Renormalization-group flow and asymptotic behaviors at the Berezinskii-Kosterlitz-Thouless transitions

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We investigate the general features of the renormalization-group flow at the Berezinskii-Kosterlitz-Thouless (BKT) transition, providing a thorough quantitative description of the asymptotic critical behavior, including the multiplicative and subleading logarithmic corrections. For this purpose, we consider the RG flow of the sine-Gordon model around the renormalizable point which describes the BKT transition. We reduce the corresponding $\beta$-functions to a universal canonical form, valid to all perturbative orders. Then, we determine the asymptotic solutions of the RG equations in various critical regimes: the infinite-volume critical behavior in the disordered phase, the finite-size scaling limit for homogeneous systems of finite size, and the trap-size scaling limit occurring in 2D bosonic particle systems trapped by an external space-dependent potential.

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I. INTRODUCTION

The Berezinskii-Kosterlitz-Thouless (BKT) theory\textsuperscript{[1–4]} describes finite-temperature transitions in two-dimensional (2D) systems with a global U(1) symmetry, which belong to the so-called 2D XY universality class. BKT transitions are quite peculiar, since the low-temperature phase is not characterized by long-range order and the emergence of a nonvanishing order parameter\textsuperscript{[5, 6]}, but rather by quasi-long range order (QLRO) with correlations decaying algebraically at large order. For example, a 2D fluid of identical bosons cannot undergo Bose-Einstein condensation. Above $T_c$, these systems show a standard disordered phase with exponentially decaying correlations. The BKT theory predicts an exponential increase of the correlation length when approaching the transition point $T_c$ from above, as $\xi \sim \exp(c/\sqrt{T})$ with $c \equiv T/T_c - 1$. BKT transitions are generally expected in 2D systems of interacting bosonic atoms, such as those investigated in experiments with trapped atomic gases\textsuperscript{[7–11]}, in liquid helium films\textsuperscript{12}, in arrays of Josephson junctions\textsuperscript{13}, etc. These experiments have provided evidence of the general features predicted by the BKT theory.

A standard representative model of the 2D XY universality class is the classical 2D XY model. Its Hamiltonian is

$$ H_{XY} = -J \sum_{\langle ij \rangle} \text{Re} \bar{\psi}_i \psi_j, \quad \psi_i \in U(1), $$

where the sum runs over the bonds of a square lattice. Its phase diagram shows a BKT transition between a high-temperature disordered phase and a low-temperature QLRO phase, at $J \beta_c = 1.1199(1)$. The asymptotic behaviors at the BKT transition, and in particular their logarithmic corrections, have been much investigated, see e.g. Refs.\textsuperscript{13, 28}, by analytical and numerical studies.

In this paper we investigate the general features of the renormalization-group (RG) flow at the BKT transition, providing a complete characterization of the asymptotic BKT behaviors, and in particular of the multiplicative and subleading logarithmic corrections. For this purpose, we exploit the mapping between the 2D XY or Coulomb-gas models and the sine-Gordon (SG) model, whose RG flow around the renormalizable point describes the BKT transition\textsuperscript{[34]}. In order to investigate its RG flow, we first reduce the SG $\beta$-functions to a canonical universal form. Explicitly, we show that we can define appropriate couplings $u$ and $v$ so that the associated $\beta$-functions have the form $\beta_u = -uv$ and $\beta_v = -u^2[1+vf(v^2)]$ to all orders of the perturbative expansion in powers of $u$ and $v$. The universal function $f(v^2)$ cannot be determined by general arguments, but only by means of detailed calculations in the SG model (at present only $f(0)$ is known). Then, generalizing the RG study of Ref.\textsuperscript{24}, we determine the asymptotic solutions of the RG equations in some different critical regimes: the infinite-volume critical behavior in the disordered phase, the finite-size scaling (FSS) limit for homogeneous systems of finite size\textsuperscript{33, 36}, and the trap-size scaling (TSS) limit\textsuperscript{37} in 2D bosonic particle systems trapped by an external space-dependent potential. The latter results are relevant for experimental investigations of trapped quasi-2D atomic gases, such as those reported in Refs.\textsuperscript{7–11}.

The paper is organized as follows. In Sec.\textsuperscript{II} we summarize some of the RG ideas that we use to analyze the BKT RG flow. Sec.\textsuperscript{III} reports the derivation of the canonical form of the $\beta$-functions and outlines the main features of the RG flow which they describe. In Sec.\textsuperscript{IV} we derive the asymptotic critical behavior of some observables, such as the correlation function $\langle \bar{\psi}(x)\psi(y) \rangle$ of the XY model and its low-momentum components, when approaching the critical point from the high-temperature phase. In Sec.\textsuperscript{V} we discuss the asymptotic behavior in the FSS limit, i.e. in the infinite-volume limit keeping the ratio between the system size and the correlation length fixed, and in particular at $T_c$. Multiplicative logarithms appear in the two-point function and in the related susceptibil-
ity. Sec. [VI] is devoted to an analysis of the TSS behavior at the BKT transition. We show that, at $T_c$, the critical behavior with respect to the trap size must include new multiplicative logarithms. Finally, in Sec. [VII] we draw our conclusions and summarize the main results of the paper. The various appendices report some technical details of the derivations of the results.

II. A SHORT SUMMARY OF THE RENORMALIZATION-GROUP IDEAS

Before discussing the RG flow at the BKT transition, we would like to recall a number of ideas concerning the RG flow, which we then apply to the study of the BKT critical behavior. We consider a generic critical system depending on a set of scaling fields $u_{10}, u_{20}$, and so on. The RG flow with respect to a length rescaling $b$ is defined by

$$b \frac{du_i}{db} = \beta_i(u_1, u_2, \ldots),$$

with boundary condition $u_i(b = 1) = u_{i0}$. Then, the scaling part of the free-energy density satisfies

$$\mathcal{F}(u_{10}, u_{20}, \ldots) = b^{-d} \mathcal{F}[u_1(b), u_2(b), \ldots],$$

where $d$ is the space dimension. Analogously, the correlation length satisfies

$$\xi(u_{10}, u_{20}, \ldots) = b \xi[u_1(b), u_2(b), \ldots].$$

An operator that renormalizes multiplicatively scales as

$$\mathcal{O}(u_{10}, u_{20}, \ldots) = b^{d_{\mathcal{O}}} Z_{\mathcal{O}}[u_1(b), u_2(b), \ldots] \mathcal{O}[u_1(b), u_2(b), \ldots],$$

where $d_{\mathcal{O}}$ is its power-counting dimension and $Z_{\mathcal{O}}$ satisfies the RG equation

$$b \frac{d \ln Z_{\mathcal{O}}}{db} = \gamma_{\mathcal{O}}(u_1, u_2, \ldots), \quad Z_{\mathcal{O}}(b = 1) = 1,$$

where $\gamma_{\mathcal{O}}$ is the anomalous dimension associated with $\mathcal{O}$.

The RG flow can be characterized in terms of characteristic surfaces. For a given set of initial conditions we consider the functions $f_i(u_1)$ for $i \geq 2$ (the choice of the first scaling field to parametrize the flow is arbitrary; any other choice would work equally well), which are solutions of the equations

$$\frac{df_i}{du_1} = \frac{\beta_i[u_1, f_2(u_1), f_3(u_1), \ldots]}{\beta_1[u_1, f_2(u_1), f_3(u_1), \ldots]}$$

with initial conditions $f_i(u_{10}) = u_{i0}$. The hypersurface $H_i$ of equation $u_i = f_i(u_1)$ is invariant under the RG flow, since

$$b \frac{d}{db}[u_i(b) - f_i(u_1(b))] = \beta_i - \frac{\beta_i}{\beta_1} \beta_1 = 0.$$

Therefore the flow line lies in the intersection of all the $H_i$ hypersurfaces.

We can also take into account the size $L$ of the system. With the usual hypotheses [38, 41] of the FSS theory, this is achieved by adding a term $L/b$ in the scaling Ansatz:

$$\mathcal{F}(u_{10}, u_{20}, \ldots, L) = b^{-d} \mathcal{F}[u_1(b), u_2(b), \ldots, L/b].$$

Also correlation functions that depend on coordinates $x, y, \ldots$ can be analyzed. In this case the RG mapping is simply $x \to x/b, y \to y/b, \ldots$

In the following we shall use the notation

$$l \equiv \ln b, \quad \frac{d}{dl} = b \frac{d}{db}.$$

III. CANONICAL FORM OF THE BKT BETA FUNCTIONS AND RENORMALIZATION-GROUP FLOW

We want to study the general features of the RG flow at the BKT transition of 2D systems with U(1) symmetry. For this purpose, we consider the SG field-theoretical model, see, e.g., Ref. [42], defined by the Lagrangian

$$\mathcal{L}_{SG} = \frac{1}{2} (\partial_\mu \phi)^2 + \frac{\alpha}{a^2 \beta^2} [1 - \cos(\beta \phi)],$$

where $\alpha$ and $\beta$ are dimensionless coupling constants, and $a$ is an ultraviolet length scale. The RG flow around the fixed point $\beta^* = \sqrt{8\pi}, \alpha^* = 0$ describes the BKT transition [34]. It can be investigated by a renormalizable two-parameter perturbative expansion in powers of $\delta$, defined by $\beta^2 = 8\pi(1 + \delta)$, and $\alpha$. Their $\beta$ functions have been computed to two-loop order [34, 43], obtaining [44]

$$\beta_\alpha = -2\alpha \delta - \frac{5}{64} \alpha^3,$$

$$\beta_\beta = -\frac{1}{32} \alpha^2 + \frac{1}{16} \alpha^2 \delta.$$

Under an appropriate analytic redefinition of the couplings $\alpha$ and $\delta$, the above two-loop $\beta$-functions can be rewritten as

$$\beta_\alpha = -uv,$n

$$\beta_\delta = -u^2 - \frac{3}{2} v^2.$$

The coefficient $-3/2$ is universal in the following sense: there is no redefinition of the couplings $u' = U(u, v)$ and $v' = V(u, v)$ such that $\beta_{u'} = -u' v'$ and $\beta_{v'} = -u'^2 - c u'^2 v' + \ldots$, with $c \neq -3/2$.

