Correlation function distributions for O(N) lattice field theories in the disordered phase

Cagin Yunus^{1,*} and William Detmold^{1,2,†}

¹Center for Theoretical Physics, Massachusetts Institute of Technology,

Cambridge, Massachusetts 02139, USA

²The NSF Institute for Artificial Intelligence and Fundamental Interactions, Cambridge, Massachusetts

01239, USA

(Received 21 June 2023; accepted 12 December 2023; published 16 February 2024)

Numerical computations in strongly interacting quantum field theories are often performed using Monte Carlo sampling methods. A key task in these calculations is to estimate the value of a given physical quantity from the distribution of stochastic samples that are generated using the Monte Carlo method. Typically, the sample mean and sample variance are used to define the expectation values and uncertainties of computed quantities. However, the Monte Carlo sample distribution contains more information than these basic properties, and it is useful to investigate it more generally. In this work, the exact form of the probability distributions of two-point correlation functions at zero momentum in O(N) lattice field theories in the disordered phase and in infinite volume are determined. These distributions allow for a robust investigation of the efficacy of the Monte Carlo sampling procedure and are shown also to allow for improved estimators of the target physical quantity to be constructed. The theoretical expectations are shown to agree with numerical calculations in the O(2) model.

DOI: 10.1103/PhysRevD.109.034512

I. INTRODUCTION

Quantum field theories (QFTs) are used pervasively in theoretical particle, nuclear, and condensed-matter physics to describe a wide range of physical phenomena. In many cases, these QFTs are strongly interacting, and numerical methods are needed in order to make predictions. In many cases, the only effective numerical approach is to discretize and compactify spacetime and use importance-sampling Monte Carlo to estimate the Euclidean path integrals that result. In many situations, this is a stochastically challenging task; numerical results for correlation functions between fields at different points usually exhibit signalto-noise ratios that degrade exponentially in the separation between the points. This makes extraction of physical information such as the masses of excitations of the theory difficult. To confront these difficulties, various strategies for the reduction of variance in the Monte Carlo procedure have been pursued [1-15]. Previous works have also investigated the nature of statistical fluctuations in specific

cyunus@mit.edu wdetmold@mit.edu QFTs empirically [16–23]. In Ref. [24], the first analytic insights into the structure of the probability distribution functions (PDFs) of correlation functions were presented in the context of a scalar field theory. In general, knowledge of the probability distributions can lead to more efficient estimators of the mean.¹ In the context of Monte Carlo sampling, knowledge of the PDF can also allow for statistical tests of thermalization and autocorrelation of the samples.

In this work, the PDFs of two-point correlation functions in the lattice O(N) model in the disordered phase at vanishing spatial momentum will be calculated, significantly extending the results in Ref. [24]. O(N) models are a generalization of the Ising model and have been studied extensively since their initial definition in Ref. [25]. These models exhibit many important phenomena; for example, in two dimensions, the O(2) model features a Berezinskii-Kosterlitz-Thouless transition at low temperatures, while O(N) models for N > 2 are asymptotically free and are therefore strongly coupled at long distances (see Ref. [26] for a review). In any dimension, the O(N) model reduces to a self-avoiding random walk as $N \rightarrow 0$ as first demonstrated in Ref. [27]. The O(N) model therefore provides an

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¹For example, for a uniform distribution on the interval [0, a] for a > 0, the minimum-variance unbiased estimator of the mean, $\hat{\mu}_{U,mvue} = \frac{N+1}{2N} \max_i x_i$, can be shown to outperform the sample mean by using specific properties of the PDF.

interesting testing ground for extensions of the previous work on PDFs of correlation functions and forms the central basis of this work.

The structure of this work is as follows. In Sec. II, the probability distributions of two-point correlation functions at vanishing spatial momentum are calculated for a free complex scalar field, equivalent to the O(2) model. In Sec. III, this is extended to the case of interacting O(N) models in the disordered phase, and the derived form is shown to hold at all temporal separations of the correlation function. In Sec. IV, numerical results are presented for interacting O(2) models in two dimensions in the disordered phase. These results confirm the predictions of Sec. III and provide support for the assumptions needed to derive the distributions. Using the PDFs of two-point correlation functions in the O(2) model, an improved estimator of the mean is constructed in Sec. V. Section VI summarizes the results and presents an outlook.

