains reliable up to \(T \approx 0.9T_{BKT}\).

This implies that for \(U \to 0\), and in practice \(mU/\hbar^2\) extremely small, there will be the above mentioned double jump phenomenon for the exponent \(C_0^{\text{Bose}}\) which will pass near below \(T_{BKT}\) from a value close to the quantity in Eq. \((54)\), \(0.912\), to \(\frac{\hbar}{2X} = 0.875\) for \(T = T_{BKT}\). Then the second Nelson-Kosterlitz jump will lead \(C_0^{\text{Bose}}\) to pass from \(7/8\) to zero. It can be seen that there is not appreciable change in this result if one goes to higher orders of approximation. Despite being not too large in absolute value, the first jump should be appreciable in experiments or simulations, one problem being that one has to go possibly to very small values of \(mU/\hbar^2\). We observe that the prediction of the double jump is based on the validity of the low \(T\) expansion and its extension near \(T_{BKT}\) for \(U\) very small – and when \(T\) is scaled in units of \(T_{BKT}\), which in turn depends in \(U\). Therefore it could be that further corrections near \(T_{BKT}\) may soften the first jump, making it a very steep decrease. Notice, that due to Eq. \((25)\), the value \(\eta = 0.176\), which is pretty far from the universal value \(\eta = 0.25\), so that going to very small \(U\) one should appreciate such relatively large variation of \(\eta\) near \(T_{BKT}\). Further simulations would be extremely useful to better quantify such steep decrease of \(\eta\) close to \(T_{BKT}\).

Interestingly enough, at low temperatures, the Bose gas can be described by the corresponding results for the XY model. Therefore, posing \(C_0^{XY} = C_0^{\text{Bose}}(0)\) \(i.e.\) equating the low temperature result of the XY model in Eq. \((58)\) to the low temperature result for the 2D Bose gas in Eq. \((51)\) for any rescaled temperature \(T/T_{BKT}\), one obtains the following value for the parameter \(\xi\):

\[
\xi = \frac{1}{2} e^{1+\frac{\pi}{2}(T^{-1})}, \tag{55}
\]

where \(T \equiv 4J/k_BT_{BKT}^{(XY)}\). When the dimensionless interaction strength satisfies the equation

\[
\frac{mU}{\hbar^2} = \frac{1}{2} e^{1+\frac{\pi}{2}} = 0.283, \tag{56}
\]

the low \(T\) predictions in Eq. \((51)\) equals Eq. \((38)\), valid respectively for the 2\(D\) Bose gas and the XY model. Since for the XY model it is \(k_BT_{BKT}^{(XY)}/J = 0.893 \pm 0.001\), one finds

\[
\xi = 321 \pm 3, \tag{57}
\]

which should be compared with the Monte Carlo result \(\xi = 380 \pm 3\). The comparison shows that this result (that depends only on the critical temperature of the 2\(D\) XY model) is not entirely unreasonable, given the non-perturbative nature of the parameter \(\xi\) and the well-known failure of mean-field calculations to determine it and in general the difficulty of obtaining analytical estimates for it.

Predictions can be made also for \(T \simeq T_{BKT}\), \(i.e.\) \(X \to 0^+\). We write the function \(\theta(X)\) as:

\[
\theta(X \to 0) = bX + \frac{1}{\pi} \ln \left( \frac{\xi}{\kappa} \right), \tag{58}\]

where \(b\) is a constant to be determined by fitting the values of \(\theta(X)\) for small \(X\) coming from Monte Carlo simulations with the law in Eq. \((58)\). It is found \(b = 1.29 \pm 0.05\).