This reduction to a universal form can be extended to all orders, leading to the most general canonical form of the $\beta$-functions which is compatible with the invariance of the model under $\alpha \to -\alpha$ (it corresponds to a shift
of $\pi/\beta$ in the field $\phi$). We prove that, by an analytic redefinition of the couplings 
\[ \alpha = a_{\alpha,10}u + \sum_{n+m \geq 2} a_{\alpha,nm}u^nv^m, \]  
\[ \delta = a_{\delta,10}v + \sum_{n+m \geq 2} a_{\delta,nm}u^nv^m, \]  
the $\beta$-functions of the SG model can be rewritten in the general form 
\[ \beta_u(u,v) = -uv, \]  
\[ \beta_v(u,v) = -u^2[1 + v f(v^2)], \]  
where $f(x)$ has an expansion of the form 
\[ f(x) = b_0 + b_1x + b_2x^2 + \ldots \]  
This representation of the $\beta$-functions is universal, in the sense that, by redefining the couplings, it is not possible to obtain $\beta$ functions of the same form, i.e., $\beta_u' = -uv'$ and $\beta_v' = -u^2[1 + v' g(u'^2)]$, with $g(x) \neq f(x)$. The proof is outlined in App. A (this result was already conjectured in Ref. [24] without proof). The coefficient $b_0$ can be read off from Eq. (13), 
\[ b_0 = 3/2, \]  
while the higher-order terms, $b_i$, $i \geq 1$, are unknown. Note that the evaluation of the next universal coefficient $b_1$ requires a perturbative calculation of the SG $\beta$-functions to four loops.

The analysis of the RG flow can be performed following the method outlined in Sec. II see also Refs. [24, 34]. First, we define the RG invariant function 
\[ Q(u,v) = u^2 - F(v), \]  
where 
\[ F(v) = 2 \int_0^v \frac{wdw}{1 + w f(w^2)} \]  
\[ = v^2 - \frac{2b_0}{3} v^3 + \frac{b_0^2}{2} v^4 + O(v^5), \]  
which satisfies 
\[ \frac{dQ}{dl} = \frac{\partial Q}{\partial u} \beta_u(u,v) + \frac{\partial Q}{\partial v} \beta_v(u,v) = 0, \]  
where $l$ is the flow parameter. The RG flow follows the lines $Q = \text{constant}$. It is thus natural to parametrize the RG flow in terms of $Q$ and $v(l)$. Since 
\[ \frac{dv}{dl} = \beta_v(u,v) = -[Q + F(v)][1 + v f(v^2)], \]  
we obtain 
\[ l = -\int_{v_0}^{v(l)} \frac{dw}{[Q + F(w)][1 + w f(w^2)]}, \]  
where $v(l = 0) = v_0$.

It is important to stress that Eqs. (17) and (18) are the two $\beta$-functions associated with the marginal operators that characterize the BKT transition. For a full understanding of the scaling corrections one should also consider the contributions of the subleading operators, which are suppressed by powers of the critical length scale. The most relevant subleading operator at the BKT transition is expected to have RG dimension $-2$, as in the Gaussian spin-wave theory, see, e.g., Ref. [13]. In the standard RG language this corresponds to a scaling-correction exponent $\omega = 2$. Thus, subleading operators induce corrections of order $\xi^{-2}$ in the high-temperature infinite-volume limit and of order $L^{-2}$ in the FSS limit (apart from corrections arising from the boundary conditions [16, 17], which are expected to be $O(L^{-1})$; they are absent in the case of boundary conditions preserving translation invariance, such as periodic boundary conditions). Additional multiplicative logarithms may also appear (hence, corrections might scale as $\xi^{-2} \ln^2 \xi$, $L^{-2} \ln^2 L$), because of the possible resonance between the subleading and the marginal operators [35]. The difference between their RG dimensions being an integer number. In the following we shall not consider these scaling corrections, since our focus will be mainly on the logarithmic corrections to the leading behavior that can be obtained by considering only the two marginal couplings.

IV. INFINITE-VOLUME RESULTS AT THE BKT TRANSITION

Let us now apply these results to the XY model. In Fig. 1 we show a sketch of the RG flow. Repeating the discussion of Refs. [3, 4, 24] the XY model can be mapped onto a line in the $(u,v)$ plane with $v > 0$. The BKT transition is the intersection of this line with the line $Q = 0$ and the high-temperature phase corresponds to $Q > 0$ (region C with $v > 0$ in Fig. 1). Thus, $Q$ plays the role of thermal nonlinear scaling field, i.e., 
\[ Q = q_1 \tau + q_2 \tau^2 + \ldots \]  
where $\tau = T/T_c - 1$, and $q_i$ are nonuniversal coefficients. In the following we shall use $Q$ instead of $\tau$.

Let us first consider the infinite-volume correlation length $\xi_\infty(\tau) = \xi_\infty(Q,v)$, which we may define by using the second-moment of the two-point correlation function 
\[ G(x,y) = \langle \tilde{\psi}(x)\tilde{\psi}(y) \rangle, \]  
or its large-distance exponential decay. For all $v > 0$ the correlation length is singular as $Q \to 0$. On the other hand, for $v < 0$, the correlation length is analytic on the line $Q = 0$ (see Ref. [24]). Hence, in order to obtain the singular behavior, we use the RG equations to flow from the starting point $v_0 > 0$ to the negative point $v = -1$.

We determine $l_0$ by requiring 
\[ v(l_0) = -1, \]
so that
\[ l_0 = \int_{-1}^{v_0} \frac{dw}{Q+F(w)[1+w^2]} = I(Q,v_0). \] (29)

Then, Eq. (4) gives
\[ \xi_\infty(Q,v_0) = e^l \xi_\infty(Q,v(l)) = e^{I(Q,v_0)} \xi_\infty(Q,-1). \] (30)

Since \( \xi_\infty(Q,-1) \) is analytic in \( Q \), the singular part is given by the exponential term. The behavior of \( \xi_\infty(\tau) \) for \( \tau \to 0 \) is obtained by computing the asymptotic expansion of \( I(Q,v_0) \) for \( Q \to 0 \), which can be written in the form
\[ I(Q,v_0) = \frac{1}{\sqrt{Q}} \sum_{n=0} \sqrt{n} Q^n + \sum_{n=0,1} Y_n(v_0) Q^n, \] (31)
see App. [13] for its derivation. The nonanalytic terms in this expansion depend only of the coefficients \( b_k \) which appear in Eq. (18). The first two coefficients are
\[ I_0 = \frac{\pi}{12}, \quad I_1 = -\frac{\pi b_0}{12} = \frac{3\pi}{16}. \] (32)

Correspondingly, we obtain
\[ \xi_\infty(\tau) = X \exp(\pi/\sqrt{Q})[1 + I_1 \sqrt{Q} + O(Q)]. \] (33)

Expanding \( Q \) in powers of \( \tau \) we obtain the celebrated BKT expression for the correlation length [1, 3]. Of course, this is also consistent with the exact result for the correlation length of the F-model, computed using transfer-matrix techniques, see e.g. [11, 29].

These results allow us to derive the critical behavior of of generic RG invariant dimensionless quantities, which we generically denote by \( R \). Examples of such quantities are ratios of length scales and the so-called zero-momentum \( 2n \)-point renormalized couplings (related to the small-magnetization expansion of the scaling free energy), see e.g. Refs. [20, 30–33]. Indeed, \( R \) satisfies the scaling relation
\[ R(Q, v_0) = R(Q, v(l)), \] (34)
for any \( l \). This implies that \( R(Q, v_0) \) is independent of \( v(l) \), hence an analytic function of \( Q \) and therefore of \( \tau \). It follows
\[ R(\tau) = R^* + \frac{c_R}{\ln^3(\xi_\infty/X)} + O(\ln^{-3} \xi_\infty), \] (35)

where the constant \( c_R \) is expected to be universal.

Let us now consider a generic operator that renormalizes multiplicatively. Writing the corresponding anomalous dimension \( \gamma_\mathcal{O}(u, v) \) in terms of \( Q \) and \( v \), from Eq. (4) we obtain
\[ \mathcal{O}(Q, v_0) = \left[ \exp \int_{v_0}^{-1} dw \frac{\gamma_\mathcal{O}(Q,w)}{\beta_c(Q,w)} \right] \mathcal{O}(Q,-1). \] (36)

Taking into account the symmetry properties of the SG model, we write the expansion of \( \gamma_\mathcal{O} \) as
\[ \gamma_\mathcal{O} = g_{00} + g_{01} v + g_{02} v^2 + g_{20} u^2 + O(v^3, u^2 v^2, u^4) = g_{00} + g_{01} v + (g_{02} + g_{20}) u^2 + g_{20} Q + O(v^3, Q v^2, Q^2). \] (37)

It is important to discuss the universality of this expansion. There is a residual transformation of the couplings that leaves the \( \beta \)-functions [17] and [18] invariant:

\[ u' = u + A_{uv} u + \ldots, \] (38)
\[ v' = v + A_{u^2} u^2 + \ldots, \] (39)

for any \( A \). The RG invariant function \( Q \) is invariant under the transformation and so are the coefficients \( g_{00}, g_{01}, \) and \( g_{02} \), hence they are universal. Instead, \( g_{20} \) can be changed at will, hence it is model dependent.