II. FREE COMPLEX FIELD

To introduce the calculation of correlation function probability distributions, the case of a single free complex scalar field is first discussed, generalizing the discussion of the real scalar field in Ref. [24]. Let $\psi(t, \vec{x}) = \phi_1(t, \vec{x}) + i\phi_2(t, \vec{x})$ be a free complex field, where $\phi_i(t, \vec{x}) \in \mathbb{R}$. A d + 1-dimensional free Euclidean lattice field theory will be considered with L being the size of each of the spatial directions in lattice units and β being the size of the temporal direction. For a free lattice field theory, volume averaged² fields $\bar{\phi}_i(t)$ will decouple from other modes due to momentum conservation. Therefore, the partition function for this sector of the theory can be written as

$$Z = \int \mathcal{D}\bar{\phi}_1 e^{-\frac{1}{2}\bar{\phi}_1^T D\bar{\phi}_1} \int \mathcal{D}\bar{\phi}_2 e^{-\frac{1}{2}\bar{\phi}_2^T D\bar{\phi}_2}, \qquad (1)$$

where the vector notation

$$\bar{\phi}_{1,2} = \begin{pmatrix} \bar{\phi}_{1,2}(0) \\ \cdots \\ \bar{\phi}_{1,2}(\beta - 1) \end{pmatrix}$$
(2)

is used, with $\mathcal{D}\bar{\phi}_i = \prod_{i'=0}^{\beta-1} d\bar{\phi}_i(t')$. *D* is a real symmetric matrix arising from the kinetic operator after integrating over the nonzero momentum modes; the exact form of *D* is not relevant in what follows. Since all integrals are Gaussian, one may choose to integrate out all of the field variables except $\bar{\phi}_1(0)$, $\bar{\phi}_1(t)$, $\bar{\phi}_2(0)$, and $\bar{\phi}_2(t)$ (in what follows, only the temporal separation between the fields is

important, so the temporal location of one pair of fields is chosen to be at 0 without loss of generality). The partition function can then be expressed as

$$Z = \mathcal{N}(t) \int d\bar{\phi}_1(0) d\bar{\phi}_1(t) d\bar{\phi}_2(0) d\bar{\phi}_2(t)$$

$$\times \exp\left(-\frac{\sigma_f^2}{2} \frac{(\bar{\phi}_1(0)^2 + \bar{\phi}_1(t)^2 + \bar{\phi}_2(0)^2 + \bar{\phi}_2(t)^2)}{\sigma_f^4 - K_f(t)^2}\right)$$

$$\times \exp\left(\frac{K_f(t)}{\sigma_f^4 - K_f(t)^2} (\bar{\phi}_1(0)\bar{\phi}_1(t) + \bar{\phi}_2(0)\bar{\phi}_2(t))\right), \quad (3)$$

where

$$\sigma_f^2 = \langle \bar{\phi}_1(0)\bar{\phi}_1(0) \rangle = \langle \bar{\phi}_2(0)\bar{\phi}_2(0) \rangle,$$

$$K_f(t) = \langle \bar{\phi}_1(t)\bar{\phi}_1(0) \rangle = \langle \bar{\phi}_2(t)\bar{\phi}_2(0) \rangle,$$
(4)

and the normalization factor $\mathcal{N}(t)$ can be calculated by performing the remaining Gaussian integrals exactly and imposing that Z = 1:

$$\mathcal{N}(t) = \frac{1}{(2\pi)^2 (\sigma_f^4 - K_f(t)^2)}.$$
(5)

For Z defined by Eq. (3) to be finite, the condition $K_f(t) < \sigma_f^{-2}$ must be satisfied. Furthermore, the inequality $K_f(t) > 0$ follows from the reflection positivity and Eq. (4).