For the function \(f(X)\) is found instead \([41, 42, 62]\):

\[
f(X \to 0) = 1 + \sqrt{2\kappa' X}, \tag{59}\]

with \(\kappa' = 0.61 \pm 0.01\). For \(\lambda(X)\), from Eq. \((58)\), is simply found that:

\[
\lambda(X \to 0) = \frac{b - 1}{2} X, \tag{60}\]
and therefore, following the same reasoning of the low $T$ case, from Eq. (43) follows that:

$$X = \frac{\ln \left( \frac{\hbar^2 \xi}{mU} \right)}{\pi (b - 1)} \left( \frac{T_{BKT}}{T} - 1 \right).$$

Finally we can substitute the above expression for $X$ into Eq. (59) and then into Eq. (42) to obtain an expression for $C_0^{\text{Bose}}(T)$ for $T \approx T_{BKT}$ which reads:

$$C_0^{\text{Bose}}(T \rightarrow T_{BKT}) \approx 1 - \frac{1}{8} \left[ 1 + \sqrt{\frac{2\kappa'}{\pi (b - 1)}} \ln \left( \frac{\hbar^2 \xi}{mU} \right) \right] \left( \frac{T_{BKT}}{T} - 1 \right)^{-1}.$$  

We report its behaviour in red solid lines in Fig. 6 along with numerical Monte Carlo results of $C_0^{\text{Bose}}$ obtained from Ref. [62] for different interactions. The agreement is good only for values $X \approx 0$ and the analytical prediction of Eq. (62) gets rapidly worst for decreasing temperatures.

Equating the two behaviours in Eqs. (51) and (62) we can find how the temperature with which the two curves intersect depends on the dimensionless interaction parameter $\frac{mU}{\hbar^2}$. Substituting this expression back to either (51) or (62), it is found that the value for $C_0^{\text{Bose}}$ at which the two limiting behaviours intersect is independent on the interaction strength, and reads:

$$C_0^{\text{Bose}}(0) = 1 - \frac{1}{8} \left[ 1 + \sqrt{\frac{2\kappa'}{\pi (b - 1)}} \right] \left( \frac{T_{BKT}}{T} - 1 \right)^{-1}.$$  

This intersection value can also be obtained using the first order approximation formula $C_0^{\text{Bose}}(1)$, for which one gets 0.915.

Let now study the scaling exponent $C_{k\neq0}$ for the eigenvalues of the 1BDM corresponding to non-vanishing momenta. As in previous Section, we have to compute the Fourier transform of the symmetrized asymptotic behaviour of the density matrix, hence:

$$n(k) \propto \lim_{L \rightarrow \infty} \frac{2\pi}{L^2} e^{i k r \cos(\theta)} d\theta \left[ \frac{L/2}{0} \int dr \frac{J_0(kr)}{r^{\eta-1}} + \frac{L}{L/2} \int (L - r)^{\eta-1} dr \right] = \lim_{L \rightarrow \infty} \frac{L}{0} \int dr \frac{J_0(kr)}{r^{\eta-1}} + \frac{L}{L/2} \int (L - r)^{\eta-1} dr,$$

where we passed to polar coordinates symmetrizing on the radial component as was done for the XY model case, $J_0(x)$ is the Bessel function of the first kind, and $\eta = \frac{m^2 k \rho T}{2 \pi \hbar^2 \rho}$ for the weakly interacting Bose gas, while $\eta = \frac{2 \pi J_0(k)}{\pi J_1(k)}$ for the XY model. Focusing only on the first half of the integration interval [67] we obtain:

$$n(k) \propto L^{2-\eta} F_2 \left( 1 - \frac{\eta}{2}, 2 - \frac{\eta}{2}; -\frac{\pi^2 l^2}{4} \right),$$

where we used $k L = 2 \pi l$ with $l \in \mathbb{N}$. Expanding the hypergeometric function for large $l$ and focusing only the leading term, we obtain finally:

$$n(k) \propto L^{2-\eta} L^{\eta-2} \propto L^0,$$

where in the last proportion we wrote $l \propto L$ in order that $k$ remains finite in the thermodynamic limit and $L \propto \sqrt{N}$, since the density $n = N/L^2$ is fixed. Therefore we simply read

$$C_{k\neq0}(T) = 0,$$

both for the XY and two–dimensional Bose gas systems for zero and finite temperatures.