We can now rewrite Eq. (36) as
\[ \mathcal{O}(Q, v_0) = e^{g_{00}} \exp \left[ \int_{v_0}^{-1} dw \frac{\gamma_\mathcal{O}(Q,w) - g_{00}}{\beta_c(Q,w)} \right] \mathcal{O}(Q,-1). \] (40)

Collecting everything together we obtain
\[ \frac{\Delta \mathcal{O}(Q,v)}{\xi_\infty(Q,v)^{d_\Delta + g_{00}}} = C(Q) \exp \int_{v_0}^{-1} dw \frac{\gamma_\mathcal{O}(Q,w) - g_{00}}{\beta_c(Q,w)}, \] (41)

where \( C(Q) \) is an analytic function of \( Q \). For \( Q \to 0 \) we obtain an expansion of the form
\[ \frac{\mathcal{O}(Q,v)}{\xi_\infty(Q,v)^{d_\mathcal{O} + g_{00}}} = a_0 C(Q)[1 + a_1 \sqrt{Q} + a_2 Q + \ldots], \] (42)

where \( a_0 \) and \( a_2 \) depend on nonuniversal details (the starting point \( v_0 \), for instance), while \( a_1 \) is universal, since it only depends on the universal coefficient \( g_{02} \):
\[ a_1 = -\pi g_{02}. \] (43)
The above result can be specialized to the susceptibility, defined as the space integral of the two-point function \[ \chi(q, v) \]. Perturbation theory for the scaling dimension of the spin correlation function gives \[ \gamma = -\frac{1}{4} + \frac{1}{8} \delta - \frac{1}{16} \delta^2 + h_1 \delta^2 + \ldots , \] (44)
where \( h_1 \) is an unknown coefficient. If we perform the redefinitions \((\alpha, \delta) \rightarrow (u, v)\) considered before, we can rewrite \( \gamma \) as
\[ \gamma = -\frac{1}{4} + \frac{1}{8} v - \frac{1}{16} v^2 + g_{20} u^2 \ldots \] (45)
with arbitrary \( g_{20} \). The previous results show that, in the infinite-volume limit, the susceptibility satisfies the scaling law
\[ \chi_{v}^{-7/4} = A(1 + c_1 \sqrt{Q} + c_2 Q + \ldots ) . \] (46)
The coefficient \( c_1 \) can be computed exactly. Since \( g_{02} = -1/16 \), we obtain
\[ c_1 = \frac{\pi}{16} . \] (47)
Using Eq. (59) we can write
\[ \sqrt{Q} = \frac{\pi}{\ln(\xi_{\infty}/X)} + O(\ln^{-2} \xi_{\infty}) \] (48)
and obtain
\[ \chi_{v}^{-7/4} = A \left[ 1 + \frac{\pi^2}{16 \ln(\xi_{\infty}/X)} + O(1/\ln^2 \xi_{\infty}) \right] . \] (49)

As already noted in Ref. [24], RG predicts the absence of a leading logarithmic singular term. Note also that, at variance with what happens with RG invariant quantities, cf. Eq. (55), corrections decay as \( 1/\ln \xi_{\infty} \) and not as \( 1/\ln^2 \xi_{\infty} \). Moreover, the coefficient of the leading logarithmic scaling correction is universal.

We should note that in the literature, see, e.g., [17–21, 22], it was often assumed that the correct scaling behavior is \( \chi_{v}^{-7/4} \sim (\ln \xi_{\infty})^{1/8} \). Such a behavior was derived as follows. Since the two-point function at the critical point scales as \[ 1 \quad 3 \quad 4 \quad G(r) \sim (\ln r)^{1/8}/r^{1/4}, \] it was assumed that
\[ \chi \sim \int_{r<\xi_{\infty}} d^2 r G(r) \sim \xi_{\infty}^{-7/4}(\ln \xi_{\infty})^{1/8} . \] (50)

However, in the presence of logarithmic corrections it is not clear if one should cutoff the integral at \( \xi_{\infty} \), or rather at \( \xi_{\infty}(\ln \xi_{\infty})^{9} \). If we use the latter cutoff we can freely change the leading logarithmic behavior by changing \( q \). In particular, if \( q = -1/4 \), we obtain Eq. (49). The most recent MC simulations of the XY model in the thermodynamic limit confirm the absence of the leading singular term [25]. The analyses of high-temperature expansions have led to apparently contradictory results: the results Ref. [27], are consistent with Eq. (49), while the analysis of Ref. [28] apparently favors the presence of a leading logarithmic correction. On the other hand, we should note that the resummation of high-temperature expansions at finite order can hardly reconstruct an asymptotic behavior at the critical point with logarithmic corrections.

V. FINITE-SIZE SCALING

A. Finite-size scaling in the high-temperature phase

In order to study the FSS regime, we add \( L/b = L e^{-l} \) in the scaling Ansatz. If \( Q \neq 0 \), i.e., we are not at the critical point, we can study the FSS regime as we did in the previous section. If we choose \( l = l_0 \) such that \( v(l_0) = -1 \), we can write
\[ L^{-l_0} = L^{-l(Q,v_0)} = \xi_{\infty}(Q, -1) \times \frac{L}{\xi_{\infty}(Q, v_0)} , \] (51)
where \( \xi_{\infty}(Q, v_0) \) is the infinite-volume correlation length, and \( \xi_{\infty}(Q, -1) \) is an analytic function of \( Q \), which is finite for \( Q \to 0 \). The finite-size correlation length must satisfy the equation
\[ \xi(Q, v_0, L) = e^{l_0} \xi(Q, -1, L e^{-l_0}) . \] (52)
For \( Q \to 0 \), introducing the FSS variable
\[ z \equiv \xi_{\infty}/L , \] (53)
we obtain
\[ \frac{\xi(Q, v_0, L)}{\xi_{\infty}(Q, v_0)} = \frac{\xi(Q, -1, L^{-l_0})}{\xi_{\infty}(Q, -1)} = A(z) + Q B(z) + O(Q^2) . \] (54)

Hence, if we use \( z \) as basic FSS variable, scaling corrections decay as \( 1/\ln^2 \xi_{\infty} \). It is clear that the same arguments apply to any observable, as long as we divide it by its infinite-volume limit. Hence
\[ \frac{O(Q, v_0, L)}{O_{\infty}(Q, v_0)} = \frac{O(Q, -1, e^{-l_0} L)}{O_{\infty}(Q, -1)} = A_0(z) + Q B_0(z) + O(Q^2) . \] (55)

All these relations hold as long as \( z \) is finite. The infinite-volume limit is not uniform in \( z \) and indeed the scaling functions \( A_0(z), B_0(z) \), etc., are singular for \( z \to \infty \). The limiting behavior for \( z \to \infty \), i.e. the asymptotic behavior at the critical point will be discussed in the next section.

B. Finite-size behavior at the critical point

The finite-size behavior at \( T_c \) is not simply obtained by extending the results of Sec. [V.A] to \( T_c \). We consider
the correlation length in a finite box of size $L$, $\xi(Q, v, L)$. For finite $L$, we can take the limit $Q \to 0$ and obtain $\xi(0, v, L)$, which is singular as $L \to \infty$. At $T = T_c$ it is convenient to fix $l = \ln L$, which gives

$$\xi(0, v, L) = e^l \xi[0, v(l), e^{-l}] = L \xi[0, v(L), 1], \quad (56)$$

where $v(L) = v(l = \ln L)$. The function $\xi[0, v(L), 1]$ is analytic for any $L$, since the size is equal to 1, hence we have

$$\xi(0, v, L) = L[s_0 + s_1 v(L) + s_2 v(L)^2 + \ldots], \quad (57)$$

where the coefficients $s_i$ are universal and $v(L)$ is defined by

$$\ln L = \int_{v(L)}^{v_0} \frac{dw}{F(w)[1 + w f(w^2)]}. \quad (58)$$

For $L \to \infty$, the effective coupling $v(L)$ vanishes as $1/\ln L$. In this limit we obtain

$$\ln L = \frac{1}{v(L)} + \frac{b_0}{3} \ln v(L) + K \quad (59)$$

$$- \int_0^{v(L)} dw \left\{ \frac{1}{F(w)[1 + w f(w^2)]} - \frac{1}{w^2 + \frac{b_0}{3w^3}} \right\},$$

where

$$K = \int_{0}^{v_0} dw \left\{ \frac{1}{F(w)[1 + w f(w^2)]} - \frac{1}{w^2 + \frac{b_0}{3w^3}} \right\}. \quad (60)$$

In Eq. (59) all terms are universal, except for the constant $K$, which encodes all microscopic details. If we define

$$\mu \equiv \ln(L e^{-K}), \quad (61)$$

for $v(L) \to 0$ we obtain the expansion

$$\mu = \frac{1}{v(L)} + \frac{b_0}{3} \ln v(L) + \frac{5b_0^2}{18} v(L) + O(v^2). \quad (62)$$