It follows from this partition function that the joint probability distribution of $\bar{\phi}_1(0)$, $\bar{\phi}_1(t)$, $\bar{\phi}_2(0)$, $\bar{\phi}_2(t)$ taking values u_0 , u_t , v_0 , v_t , respectively, is given by

$$P_{\bar{\phi}_{1}(0),\bar{\phi}_{1}(t),\bar{\phi}_{2}(0),\bar{\phi}_{2}(t)}(u_{0},u_{t},v_{0},v_{t}) = \frac{1}{(2\pi)^{2}(\sigma_{f}^{4}-K_{f}(t)^{2})} \times \exp\left(-\frac{\sigma_{f}^{2}}{2(\sigma_{f}^{4}-K_{f}(t)^{2})}(u_{0}^{2}+u_{t}^{2}+v_{0}^{2}+v_{t}^{2}) + \frac{K_{f}(t)}{\sigma_{f}^{4}-K_{f}(t)^{2}}(u_{0}u_{t}+v_{0}v_{t})\right).$$

$$(6)$$

Since $\langle \bar{\phi}_i(t) \bar{\phi}_i(0) \rangle \propto e^{-mt}$ for $i \in \{1, 2\}$ and $t \gg \frac{1}{\bar{m}-m}$, where *m* is the energy of the first excited state and \tilde{m} is the energy of the second excited state with vanishing spatial momentum, it follows that $K_f(t) \propto e^{-mt}$ in the same large-time limit. The distributions of

$$C_{\text{Re}}(t) = \text{Re}(\bar{\psi}(t)\bar{\psi}^*(0)) = \bar{\phi}_1(t)\bar{\phi}_1(0) + \bar{\phi}_2(t)\bar{\phi}_2(0)$$
(7)

and

$$C_{\rm Im}(t) = {\rm Im}(\bar{\psi}(t)\bar{\psi}^*(0)) = \bar{\phi}_2(t)\bar{\phi}_1(0) - \bar{\phi}_1(t)\bar{\phi}_2(0) \qquad (8)$$

²In what follows, fields with bars will denote spatially averaged fields: $\overline{\mathcal{O}}(t) = L^{-\frac{d}{2}} \sum_{\vec{x}} \mathcal{O}(t, \vec{x})$. The scaling with $L^{-\frac{d}{2}}$ is fixed by requiring that $\overline{\mathcal{O}}(t)$ has finite and nonzero variance as $L \to \infty$.

can be calculated from this joint probability density. The corresponding characteristic functions³ can be calculated from Eq. (6), giving

$$\begin{split} \Phi_{C_{\text{Re}}(t)}(\omega) &= \langle e^{-i\omega C_{\text{Re}}(t)} \rangle \\ &= \langle e^{-i\omega \bar{\phi}_1(t)\bar{\phi}_1(0)} \rangle \langle e^{-i\omega \bar{\phi}_2(t)\bar{\phi}_2(0)} \rangle \\ &= \frac{\omega_{R,+}(t)\omega_{R,-}(t)}{(\omega - i\omega_{R,+}(t))(\omega + i\omega_{R,-}(t))}, \\ \Phi_{C_{\text{Im}}(t)}(\omega) &= \frac{\omega_I(t)^2}{(\omega - i\omega_I(t))(\omega + i\omega_I(t))}, \end{split}$$
(9)

where the independence of $\bar{\phi}_1(t)$ and $\bar{\phi}_2(t)$ has been used and $\omega_{R,+}(t), \omega_{R,-}(t), \omega_I(t)$ are defined by

$$\omega_{R,+}(t) = \frac{1}{\sigma_f^2 + K_f(t)},
\omega_{R,-}(t) = \frac{1}{\sigma_f^2 - K_f(t)},
\omega_I(t) = \frac{1}{\sqrt{\sigma_f^4 - K_f(t)^2}}.$$
(10)