**VI. CONCLUSIONS**

The goal of the present paper has been to characterize the off–diagonal long-range order (ODLRO) properties
of interacting bosons at finite temperatures through the study of the eigenvalues’ scaling of the one–body density matrix (1BDM) vs the number of particles \(N\). For translational invariant systems, denoting by \(\lambda_0\) the eigenvalues of the (1BDM) and by \(\lambda_0\) the largest among them, one can define the scaling exponents \(C_k\) from the relation \(\lambda_k \sim N^{C_k}\). The exponents \(C_k\) depend on the temperature \(T\) and on the strength of the interaction (which we assume short-ranged), and as well on the dimension \(D\). According the Penrose-Onsager criterion, \(C_0 = 1\) corresponds to ODLRO, while at variance the opposite limit \(C_0 = 0\) corresponds to the single-particle occupation of the natural orbital associated to \(\lambda_0\). The intermediate case, \(0 < C_0 < 1\), is associated for translational invariant systems to the power-law decaying of non-connected correlation functions and it can be seen as identifying quasi-long-range order.

After introducing some basic definitions and properties of the 1BDM, we discussed how to obtain the exponents \(C_k\) directly from the large distance behaviour of the 1BDM. The ODLRO in the three–dimensional case for temperatures below the Bose-Einstein critical temperature has been described, as well as quasi-long-range order in the one– and two–dimensional Bose gases for different interactions and temperatures, discussing the connection of the Mermin-Wagner theorem with the occurrence of mesoscopic condensation. We showed that in 1D it is \(C_0 = 0\) for non-vanishing temperature, while in 3D \(C_0 = 1\) (\(C_0 = 0\)) for temperatures smaller (larger) than the Bose-Einstein critical temperature. We then focused on the two–dimensional case. We presented the application of our methods to the XY and Villain models, where ODLRO is translated as a fully magnetization of the system, and to the 2D Bose gases. A universal jump of the power \(C_0\) from \(\frac{T}{8}\) to 0 is found at the Berezinskii–Kosterlitz-Thouless temperature \(T_{BKT}\), reflecting the universal jump for the superfluid stiffness. The dependence of \(C_0\) between \(T = 0\) (at which \(C_0 = 1\)) and \(T_{BKT}\) is studied in the different models. We found a weak dependence of it when the reduced temperature \(T/T_{BKT}\) is used. An estimate for the (non-perturbative) parameter \(\xi\) entering the equation of state of the 2D Bose gases was obtained using low temperature expansions and compared with the Monte Carlo result. We also unveiled a “double jump”–like behaviour for \(C_0\), and correspondingly of the anomalous dimension \(\eta\), right below \(T_{BKT}\) in the limit of vanishing interactions. When the dimensionless parameter \(mU/\hbar^2\) is very small, the validity region of the low-temperature expansions enlarges towards \(T_{BKT}\) as soon as that \(mU/\hbar^2\) decreases. When such regime is reached, then \(C_0\) tends to the value \(\approx 0.912\), and again moving towards \(T_{BKT}\) from below it abruptly (or, at least, in a very steep way) decreases to the universal value 7/8, then jumping again to 0. We presented a detailed discussion of the weakly interacting regime and we commented how the double jump behaviour could be appreciable for very low values of the parameter \(mU/\hbar^2\). Then we analyzed the behaviour of \(C_k\neq 0\), finding that in none of the cases presented there is quasi-fragmentation, i.e. \(C_k\neq 0 = 0\).

Our investigation is based both on the homogeneity of space and the thermodynamic limit, therefore will be interesting to study in a future work whether adding a confining external potential could change our predictions and how finite number of particles affects the results. Moreover, it would be of interest to consider long-range interactions and the presence of disorder, where rigorous results are available in literature. We also mention that for 2D anyonic gases, despite the presence of a considerable literature, see e.g. [71–74] and refs. therein, to the best of our knowledge no results for the scaling exponents \(C_k(T)\) are available at date.

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