The general solution is

$$v(L) = \frac{1}{\mu} + \sigma_1 \ln \frac{\mu}{\mu^2} + \sigma_2 \ln^2 \frac{\mu}{\mu^3} + \sigma_3 \frac{\ln \mu}{\mu^3} + \sigma_4 \frac{1}{\mu^3} + O(\mu^{-4} \ln^3 \mu), \quad (63)$$

where all coefficients of the expansion are universal, and $\sigma_i$, up to $i = 4$, can be computed in terms of $b_0$ only. The terms of order $\ln^{i-1} \mu/\mu^i$ can be resummed, obtaining

$$v(L) = \frac{1}{\mu} + \frac{b_0}{3} \ln \mu + O(\mu^{-3} \ln \mu). \quad (64)$$

We can rewrite Eq. (64) as

$$\frac{1}{v} \approx \mu - \frac{b_0}{3} \ln v \approx \mu + \frac{b_0}{3} \ln \mu = \mu + \frac{1}{2} \ln \mu. \quad (65)$$

The above results allow us to derive the asymptotic finite-size behavior at $T_c$ of generic RG invariant dimensionless quantities $R$, such as ratios $\xi/L$ for any definition of length scale, Binder cumulants and the helicity modulus $\Upsilon$. They are expected to behave as

$$R(l) = R^* + C_R v(L) + O(v^2) \quad (66)$$

where the $R^*$ and $C_R$ are universal, although they may depend on the shape of the finite volume and the boundary conditions. Then, using Eq. (61), we obtain

$$R \approx R^* + \frac{C_R}{\mu + \frac{1}{2} \ln \mu} + O(\mu^{-2}). \quad (67)$$

This result improves earlier asymptotic expansions, see, e.g., Refs. [15, 48–50]. The asymptotic values $R^*$ and $C_R$ can be computed within the spin-wave theory, as shown in Refs. [15, 48]. For example, in the case of the helicity modulus in a square lattice with periodic boundary conditions, $\Upsilon^* = 0.636508...$ and $C_\Upsilon = 0.318899...$ [15].

An analogous result applies to the exponential correlation length $\xi$, in a strip $L \times \infty$, i.e. for $R_{\xi,c} = \xi_c/L$, with $R_{\xi,c}^* = 4/\pi$ and $C_{\xi,c} = 2/\pi$ [15].

It is worth noting that the behavior of RG invariant quantities at $T_c$ has different features with respect to the infinite-volume case. Here corrections decay as $1/\ln L$, while in the infinite-volume case, see Eq. (65), they decay as $1/(\ln \xi_c)^2$, i.e. with the square of the logarithm of the relevant length scale.

The finite-size behavior of observables $O$ with anomalous RG dimension can be obtained in a similar fashion. We need to compute the behavior of the integral

$$\int_{v_0}^{v(L)} dw \gamma_O(0, w) = \int_{v(L)}^{v_0} dw \frac{\gamma_O(0, w)}{F(w)[1 + w f(w^2)]} = \int_{v_0}^{v(L)} dw \frac{\gamma_O(0, w) - g_00}{F(w)[1 + w f(w^2)]} \quad (68)$$

$$= g_{00} \ln L + g_{01} \ln v(L) + K' + O(v),$$

where $\gamma_O(Q, v)$ is the anomalous dimension as a function of $Q$ and $v$, and $K'$ is a nonuniversal constant. Hence

$$Z[0, v(L)] = L^{g_{00} v(L)^{g_{01}}} e^{K'} [1 + O(v)] Z(0, v_0). \quad (69)$$

We end up with

$$\frac{O(0, v_0, L)}{L^{g_{00}}} = K' \left( \mu + \frac{1}{2} \ln \mu \right)^{g_{01}} [1 + O(\mu^{-1})]. \quad (70)$$

The above results imply that the two-point function at $T_c$ behaves as

$$G(x, y) \approx L^{-1/4} \left( \mu + \frac{1}{2} \ln \mu \right)^{1/8} \mathcal{G}(x/L, y/L). \quad (71)$$

In particular, its space integral, i.e. the susceptibility, scales at the critical point as

$$\chi L^{-7/4} = K' \left( \mu + \frac{1}{2} \ln \mu \right)^{1/8} [1 + O(\mu^{-1})]. \quad (72)$$
where we used \( g_{01} = 1/8 \). A numerical analysis of the 2D XY model providing evidence of the leading multiplicative logarithm is reported in Refs. [13, 10]. Note that a naive integration of the infinite-volume two-point function \( G(r) \) up to \( r \sim L \) would give the same result, \( \chi \sim L^{7/4}/(\ln L)^{1/8} \). The critical-point behavior (72) should be contrasted with Eq. (49): in infinite-volume \( \chi \sim \xi^7/4 \) without additional leading logarithms.

VI. TRAP-SIZE SCALING

Statistical systems are generally inhomogeneous in nature, while homogeneous systems are often an ideal limit of experimental conditions. Thus, in the study of critical phenomena, an important issue is how critical behaviors develop in inhomogeneous systems. Particularly interesting physical systems are interacting particles constrained within a limited region of space by an external force. This is a common feature of recent experiments with diluted atomic vapors [51] and cold atoms in optical lattices [52], which have provided a great opportunity to investigate the interplay between quantum and statistical behaviors in particle systems.

Experimental evidences of BKT transitions in trapped quasi-2D atomic gases have been reported in Refs. [6–11]. The inhomogeneity due to the trapping potential drastically changes, even qualitatively, the general features of the critical behavior. For example, the correlation functions of the critical modes do not develop a diverging length scale in a trap. Nevertheless, when the trap size becomes large the system develops a critical scaling behavior, which can be described in the framework of the TSS theory [37, 53]. TSS has some analogies with the standard FSS for homogeneous systems with two main differences: the inhomogeneity due to the space-dependence of the external field, and a nontrivial dependence of the correlation length on the trap size at the critical point.

The above considerations apply to general quasi-2D systems of interacting bosonic particles trapped by an external harmonic potential. In particular, we mention systems of bosonic cold atoms in quasi-2D optical lattices [52], which can be effectively described [54] by the Bose-Hubbard (BH) model [55]

\[
H_{\text{BH}} = - \frac{J}{2} \sum_{(ij)} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1) - \mu \sum_i n_i,
\]

where \( b_i \) is the bosonic operator, \( n_i = b_i^\dagger b_i \) is the particle density operator, and the sums run over the bonds \( (ij) \) and the sites \( i \) of a square lattice. The phase diagram of the 2D BH model presents finite-temperature BKT transition lines, connecting \( T = 0 \) quantum transitions, such as those from the vacuum state to the superfluid phase, and from the superfluid phase to Mott phases [53]. Experiments with cold atoms [51, 52] are usually performed in the presence of a trapping potential, which can be taken into account by adding a corresponding term in the Hamiltonian:

\[
H_{\text{BH}} = H_{\text{BH}} + \sum_i V(r_i)n_i,
\]

\[
V(r) = w^{p}r^{p},
\]

where \( r \) is the distance from the center of the trap, and \( p \) is a positive even exponent. A natural definition of trap size is provided by

\[
l_t \equiv J^{1/p}/w.
\]

Far from the origin the potential \( V(r) \) diverges, therefore \( \langle n_i \rangle \) vanishes and the particles are trapped. The trapping potential is effectively harmonic in most experiments, i.e. \( p = 2 \).

The trapped 2D BH model has been numerically investigated in Ref. [56], by quantum Monte Carlo simulations, showing that the BKT critical behavior is significantly modified by the presence of the trap. Analogously, an accurate experimental determination of the critical parameters, such as the critical temperature, critical exponents, etc..., in trapped particle systems requires a quantitative analysis of the trap effects. In the following we investigate this issue at the BKT transition and derive the asymptotic TSS behavior from the BKT RG flow.

A. General features of trap-size scaling

Let us first describe the general TSS approach to standard continuous transitions [33], characterized by two relevant parameters \( \tau \) and \( h \) (usually \( \tau \sim T/T_c - 1 \) and \( h \) is the external field coupled to the order parameter), whose RG dimensions are \( y_{\tau} = 1/\nu \) and \( y_h = (d + 2 - \eta)/2 \). The presence of an external space-dependent field \( V(r) = (wr)^{p} \) significantly affects the critical modes, introducing another length scale, the trap size \( l_t \sim 1/w \). Within the TSS framework [37, 53], the scaling of the singular part of the free-energy density around the center of the trap is generally written as

\[
F(x, T, h) = l_t^{-\theta}F(xl_t^{-\theta}, r_t^{-\theta}y_t^{-\theta/\nu}, h_t^{\beta_1}),
\]

where \( r_t \) is the distance from the center of the trap, and \( \theta \) is the trap exponent. TSS implies that at the critical point \( (\tau = 0) \) the correlation length \( \xi \) of the critical modes is finite, but increases as \( \xi \sim l_t^{\theta} \) with increasing the trap size \( l_t \). TSS equations can be derived for the correlation functions of the critical modes. For example, the correlation function of the fundamental field \( \psi(x) \) (the quantum field \( \phi \) in the BH model) is expected to behave as

\[
G(x, y) \equiv \langle \psi(x)\psi(y) \rangle_c = l_t^{-\theta}G(xl_t^{-\theta}, y_l^{-\theta}, \tau_l^{\theta/\nu}),
\]

where \( \theta \) is the trap exponent.
where $G$ is a scaling function.