Consequently, the probability distributions $P_{C_{\text{Re},Im}(t)}(x) = \int d\omega e^{i\omega x} \tilde{P}_{C_{\text{Re},Im}(t)}(\omega)$ are given by

$$P_{C_{\text{Re}}(t)}(x) = \begin{cases} \frac{\omega_{R,+}(t)\omega_{R,-}(t)}{\omega_{R,+}(t)+\omega_{R,-}(t)}e^{-\omega_{R,+}(t)x} & \text{for } x > 0\\ \frac{\omega_{R,+}(t)\omega_{R,-}(t)}{\omega_{R,+}(t)+\omega_{R,-}(t)}e^{\omega_{R,-}(t)x} & \text{for } x < 0 \end{cases},$$

$$P_{C_{\text{Im}}(t)}(x) = \frac{\omega_{I}(t)}{2}e^{-\omega_{I}(t)|x|}.$$
(11)

Since there is strong evidence that phase fluctuations rather than magnitude fluctuations are central to signal-tonoise degradation in many QFT contexts [8–10], it is also of interest to calculate $P_{R_t}(x)$ and $P_{\theta_t}(x)$ where $R_t = |\bar{\psi}(t)\bar{\psi}^*(0)|$ is the magnitude and $\theta_t = \arg(\bar{\psi}(t)\bar{\psi}^*(0))$ is the phase of the correlation function. For this purpose, it is useful to express the partition function in Eq. (3) in terms of the polar fields defined by the relations

$$r_{0} = \sqrt{\phi_{1}(0)^{2} + \phi_{2}(0)^{2}},$$

$$\xi_{0} = \arctan\left(\frac{\phi_{2}(0)}{\phi_{1}(0)}\right),$$

$$r_{t} = \sqrt{\phi_{1}(t)^{2} + \phi_{2}(t)^{2}},$$

$$\xi_{t} = \arctan\left(\frac{\phi_{2}(t)}{\phi_{1}(t)}\right).$$
(12)

With this substitution, Eq. (3) becomes

$$Z = \frac{1}{(2\pi)^2 (\sigma_f^4 - K_f(t)^2)} \int dr_0 dr_t d\xi_0 d\xi_t r_0 r_t$$

$$\times \exp\left(-\frac{\sigma_f^2}{2(\sigma_f^4 - K_f(t)^2)} \left[(r_0^2 + r_t^2) + 2\frac{K_f(t)}{\sigma_f^2} r_0 r_t \cos(\xi_t - \xi_0) \right] \right).$$
(13)

Since this is independent of $\xi_0 + \xi_t$, the partition function can be integrated over this combination to give

$$Z = \frac{1}{2\pi(\sigma_f^4 - K_f(t)^2)} \int dr_0 dr_t d\theta_t r_0 r_t \exp\left(-\frac{\sigma_f^2}{2(\sigma_f^4 - K_f(t)^2)} \left[(r_0^2 + r_t^2) + 2\frac{K_f(t)}{\sigma_f^2} r_0 r_t \cos(\theta_t) \right] \right),$$
(14)

where $\theta_t = \xi_t - \xi_0$.

To find $P_{\theta_t}(x)$, one integrates over r_0 and r_t in Eq. (14) to obtain

$$Z = \frac{1 - \frac{K_{f}(t)^{2}}{\sigma_{f}^{4}}}{4\pi} \int \frac{d\theta_{t}}{\left(1 - \frac{K_{f}(t)^{2}}{\sigma_{f}^{4}}\cos\left(\theta_{t}\right)^{2}\right)^{2}} \left[2\left(1 - \frac{K_{f}(t)^{2}}{\sigma_{f}^{4}}\cos\left(\theta_{t}\right)^{2}\right) + \pi \frac{K_{f}(t)}{\sigma_{f}^{2}}\sqrt{1 - \frac{K_{f}(t)^{2}}{\sigma_{f}^{4}}\cos\left(\theta_{t}\right)^{2}}\cos\left(\theta_{t}\right)^{2}} + 2\cos(\theta_{t})\frac{K_{f}(t)}{\sigma_{f}^{2}}\sqrt{1 - \frac{K_{f}(t)^{2}}{\sigma_{f}^{4}}\cos\left(\theta_{t}\right)^{2}} + \arctan\left(\frac{K_{f}(t)^{2}\cos(\theta_{t})}{\sigma_{f}^{4}\sqrt{1 - \frac{K_{f}(t)}{\sigma_{f}^{2}}\cos\left(\theta_{t}\right)^{2}}}\right)\right].$$
(15)

³The characteristic function $\Phi_A(\omega)$ of a random variable A is defined as $\Phi_A(\omega) = \int dx e^{-i\omega x} P_A(x)$, where $P_A(x)$ is the probability density function of A.

For $K_f(t) \ll \sigma_f^{-2}$, Eq. (15) can be expressed as a series in $K_f(t)/\sigma_f^2$ as

$$Z = \int d\theta_t \left(\frac{1}{2\pi} + \frac{K_f(t)}{4\sigma_f^2} \cos(\theta_t) + \mathcal{O}\left(\left(\frac{K_f(t)}{\sigma_f^2} \right)^2 \right) \right), \quad (16)$$

and therefore the angular probability density is

$$P_{\theta_t}(x) = \frac{1}{2\pi} + \frac{K_f(t)}{4\sigma_f^2} \cos(x) + \mathcal{O}\left(\left(\frac{K_f(t)}{\sigma_f^2}\right)^2\right), \quad (17)$$

where the domain of x is $-\pi \le x < \pi$.

To find $P_{R_t}(x)$, one integrates over θ_t in Eq. (14) and can define $R_t = r_0 r_t$, leading in the limit $K_f(t) \ll \sigma_f^{-2}$ to

$$Z = \frac{1}{\sigma_f^4} \int dr_0 dr_t r_0 r_t I_0 (K_f(t) r_0 r_t / \sigma_f^4) e^{-\frac{1}{2\sigma_f^2} (r_0^2 + r_t^2)}$$

$$= \frac{1}{\sigma_f^4} \int dR_t dr_0 dr_t r_0 r_t \delta(R_t - r_0 r_t)$$

$$\times I_0 (K_f(t) r_0 r_t / \sigma_f^4) e^{-\frac{1}{2\sigma_f^2} (r_0^2 + r_t^2)}$$

$$= \frac{1}{\sigma_f^4} \int_0^\infty dR_t I_0 \left(\frac{K_f(t) R_t}{\sigma_f^4}\right) K_0 \left(\frac{R_t}{\sigma_f^2}\right) R_t,$$
(18)

after $r_{0,t}$ are integrated out, where $I_n(x)$ and $K_n(x)$ are modified Bessel functions of the first and second kinds, respectively. Therefore, the radial probability density is

$$P_{R_t}(x) = \frac{1}{\sigma_f^4} I_0\left(\frac{K_f(t)x}{\sigma_f^4}\right) K_0\left(\frac{x}{\sigma_f^2}\right) x.$$
(19)

III. PROBABILITY DISTRIBUTIONS OF O(N)MODELS IN THE DISORDERED PHASE

In this section, an interacting Euclidean lattice field theory with N real bosonic fields, $\phi_a(t, \vec{x})$, where $a \in \{1, ..., N\}$ will be considered such that:

- (i) The Euclidean action of the theory is real.
- (ii) There is a unique, translationally invariant, gapped vacuum $|\Omega\rangle$.
- (iii) $\phi_a(t, \vec{x})$ is covariant under temporal and spatial translations for $a \in \{1, ..., N\}$.
- (iv) The vacuum expectation value of $\phi_a(t, \vec{x})$, $\langle \Omega | \phi_a(t, \vec{x}) | \Omega \rangle$, vanishes for $a \in \{1, ..., N\}$.

In the following subsections, probability distributions of the volume averaged fields defined at different times will be presented⁴ in increasing generality. While the methods work in the general case, some of the results will be presented for the specific case where the theory is invariant under an O(N) symmetry relating the N fields. As in the previous section, L is the extent of each of the d spatial directions, and β is the extent of the temporal direction.

A. Large-time limit

In this subsection, it will be shown that the distributions of two-point correlation functions in O(N) models in the disordered phase have a universal large-time limit.