The trap exponent $\theta$ generally depends on the universality class of the transition, on its space dependence (in experiments the external potential is usually harmonic), and on the way it couples to the particles. Its value can be inferred by an RG analysis of the perturbation $P_V$ representing the external trapping potential coupled to the particle density. The universality class of the superfluid transition can be represented by a $\Phi^4$ theory for a complex field $\psi$ associated with the order parameter, see, e.g., Ref. [42].

$$H_{\Phi^4} = \int d^d x \left[ |\partial_\mu \psi(x)|^2 + r|\psi(x)|^2 + u|\psi(x)|^4 \right]. \quad (79)$$

Since the particle density corresponds to the energy operator $|\psi|^2$, we write the perturbation $P_V$ as

$$P_V = \int d^d x V(x)|\psi(x)|^2. \quad (80)$$

The exponent $\theta$ is related to the RG dimension $y_w$ of the coupling $w$ of the external field $V = (wr)^p$ by $\theta = 1/y_w$. Then, a standard RG argument gives

$$p y_w - p + y_n = d, \quad (81)$$

where $y_n = d - 1/\nu$ is the RG dimension of the density/energy operator $|\psi|^2$. We eventually obtain

$$\theta = \frac{1}{y_w} = \frac{p \nu}{1 + p \nu}. \quad (82)$$

We may derive the value of $\theta$ at the BKT transition by formally setting $\nu = \infty$ in Eq. (82), somehow corresponding to the BKT exponential behavior of the correlation length $\xi \sim \exp(\tau^{-1/2})$, where $\tau = T/T_c - 1 \to 0^+$. This would give $\theta = 1$ for any power $p$ of the potential. This result is also obtained by extending to the BKT transition point the result $\theta = 1$ for the TSS in the whole QLRO phase [53], which can be inferred by a RG analysis of the trap perturbation along the low-temperature line of Gaussian fixed points where spin-wave theory applies.

The trap-size dependence predicted by TSS has been verified at various phase transitions, for example at the Ising transition of lattice gas models [57, 58], at the 3D superfluid transition of bosonic particle systems such as those described by the 3D BH model [55], and at the quantum $T = 0$ Ising and Mott transitions [53, 60-62]. Multiplicative logarithms are generally expected at the upper dimension of the given universality class. We shall show that they also appear at the BKT transition, which should not be surprising because they are already present in the scaling behavior of homogeneous systems, as discussed in the previous sections.

Note that the RG dimension associated with the size $L$ is also 1 (in length units). This might suggest that TSS is analogous to FSS, i.e. characterized by the same power laws and similar multiplicative logarithms. However, as we shall see below, the analysis of the RG flow taking into account the trapping potential shows that the asymptotic trap-size dependence at the BKT transition presents multiplicative logarithms which turn out to depend on the power law of the trapping potential. Therefore, at a BKT transition the TSS relations (77) and (78) must be revised, including multiplicative logarithms, which differ from those observed in the FSS case.

### B. Renormalization-group analysis of trap-size scaling

To investigate the TSS regime, we extend the RG analysis presented above. It is quite obvious that the presence of the trap does not change the short-distance behavior of the model, hence no change should be made on the scaling behavior of the couplings. Let us now consider the flow of the coupling $w$ entering the potential (74), which, in full generality, can have the form

$$\frac{dw}{dl} = \beta_w(u, v, w). \quad (83)$$

If we start from $w = 0$ (no trap), we should always have $w(l) = 0$, hence the $\beta$-function should have the form

$$\beta_w(u, v, w) = w H(u, v, w). \quad (84)$$

Assuming $y_w = \theta^{-1} = 1$, we have

$$H(0, 0, 0) = y_w = 1. \quad (85)$$

In App. C we show that we can define a nonlinear scaling field $z(u, v, w)$ so that the $\beta$-function (84) becomes

$$\beta_z(u, v, z) = z T(Q, v), \quad (86)$$

where, as before, we have replaced $u$ with the RG invariant quantity $Q$ and $T(0, 0) = 1$. The RG flow of $z$ is particularly simple:

$$z(l) = z_0 \exp \left\{ \int_0^l T(Q, v(l))dl' \right\} \quad (87)$$

$$= z_0 e^{\nu l} \exp \left\{ - \int_{v_0}^{v(l)} dw \frac{T(Q, w) - 1}{[Q + F(w)][1 + w f(w^2)]} \right\}, \quad (88)$$

where $z_0 \sim 1/l_4$ is the starting point of the flow. Below, we shall consider two cases: first, we consider the high-temperature phase $T > T_c$, then TSS at the critical point. In both cases, we assume that the infinite-volume limit has been attained, i.e. that $L \gg l_4$.

#### 1. TSS in the high-temperature phase

We start from the general scaling relation for the two-point correlation function

$$G(x, y; Q, v_0, z_0) = Z[Q, v(l)]G[x e^{-l}, y e^{-l}, Q, v(l), z(l)]. \quad (88)$$
Note that the renormalization function $Z(Q, v)$ does not depend on the scaling field $z$, since the renormalization constant is only determined by the short-distance behavior of the operators — the fundamental field in this case — defining the correlation function. As in Sec. IV we fix $l = l_0$ by requiring $v(l_0) = -1$. Then, by using Eq. (80) we can write

$$e^{l_0} = \frac{\xi_\infty(Q, v_0)}{\xi_\infty(Q, -1)} \approx a\xi_\infty(Q, v_0)[1 + O(Q)],$$

where $a = 1/\xi_\infty(Q = 0, -1)$ is a constant. To obtain the trap corrections, we must evaluate $z(l_0)$. Eq. (81) allows us to write

$$z(l_0) = z_0a\xi_\infty(Q, v_0)$$

$$\times \exp \left\{ -\int_{v_0}^{1} dw \frac{T(Q, w) - 1}{[Q + F(w)](1 + w f(w^2))} \right\}.$$  

The integral is finite for $Q \to 0$, with corrections of order $\sqrt{Q}$, see App. B. Hence

$$z(l_0) \sim z_0a\xi_\infty(Q, v_0)[1 + O(Q^{1/2})].$$

Since $l_0 \sim 1/z_0$, we obtain the general scaling form

$$G(x, y; \tau) = G(\xi^{-1}_\infty, y, \xi^{-1}_\infty, t\xi^{-1}_\infty) + O(\sqrt{Q}).$$

2. TSS at the critical point

Let us now consider TSS at criticality ($Q = 0$). In this case it is convenient to fix $l = l_0$ by setting $z(l_0) = 1$. For $l \to \infty$, $v(l) \to 0$, hence we can rewrite Eq. (81) as

$$1 = z_0T_0e^{-l_0}v(l_0)^{-t_1i}[1 + O(v(l_0))],$$

where $t_1$ is defined by the expansion

$$T(0, w) = 1 + t_1 w + O(w^2),$$

and $T_0$ is a nonuniversal constant given by

$$T_0 = v_0^{-t_1} \exp \left\{ \int_{v_0}^{1} dw \left[ \frac{T(0, w) - 1}{F(w)[1 + w f(w^2)]} - t_1 \right] \right\}.$$  

The flow of $v(l)$ follows from Eq. (25). Using the results of Sec. V B and in particular Eq. (59), we have $v(l) = l^{-1} + O(l^{-2} \ln l)$, so we obtain

$$1 = z_0T_0e^{l_1}t_1[1 + O(l^{-1} \ln l)].$$

Inverting this equation we obtain

$$e^{l_1} \approx \frac{\ln z_0T_0}{z_0T_0}. $$

To obtain the scaling behavior, we need to determine the large-$l$ behavior of $Z(0, v(l))$. Using the results of Sec. V B and in particular Eq. (69), we obtain

$$Z(0, v(l)) \approx e^{g_0v(l) - g_0v_0}e^{Kl}Z(0, v_0)$$

$$\approx \frac{\ln z_0T_0}{(z_0T_0)^{g_0}}e^{Kl}Z(0, v_0).$$

Substituting this result into Eq. (88), and choosing the length scale so that $z_0T_0 \approx 1/l + O(l^{-2})$, we obtain the TSS of the two-point function at $T_c$. We write it as (using $g_00 = -1/4$ and $g_01 = 1/8$)

$$G(x, y) = l_0^{-1/4}[(\ln l_0)^{1/8+\kappa/4} \times$$

$$\times G[x(\ln l_0)^\kappa/l_0, y(\ln l_0)^\kappa/l_0],$$

where $\kappa = t_1$.

We may also define the trap susceptibility $\chi_t$,

$$\chi_t = \sum_x G(0, x),$$

and the trap correlation length $\xi_t$,

$$\xi_t^2 = \frac{1}{4\kappa} \sum_x |x|^2 G(0, x).$$

Eq. (99) implies the asymptotic behaviors

$$\chi_t \sim t_1^{7/4}[(\ln l_0)^{1/8-7\kappa/4},$$

$$\xi_t \sim l_0[(\ln l_0)^{-\kappa}].$$

We do not know the value of the coefficient $t_1$ appearing in the expansion (101), which provides the exponent $\kappa$ in the asymptotic formulas. We generally expect that it depends on the power $p$ of the trapping potential. Note that $\kappa$ must vanish in the limit $p \to \infty$. Indeed, in this limit the trapped system is equivalent to a homogenous system confined in a circle of radius $l_0 = 1/w$ with open boundary conditions. Therefore, TSS is equivalent to standard FSS with $L \sim l_0$, hence $\kappa = 0$. We anticipate that the numerical analysis that we present below provides a strong evidence that $\kappa$ depends on $p$; in particular, it suggests $\kappa = 2/p$.