The components of the (spatially averaged) *N*-component field can be collected as a vector,

$$\vec{\phi}(t) = \begin{pmatrix} \bar{\phi}_1(t) \\ \vdots \\ \bar{\phi}_N(t) \end{pmatrix}, \qquad (20)$$

and a natural object to consider is the PDF $P_{\vec{a},\vec{b}(0)}(u)$ that

represent the probability $\vec{q} \cdot \vec{\phi}(0)$ takes the value *u* for some fixed vector $\vec{q} \in \mathbb{R}^N$. In the limit where the temporal extent β is taken to infinity, this is given by

$$P_{\vec{q}\cdot\vec{\phi}(0)}(u) = \lim_{\beta \to \infty} \operatorname{Tr}\left(e^{-\beta H} \delta\left(\vec{q}\cdot\vec{\phi}(0) - u\right)\right)$$
$$= \langle \Omega | \delta\left(\vec{q}\cdot\vec{\phi}(0) - u\right) | \Omega \rangle.$$
(21)

In Ref. [24], the large-time behavior of the analogous quantity for a single field was derived. Generalizing this to the present case leads to

$$\lim_{L \to \infty} \langle \Omega | \delta(\vec{q} \cdot \vec{\phi}(0) - u) | \Omega \rangle = \frac{1}{\sqrt{2\pi\sigma(\vec{q})}} e^{-\frac{u^2}{2\sigma(\vec{q})^2}}.$$
 (22)

Here, the quantity $\sigma(\vec{q})$ can be shown to be given by

$$\sigma(\vec{q})^2 = \vec{q}^T \Sigma \vec{q} \tag{23}$$

in terms of a symmetric matrix Σ with components

$$\Sigma_{ab} = \lim_{L \to \infty} \langle \Omega | \bar{\phi}_a(0) \bar{\phi}_b(0) | \Omega \rangle.$$
 (24)

The characteristic function

$$\Phi_{\vec{q}\cdot\vec{\phi}(0)}(\omega) = \int dx e^{-i\omega x} P_{\vec{q}\cdot\vec{\phi}(0)}(x)$$
(25)

of $\vec{q} \cdot \vec{\phi}(0)$ evaluated at $\omega = 1$ can be calculated in the large volume limit as

⁴Some of the arguments used in this section are closely related to the proofs of the Central Limit Theorem for random vectors; see for example Ref. [28].

$$\Phi_{\vec{q}\cdot\vec{\phi}(0)}(1) = \lim_{L \to \infty} \langle \Omega | e^{-i\vec{q}\cdot\vec{\phi}(0)} | \Omega \rangle$$
$$= e^{-\frac{1}{2}\sigma(\vec{q})^2}$$
$$= e^{-\frac{1}{2}\vec{q}^T \Sigma \vec{q}}, \qquad (26)$$

where the second equality follows from Eq. (22).

By making use of the numerical equivalence between the characteristic function of $\vec{\phi}$ evaluated at \vec{q} and the characteristic function of $\vec{q} \cdot \vec{\phi}(0)$ evaluated at 1, this leads to

$$\Phi_{\vec{\phi}(0)}(\vec{q}) = \lim_{L \to \infty} \langle \Omega | e^{-i\vec{q}\cdot\vec{\phi}} | \Omega \rangle$$
$$= \Phi_{\vec{q}\cdot\vec{\phi}(0)}(1)$$
$$= e^{-\frac{1}{2}\vec{q}^T \Sigma \vec{q}}.$$
(27)

By performing the inverse Fourier transform the large volume probability density function $P_{\vec{\phi}(0)}(\vec{u})$ of $\vec{\phi}(0)$ can be determined and is given by

$$P_{\vec{\phi}(0)}(\vec{u}) = \frac{1}{\sqrt{(2\pi)^N \det \Sigma}} e^{-\frac{1}{2}\vec{u}^T \Sigma^{-1} \vec{u}}.$$
 (28)

Thus, the probability distribution of an *N*-component field is an *N*-dimensional correlated Gaussian. This will be useful in defining more complicated joint and product distributions.