C. Numerical results in the presence of an external space-dependent field

The main features of TSS are expected to be universal, hence the RG results should apply to generic 2D systems characterized by a U(1) symmetry in the presence of an external space-dependent field coupled to the energy density. For a numerical check of the RG predictions, we consider the classical 2D XY model in the presence of an external space-dependent field coupled to the energy density. The Hamiltonian is given by

$$H_U = -J \sum_{(ij)} \text{Re} \bar{\psi}_i U_{ij} \psi_j,$$

$$U_{ij} = [1 + V(r_{ij})]^{-1}, \quad V(r) = w^p r^p,$$  

where $p$ is an even positive integer, $r_{ij}$ is the distance from the origin of the midpoint of the lattice link connecting the nearest-neighbor sites $i$ and $j$. We set $J = 1$. The inhomogeneity arising from the space dependence of
$U_{ij}$ is analogous to that arising from a trapping potential in particle systems. Thus, $l_t \equiv 1/w$ may be considered as the analog of the trap size \((79)\). For $p \to \infty$, $V(r) = 0$ for $r < l_t$ and $V(r) = \infty$ for $r > l_t$. Hence, the system is equivalent to a homogeneous system confined in a circle of radius $l_t$ with open boundary conditions. Therefore, in this limit TSS must reproduce standard FSS. A study of the trap effects in the low-temperature phase is reported in Ref. \([57]\). Here we focus on the trap-size dependence at the BKT critical temperature $T_c = 0.89294(8) \[14, 15\]$ of the homogeneous XY model \([1\]) which is also the model \([104]\) with $U_{ij} = 1$.

We present results of Monte Carlo (MC) simulations of model \([104]\). We use a mixture of Metropolis and over-relaxation updates of the spin variables \([50]\). We consider square lattices with $L^2$, odd $L$, sites and open boundary conditions. Lattice points have coordinates $(x, y)$ with $-(L-1)/2 \leq x, y \leq (L-1)/2$, so that the origin $(0, 0)$ is at the center of the lattice. The external potential is given by $V(x) = (r/l_t)^p$, where $r \equiv |x|$ and $l_t$ is the trap size. The lattice size $L$ is taken sufficiently large to avoid finite-size effects. We check that they are negligible compared with the statistical errors by comparing results at fixed trap size $l_t$ for different lattice sizes $L$.

We want to check the TSS equation \([103]\) for the correlation function at $T_c$. For this purpose we report results at $T_c$ for the correlation function $G(0, x) \equiv \langle \psi(0)\psi(x) \rangle$, which is expected to scale as

$$G(0, x) = l_t^{-1/4}(\ln l_t)^{1/8+\kappa/4} G_p \left[r(\ln l_t)^\kappa/l_t \right],$$

where $r \equiv |x|$, and the exponent $\kappa$ is expected to depend on the power of the external potential.

We first check the FSS behavior of the homogeneous XY model with open boundary conditions (OBC), which is formally equivalent to the limit $p \to \infty$ of model \([105]\) with $L = 2l_t + 1$ and $l_t$ integer. Note that translation invariance is lost in systems with OBC. Fig. 3 shows the data for $x = (r, 0)$, which clearly support the expected

$$G(0, x) = L^{-1/4}(\ln L)^{1/8}g(x/L).$$

Note that OBC breaks translation invariance, and gives rise to power-law boundary corrections \([16, 17]\) which are expected to be $O(L^{-1})$. In Figs. 3 and 4 we show the results of the simulations for two different values of $p$, $p = 2$ and $p = 4$. In order to check the scaling behavior \([106]\), we present TSS plots with $\kappa = 0$, using the analog of the FSS formula \([107]\), and with an optimal nonzero value of the coefficient $\kappa$, which is determined by looking for the best collapse of the data. Optimal scaling is obtained by setting $\kappa \approx 1$ for $p = 2$ and $\kappa \approx 1/2$ for $p = 4$, with an uncertainty which we estimate to be approximately $10\%$. This simple scaling test clearly favors a nonzero $p$-dependent value for $\kappa$. Taking also into account that $\kappa = 0$ for $p \to \infty$, the above numerical results hint at the simple formula $\kappa = 2/p$. These results should be universal, hence they also apply to the BKT transitions of general systems of 2D interacting bosonic particles trapped by an external space-dependent potential, such as those which have been investigated experimentally \([7, 11, 52]\).

Finally, in Fig. 4 we compare the scaling functions associated with $G(0, x)$ for $p = 2$, $p = 4$, and for the homogeneous system with OBC. We plot $G_{\tau}(x) \equiv$ 1.0, 0.2, 0.4, 0.6, 0.8, 1.0
VII. CONCLUSIONS AND SUMMARY OF THE MAIN RESULTS

We have investigated the general features of the RG flow at the BKT transition, providing a definite characterization of the asymptotic critical behavior including the universal multiplicative or subleading logarithmic corrections, in different critical regimes: (i) in the infinite-volume critical disordered phase; (ii) in the FSS limit, both for $T > T_c$ and $T = T_c$; (iii) in the TSS limit, again both above and at the critical temperature.

For this purpose, we exploit the mapping between the standard XY or Coulomb gas models and the SG model, whose RG flow around the renormalizable fixed point describes the BKT transition \[34\]. To determine the RG flow, we first derive a simple canonical universal expression for the $\beta$-functions. Then, we determine the asymptotic solutions of the RG equations in the different situations mentioned above. For the TSS case, numerical simulations confirm the RG predictions.

We summarize our main results:

(a) We prove that an appropriate analytical redefinition of the couplings of the SG model, cf. Eq. (11), allows us to write the $\beta$-functions as

$$\beta_u(u, v) = -uv,$$
$$\beta_v(u, v) = -u^2[1 + vf(v^2)],$$

to all orders of perturbation theory. The universal function $f(x)$ can be expanded as $f(x) = b_0 + b_1 x + b_2 x^2 + \ldots$. The zeroth-order term $b_0 = 3/2$ can be obtained from the two-loop results of Refs. \[34, 43\], while the next coefficient $b_1$ can only be determined by means of a four-loop calculation in the SG model. In practice, our results extend the knowledge of the RG flow of the SG model to three loops. Under the same redefinition of the couplings, the anomalous dimension $\gamma(u, v)$ of the fundamental field becomes $\gamma = -1/4 + v/8 - v^2/16 + g_{20} u^2 + \ldots$, where $g_{20}$ is a nonuniversal constant which does not enter the universal scaling behavior of the two-point function.

(b) In the high-temperature critical regime and in the infinite-volume limit, the RG flow implies the BKT asymptotic behavior (setting $T = T_c - 1$) \[11\]

$$\xi_\infty(\tau) = X e^{c/\sqrt{\tau}} \; [1 + O(\sqrt{\tau})],$$

for the infinite-volume correlation length, where $X$ is a nonuniversal constant. In the case of RG invariant quantities $R$, such as the ratio of two different definitions of correlation lengths and the zero-momentum four-point renormalized coupling \[33\], we have

$$R(\tau) = R^* + O(1/\ln^2 \xi_\infty).$$

Corrections of order $1/\ln \xi_\infty$ are absent. The susceptibility, defined as the space-integral of the two-point function...
of the fundamental field, behaves as
\[ \chi = A_\chi e^{7/4} \left[ 1 + \frac{\pi^2}{16 \ln(\xi/\sqrt{X})} + O \left( \frac{1}{\ln^2 \xi} \right) \right] \]  \hspace{1cm} (111)
where \( A_\chi \) is a nonuniversal constant. The correction term behaving as \( 1/\ln \xi \) is universal.

(c) We have studied the FSS behavior. In the high-temperature phase, for any observable \( \mathcal{O} \), the ratio \( \mathcal{O}(L)/\mathcal{O}(L \to \infty) \) approaches a universal function \( \mathcal{A}(L/\xi) \) with \( O(1/\ln^2 L) \) corrections. The approach to the \( L \to \infty \) limit is not uniform in \( T \). At \( T = T_c \), further logarithms appear. Indeed, setting \( \mu \equiv \ln(L/\lambda) \) where \( \lambda \) is an appropriate nonuniversal length scale, we have
\[ R_\xi = R_\xi^* + \frac{C_\xi}{\mu + \frac{1}{2} \ln \mu} + O(\mu^{-2}), \]  \hspace{1cm} (112)
where \( R_\xi^* \) and \( C_\xi \) are universal, depending only on the shape of the systems and their boundary conditions. An analogous formula is obtained for any RG invariant quantity, such as the helicity modulus and the Binder cumulant. Moreover, the asymptotic behavior of the susceptibility reads
\[ \chi L^{-7/4} = \hat{A}_\chi \left[ \mu + \frac{1}{2} \ln \mu \right]^{1/8} \left[ 1 + O(\mu^{-1}) \right], \]  \hspace{1cm} (113)
where \( \hat{A}_\chi \) is a nonuniversal constant. Note two important differences between the behavior at \( T_c \) and in the high-temperature critical regime (b). For RG invariant quantities corrections decay as \( 1/\ln L \) in the first case; in the second one corrections of order \( 1/\ln \xi \) are instead absent. Second, the behavior of the susceptibility is characterized by a leading logarithmic term at \( T_c \), while no such term is present in the high-temperature case, see Eq. \( \text{(111)} \).