The joint probability distribution of $\vec{\phi}(t)$ and $\vec{\phi}(0)$ taking vector values \vec{u} and \vec{v} , respectively, is defined by

$$P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = \lim_{\beta \to \infty} \operatorname{Tr}[e^{-\beta H} \delta(\vec{\phi}(t) - \vec{u}) \delta(\vec{\phi}(0) - \vec{v})]$$

$$= \sum_{n} e^{-E_{n}t} \langle \Omega | \delta(\vec{\phi}(0) - \vec{u}) | n \rangle$$

$$\times \langle n | \delta(\vec{\phi}(0) - \vec{v}) | \Omega \rangle$$

$$\equiv \sum_{n} P_{\vec{\phi}(t),\vec{\phi}(0)}^{(n)}(\vec{u},\vec{v}), \qquad (29)$$

where each term in the summation in the last line arises from the contributions of successively higher energy states. That is, $E_n \leq E_{n+1}$ with $E_0 = 0$, and the sum is over states $|n\rangle$ with vanishing spatial momentum such that $\langle \Omega | \delta(\vec{\phi}(t) - \vec{u}) | n \rangle \neq 0$ for some $\vec{u} \in \mathbb{R}^N$.

In the large-time limit, only the vacuum intermediate state is relevant in Eq. (29), and the leading term is given by

$$P_{\vec{\phi}(t),\vec{\phi}(0)}^{(0)}(\vec{u},\vec{v}) = \lim_{t \to \infty} P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = \langle \Omega | \delta(\vec{\phi}(t) - \vec{u}) | \Omega \rangle \langle \Omega | \delta(\vec{\phi}(0) - \vec{v}) | \Omega \rangle = P_{\vec{\phi}(0)}(\vec{u}) P_{\vec{\phi}(0)}(\vec{v}) = \frac{1}{(2\pi)^N \det \Sigma} e^{-\frac{1}{2}\vec{u}^T \Sigma^{-1} \vec{u} - \frac{1}{2}\vec{v}^T \Sigma^{-1} \vec{v}}.$$
(30)

In the case of a theory with O(N) symmetry, further simplifications occur as it can be shown⁵ for that case that

$$\Sigma_{ab} = \sigma^2 \delta_{ab},\tag{31}$$

for some $\sigma > 0$.

For N > 2, the only O(N)-invariant quadratic bilocal operator is $C_{\bullet}(t) = \sum_{a=1}^{N} \bar{\phi}_a(t) \bar{\phi}_a(0)$, and the product distribution for this quantity is

$$P_{C_{\bullet}(t)}(x) \equiv \int d\vec{u} d\vec{v} P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v})\delta(\vec{u}\cdot\vec{v}-x), \quad (32)$$

which, as in Eq. (29), can be expanded in terms of the contributions of intermediate states as

$$P_{C.(t)}(x) = \sum_{n} P_{C.(t)}^{(n)}(x).$$
(33)

The large-time limit of $P_{C}(t)$ will be derived below; see Eq. (63).

Similarly, the characteristic function of $C_{\bullet}(t)$ can be expanded in partial contributions as

$$\Phi_{C.(t)}(\omega) \equiv \int dx \, e^{-i\omega x} P_{C.(t)}(x)$$
$$= \sum_{n} \Phi_{C.(t)}^{(n)}(\omega)(\vec{u}, \vec{v}). \tag{34}$$

B. Leading corrections

In this section, the leading correction $P_{\vec{\phi}(t),\vec{\phi}(0)}^{(1)}(\vec{u},\vec{v})$ in $P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v})$ away from the $t \to \infty$ limit will be derived. For this purpose, it is assumed that the first multiplet of excited states with vanishing spatial momentum transform in the fundamental representation of O(N) and may be labeled as $|m, a\rangle$ for $a \in \{1, ..., N\}$. The state $|m, a\rangle$ can be created by acting⁶ with $\vec{\phi}_a(t)$ on the vacuum

$$|m,a\rangle = \lim_{T \to -\infty} e^{-mT} \bar{\phi}_a(T) |\Omega\rangle$$
 (35)

as $\langle \Omega | \bar{\phi}_a(0) | \Omega \rangle = 0$ by assumption. The leading correction as $t \to \infty$ is given by