(d) Finally, we consider BKT transitions in 2D interacting bosonic particles which are trapped within a limited region of space by an external space-dependent force, which is a common feature of experiments with diluted atomic vapors and cold atoms in optical lattices. We investigate how the BKT critical behavior is affected by the presence of the external space-dependent trapping potential \( V(r) = (r/l_t)^p \) coupled to the particle (energy) density. We consider observables derived from the two-point function \( G(x,y) \) of the fundamental field describing the critical modes, such as the one-particle correlation function \( \langle b_1 b_2 \rangle \) of the BH model, which describes trapped bosonic atoms in an optical lattice. The analysis of the RG flow shows that TSS at the BKT transitions is characterized by a trap exponent \( \theta = 1 \), with additional multiplicative logarithms at \( T = T_c \). For example, at \( T_c \) the two-point function scales as
\[ G(0,x) = l_t^{-1/4} \ln(l_t) \left[ 1 + \sum_{n,m} b_{\alpha,nm} \alpha^n \delta^m \right], \]  \hspace{1cm} (114)
where \( \kappa \) is a new exponent which arises from the analysis of the RG flow of the external potential and which is expected to depend on the power \( p \) characterizing the trap potential. Of course, in the limit \( p \to \infty \) we must have \( \kappa = 0 \), since we must recover the known FSS behavior of a homogeneous system. The scaling equation \( \text{(114)} \) implies also that the correlation length \( \xi_t \) of the critical modes behaves asymptotically as
\[ \xi_t \sim l_t \ln(l_t)^{-\kappa}. \]  \hspace{1cm} (115)
These results are supported by Monte Carlo simulations of a 2D XY model with a space-dependent potential coupled to the energy density. They provide a clear evidence of the multiplicative logarithms in Eqs. \( \text{(114)} \) and \( \text{(115)} \) and are numerically consistent with the conjecture \( \kappa = 2/p \).

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Appendix A: Canonical form of the BKT \( \beta \)-functions

In the following we prove that the SG \( \beta \)-functions can be simplified by a redefinition of the couplings, reducing them to the canonical form given by Eqs. \( \text{(17)} \) and \( \text{(18)} \). For a general discussion of the mathematical problem of the reduction of coupled differential equations to canonical form, see, e.g., Refs. \[ \text{[63, 64]} \].

To all orders in the couplings \( \alpha \) and \( \delta \), the \( \beta \)-functions of the SG model have the generic form
\[ \beta_\alpha = -2\alpha \delta + \sum_{n+m>2} b_{\alpha,nm} \alpha^n \delta^m, \]  \hspace{1cm} (A1)
\[ \beta_\delta = -\frac{1}{32} \alpha^2 + \sum_{n+m>2} b_{\delta,nm} \alpha^n \delta^m. \]  \hspace{1cm} (A2)
In the SG model the sign of \( \alpha \) is irrelevant, which implies the symmetry relations
\[ \beta_\alpha(\alpha, \delta) = -\beta_\alpha(-\alpha, \delta), \]  \hspace{1cm} (A3)
\[ \beta_\delta(\alpha, \delta) = \beta_\delta(-\alpha, \delta). \]  \hspace{1cm} (A4)
As a consequence, \( b_{\alpha,nm} = 0 \) if \( n \) is even and \( b_{\delta,nm} = 0 \) if \( n \) is odd. Moreover, for \( \alpha = 0 \) the theory is free and \( \delta \) does not flow. Hence
\[ \beta_\delta(\alpha = 0, \delta) = 0, \]  \hspace{1cm} (A5)
which implies \( b_{\delta,nm} = 0 \) if \( n = 0 \).

We wish now to prove that, by an analytic redefinition of the couplings,
\[ \alpha = a_{\alpha,10} u + \sum_{n+m \geq 2} a_{\alpha,nm} u^n v^m, \]  \hspace{1cm} (A6)
\[ \delta = a_{\delta,10} v + \sum_{n+m \geq 2} a_{\delta,nm} u^n v^m, \]  \hspace{1cm} (A7)
we can rewrite the $\beta$-functions of the SG model in the form
\[
\beta_u(u, v) = -uv, \quad \beta_v(u, v) = -u^2 \left(1 + \sum_{k=0}^{\infty} b_k v^{2k+1}\right).
\] (A8)

To prove the general result, we shall work by perturbative induction. We assume that we have already proved the result to order $n - 1$, i.e. that we redefined couplings so that
\[
\beta_u = -uv + u \sum_{k=0}^{\infty} H_{k-1}(u, v),
\] (A9)
\[
\beta_v = -u^2 \left(1 + \sum_{k=0}^{m-2} b_k v^{2k+1}\right) + u^2 \sum_{k=0}^{\infty} G_{k-2}(u, v),
\]
where $m = \lfloor n/2 \rfloor$, and $H_k(u, v)$ and $G_k(u, v)$ are homogeneous polynomials satisfying
\[
H_k(\lambda u, \lambda v) = \lambda^k H_k(u, v), \quad G_k(\lambda u, \lambda v) = \lambda^k G_k(u, v).
\] (A10)

Moreover, they are even functions of $u$. We now consider the change of variables
\[
u' = u + u A_{n-2}(u, v),
\] (A11)
\[
u'' = v + B_{n-1}(u, v),
\]
where $A_{n-2}(u, v)$ and $B_{n-1}(u, v)$ are homogeneous polynomials even in $u$ and satisfying
\[
A_{n-2}(\lambda u, \lambda v) = \lambda^{n-2} A_{n-2}(u, v),
\]
\[
B_{n-1}(\lambda u, \lambda v) = \lambda^{n-1} B_{n-1}(u, v).
\] (A12)

We wish to show that, by a proper choice of $A_{n-2}$ and $B_{n-1}$, we can cancel all terms of order $n$ except, if $n$ is odd, the term of order $u^2 v^{n-2}$ in $\beta_v$. Hence we can obtain
\[
\beta_{u'}(u', v') = -u' v' + u' \sum_{k=n+1}^{\infty} \tilde{H}_{k-1}(u', v'),
\] (A13)
\[
\beta_{v'}(u', v') = -u'^2 \left(1 + \sum_{k=0}^{m'-2} b_k v'^{2k+1}\right)
+ u'^2 \sum_{k=n+1}^{\infty} \tilde{G}_{k-2}(u', v'),
\]
with different \( \tilde{H} \) and \( \tilde{G} \) and \( m' = \lfloor (n + 1)/2 \rfloor \).

Requiring all terms (except the one mentioned above) to cancel, we obtain the equations
\[
u A_{n-2} + u B_{n-1} - uv \frac{\partial (u A_{n-2})}{\partial u} = 0
\] (A14)
\[
u^2 \frac{\partial A_{n-2}}{\partial v} + u H_{n-1} = 0
\]

and
\[
2u^2 A_{n-2} - uv \frac{\partial B_{n-1}}{\partial u} - u^2 \frac{\partial B_{n-1}}{\partial v} + u^2 G_{n-2} = R_n
\] (A15)

where $R_n = 0$ for $n$ even, and $R_n = b_{(n-3)/2} u^2 v^{n-2}$ if $n$ is odd. Eq. (A14) gives us the function $B_{n-1}$:
\[
B_{n-1} = u \frac{\partial A_{n-2}}{\partial u} + u v \frac{\partial A_{n-2}}{\partial v} - H_{n-1}.
\] (A16)

Substituting it in Eq. (A15), we obtain
\[
u^2 v \frac{\partial^2 A_{n-2}}{\partial u^2} + 2u^3 v \frac{\partial^2 A_{n-2}}{\partial u \partial v} + u^4 \frac{\partial^2 A_{n-2}}{\partial v^2} + \nu (u^2 + v^2) \frac{\partial A_{n-2}}{\partial u} + 2u^2 v \frac{\partial A_{n-2}}{\partial v} - 2u^2 A_{n-2} - R_n
= u^2 G_{n-2} + u v \frac{\partial H_{n-1}}{\partial u} + v \frac{\partial H_{n-1}}{\partial v}.
\] (A17)

Now, we expand
\[
A_{n-2}(u, v) = \sum_{k=0}^{n-2} a_k u^k v^{n-2-k}
\] (A18)

with $a_k = 0$ for $k$ odd. Then, we must show that we can find $a_0, a_2, \ldots$, so that the following equations are satisfied. For $k$ even, with $k \geq 4$ and $k < n - 1$, we must satisfy
\[
E_k = -k^2 a_k + (4 - 3k + 2k^2 + 2n - 2kn) a_{k-2}
- (2 + k^2 + 3n + n^2 - k(3 + 2n) a_{k-4} - \tilde{g}_k = 0.
\]

Here $\tilde{g}_k$ is the coefficient of order $u^k v^{n-k}$ in the expansion of the r.h.s. of Eq. (A17). Moreover, we should satisfy
\[
E_n = (4 - n) a_{n-2} - 2a_{n-4} - \tilde{g}_n = 0 \quad \text{n even},
\]
\[
E_{n-1} = 3(3 - n) a_{n-3} - 6a_{n-5} - \tilde{g}_{n-1} = 0 \quad \text{n odd},
\]
\[
E_2 = 2(3 - n) a_0 - 4a_2 - \tilde{g}_2 = 0 \quad \text{n even}.
\]

$E_2$ cannot be satisfied for $n$ odd—hence the necessity for the coefficients $b_k$, which are defined by
\[
b_{(n-3)/2} = E_2 = 2(3 - n) a_0 - 4a_2 - \tilde{g}_2.
\] (A19)

We now redefine $a_{2k}$ for $k \geq 1$ as
\[
a_{2k} = \frac{(-1)^k}{k!} a_0 \prod_{j=1}^{k} \left(\frac{n-1}{2} - j\right) + c_{2k}.
\] (A20)

With this redefinition, we obtain
\[
E_4 = 6(4 - n) c_2 - 16c_4 - \tilde{g}_4 = 0
\] (A21)
\[
E_k = -k^2 c_k + (4 - 3k + 2k^2 + 2n - 2kn) c_{k-2}
- (2 + k^2 + 3n + n^2 - k(3 + 2n) c_{k-4} - \tilde{g}_k = 0,
\]

where $6 \leq k < n - 1$. For $n$ even we should also consider
\[
E_2 = -4c_2 - \tilde{g}_2 = 0,
\] (A22)
\[
E_n = p_n a_0 + (4 - n)c_{n-2} - 2c_{n-4} - \tilde{g}_n = 0,
\]
where
\[ p_n = \frac{2(-1)^{n/2}}{\sqrt{\pi} (2 - n)(n/2 - 2)!} \Gamma(n/2 - 1/2), \quad (A23) \]
while for odd \( n \) we also have
\[ E_{n-1} = 3(3 - n)c_{n-3} - 6c_{n-5} - \tilde{g}_{n-1} = 0. \quad (A24) \]
The parameter \( b_{(n-3)/2} \) is defined by (odd)
\[ b_{(n-3)/2} = E_2 = -4c_2 - \tilde{g}_2. \quad (A25) \]
For \( n \) even it is evident that all equations can be solved. \( E_n \) can be satisfied by fixing \( a_0 \), while \( E_k, k \leq n - 2 \), can be satisfied by fixing \( c_k \). For odd one, \( a_0 \), is no longer present: this explains why we are not able to satisfy all equations and we need to introduce the parameter \( b_{(n-3)/2} \). In practice, we can satisfy \( E_n \) by fixing \( c_4 \) as a function of \( c_2 \), \( E_6 \) by fixing \( c_6 \) and so on. This allows us to solve all equations except \( E_n \). However, there is still one free parameter, \( c_2 \). Substituting the expression of \( c_{n-2} \) and \( c_{n-4} \) as a function of \( c_2 \), we obtain \( E_n = \alpha_1 c_2 + \alpha_2 \), with
\[ \alpha_1 = \frac{(-1)^{(n-3)/2}(7-n)/2(n-2)!!}{(n/2 - 3/2)!}. \quad (A26) \]
Since \( \alpha_1 \neq 0 \), also \( E_n \) can be satisfied, concluding the proof.

**Appendix B: Asymptotic expansions**

We wish now to discuss the computation of the asymptotic behavior of integrals of the form
\[ I = \int_a^b dw \frac{h(w)}{Q + F(w)}, \quad (B1) \]
where \( b > a \), \( h(w) \) and \( F(w) \) are analytic functions and \( F(w) \approx w^2 \) for \( w \to 0 \). The integral \( I \) diverges as \( Q \to 0 \) if \( h(0) \neq 0 \). The leading behavior can be computed by approximating \( F(w) \approx w^2 \):
\[ I \approx \int_a^b dw \frac{h(0)}{Q + w^2} \approx \pi h(0) \sqrt{Q}. \quad (B2) \]
To compute the next nonanalytic term in the expansion, we consider
\[ J = \int_a^b dw \frac{h(w)}{(Q + F(w))^2}. \quad (B3) \]
If \( x = w/\sqrt{Q} \), we consider the expansion in powers of \( \sqrt{Q} \) at fixed \( x \):
\[ \frac{h(x\sqrt{Q})}{(Q + F(x\sqrt{Q}))^2} = \sum_{n=-4} Q^{n/2} g_n(x), \quad (B4) \]
We define
\[ G(x, Q) = \sum_{n=-4} Q^{n/2} g_n(x), \quad (B5) \]
i.e. the sum of the terms that diverge as \( Q \to 0 \), and
\[ g(w) = \lim_{Q \to 0} G(w/\sqrt{Q}, Q) \quad (B6) \]
where the limit is taken at fixed \( w \). It is easy to convince oneself that \( g(w) \) gives the principal part of the Laurent series of \( h(w)/F(w)^2 \), so that \( h(w)/F(w)^2 - g(w) \) is finite for \( w \to 0 \). We can thus rewrite
\[ J = \int_a^b dw \left\{ \frac{h(w)}{(Q + F(w))^2} - G(w/\sqrt{Q}, Q) \right\} \]
\[ + \int_a^b dw G(w/\sqrt{Q}, Q). \quad (B7) \]
The first integral is finite as \( Q \to 0 \), hence it does not contribute to the singular part of \( J \). We can thus limit ourselves to considering the second term which can be rewritten as
\[ J \approx \int_{a/\sqrt{Q}}^{b/\sqrt{Q}} dx \left[ Q^{-3/2} g_{-4}(x) + Q^{-1} g_{-3}(x) + \right. \]
\[ + \left. Q^{-1/2} g_{-2}(x) + g_{-1}(x) \right]. \quad (B8) \]
For \( x \to \infty \), we have \( g_{-n}(x) \sim x^{-n} \) (it is easy to prove it, using the fact that the expansion \( (B4) \) is indeed in powers of \( x/\sqrt{Q} \)). This implies that
\[ \int_{a/\sqrt{Q}}^{b/\sqrt{Q}} dx g_{-n}(x) \approx \int_{-\infty}^{\infty} dx g_{-n}(x) + O(Q^{(n-1)/2}) \quad (B9) \]
for \( n = 2, 3, 4 \). For \( n = 1 \) we must be a little more careful. Assume that \( g_{-1}(x) \approx g_{-1,\infty}/x \) for \( x \to \infty \). Then,
\[ \int_{a/\sqrt{Q}}^{b/\sqrt{Q}} dx g_{-1}(x) = \int_{a/\sqrt{Q}}^{b/\sqrt{Q}} dx \left[ g_{-1}(x) - g_{-1,\infty} x \right] + \int_{a/\sqrt{Q}}^{b/\sqrt{Q}} dx \frac{g_{-1,\infty} x}{1 + x^2} \quad (B10) \]
The first integral now decays as \( 1/x^2 \), hence we can extend the integration limits to \( \pm \infty \) with corrections of order \( 1/x^2 \): the second can be computed exactly and is finite for \( Q \to 0 \). Hence the singular part of \( J \) is given by
\[ J \approx \int_{-\infty}^{+\infty} dx \left[ Q^{-3/2} g_{-4}(x) + Q^{-1} g_{-3}(x) + \right. \]
\[ + \left. Q^{-1/2} g_{-2}(x) + g_{-1}(x) - g_{-1,\infty} x \right]. \quad (B11) \]
Using again the fact that the expansion \( (B4) \) is in powers of \( x/\sqrt{Q} \), we observe the \( g_{2n}(x) \) is even under \( x \to -x \), while \( g_{2n+1}(x) \) is odd. We obtain finally
\[ J = J_{-3/2} Q^{-3/2} + J_{-1/2} Q^{-1/2} + O(1), \quad (B12) \]
with

\[ J_{-3/2} = \int_{-\infty}^{+\infty} dx \, g_{-4}(x), \quad (B13) \]

\[ J_{-1/2} = \int_{-\infty}^{+\infty} dx \, g_{-2}(x). \quad (B14) \]

If we now write \( F(w) = w^2 + \sum_{n \geq 3} F_n w^n \), \( h(w) = \sum_n h_n w^n \), we obtain

\[ J_{-3/2} = \frac{\pi h_0}{2}, \quad (B15) \]

\[ J_{-1/2} = \frac{\pi}{16} (15 F_3^2 h_0 - 12 F_4 h_0 - 12 F_3 h_1 + 8 h_2). \]

From the expansion of \( J \) we can easily derive the expansion of \( I \):

\[ I = I_{-1/2} Q^{-1/2} + I_0 + I_{1/2} Q^{1/2} + O(Q), \quad (B16) \]

with \( I_{-1/2} = 2 J_{-3/2} \) and \( I_{1/2} = -2 J_{-1/2} \).

### Appendix C: The canonical form of the trap \( \beta \)-function

We wish now to prove that the trap \( \beta \)-function can be rewritten as in Eq. (80). As in App. A we work by perturbative induction. We assume that we have proved the result at order \( n - 1 \), i.e. that the \( \beta \)-function has the form

\[ \beta_w(u, v, w) = w T(u, v) + w^2 \sum_{k=n} H_{k-2}(u, v, w), \quad (C1) \]

where \( T(0, 0) = 1 \) and \( H_k(u, v, w) \) are homogeneous polynomials of order \( k \), i.e. satisfy

\[ H_k(\lambda u, \lambda v, \lambda w) = \lambda^k H_k(u, v, w). \quad (C2) \]

Then, we perform the change of variables

\[ z = w + w G_{n-1}(u, v, w), \quad (C3) \]

where \( G_k(u, v, w) \) is homogeneous polynomial of degree \( k \). If we now compute the \( \beta \)-function associated with \( z \),

\[ \beta_z(u, v, z) = \frac{dz}{dt}, \quad (C4) \]

we obtain

\[ \beta_z = z T(u, v) + z^2 \left[ H_{n-2}(u, v, z) + \frac{\partial G_{n-1}}{\partial z} \right] \quad (C5) \]

where we neglect terms of order \( n + 1 \) in the variables. Hence, if we define

\[ G_{n-1}(u, v, w) = - \int_0^w dx H_{n-2}(u, v, x), \quad (C6) \]

where the integral is performed at fixed \( u \) and \( v \), we cancel all unwanted terms, proving the result.

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