⁵The fact that Σ_{ab} is diagonal follows from invariance under the O(N) transformation $\phi_a(t, \vec{x}) \rightarrow -\phi_a(t, \vec{x})$ for fixed *a* with $\phi_b(t, \vec{x})$ invariant for $b \neq a$. The fact that Σ is proportional to the identity follows from the requirement of invariance under the O(N) transformation $\phi_a(t, \vec{x}) \rightarrow -\phi_b(t, \vec{x}), \phi_b(t, \vec{x}) \rightarrow \phi_a(t, \vec{x})$ for fixed *a* and *b* with $\phi_c(t, \vec{x})$ invariant for $c \notin \{a, b\}$. ^{The} factor of e^{-mT} is included so that in an expansion of

^bThe factor of e^{-mT} is included so that in an expansion of $e^{-mT}\bar{\phi}_a(T)|\Omega\rangle$ in terms of the eigenstates of the theory, the coefficient $|m, a\rangle$ is independent of T and the coefficients of all other terms vanish in the limit $T \to -\infty$.

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$$P^{(1)}_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = e^{-mt} \sum_{a} \langle \Omega | \delta \left(\vec{\phi}(0) - \vec{u} \right) | m, a \rangle \langle m, a | \delta \left(\vec{\phi}(0) - \vec{v} \right) | \Omega \rangle.$$
(36)

To calculate this expression, $\langle \Omega | \delta (\vec{\phi}(0) - \vec{u}) | m, a \rangle$ must be determined. From Eq. (35), it follows that

$$\langle \Omega | \delta \left(\vec{\phi}(0) - \vec{u} \right) | m, a \rangle = \lim_{T \to -\infty} e^{-mT} \langle \Omega | \delta \left(\vec{\phi}(0) - \vec{u} \right) \bar{\phi}_a(T) | \Omega \rangle.$$
(37)

The insertion of $\bar{\phi}_a(T)$ can be obtained through the response to a time-dependent, but spatially constant source term as

$$\langle \Omega | \delta \Big(\vec{\phi}(0) - \vec{u} \Big) \bar{\phi}_a(T) | \Omega \rangle = \frac{\partial}{\partial J_a} \langle \Omega | \delta \Big(\vec{\phi}(0) - \vec{u} \Big) e^{\vec{J} \cdot \vec{\phi}(T)} | \Omega \rangle |_{\vec{J}=0}.$$
(38)

For the infinite temporal extent, $\langle \Omega | \delta \left(\vec{\phi}(0) - \vec{u} \right) e^{\vec{J} \cdot \vec{\phi}(T)} | \Omega \rangle$ is equal to a path integral expression:

$$\langle \Omega | \delta \left(\vec{\phi}(0) - \vec{u} \right) e^{\vec{J} \cdot \vec{\phi}(T)} | \Omega \rangle = \lim_{\beta \to \infty} \oint_{\vec{\phi}(0,\vec{x}) = \vec{\phi}(\beta,\vec{x})} \mathcal{D} \phi e^{-S[\vec{\phi}(t,\vec{x})] + \vec{J} \cdot \vec{\phi}(T)} \delta \left(\vec{\phi}(0) - \vec{u} \right).$$
(39)

The above expression has the interpretation as the probability of $\bar{\phi}(0)$ having the value \vec{u} in the presence of the source term $\vec{J} \cdot \vec{\phi}(T)$. Under the assumption that there is still a unique vacuum in the presence of an infinitesimal source term (that is, no spontaneous symmetry breaking), the vacuum expectation value of $\delta(\bar{\phi}(0) - \vec{u})$ will change infinitesimally for an infinitesimal source, and the system observed at t = 0 will continue to have a finite correlation length. Moreover, as the source is chosen to be spatially constant, the system will remain uniform in space. In the present discussion, it is assumed that the expectation value of $\langle \vec{\phi}(0, \vec{x}) \rangle$ vanishes. In the presence of an infinitesimal source term at time T, indicated by a subscript J, T, the expectation value may shift infinitesimally as $\langle \vec{\phi}(0, \vec{x}) \rangle_{IT} = W(T)\vec{J}$, where W(T)is an undetermined $N \times N$ matrix. From O(N) invariance, it follows that $W(T) = \rho(T)I$, where I is the identity matrix and $\rho(T)$ is a real function. It follows that the results of Sec. III A can be used for the shifted fields $\vec{\phi}'(0, \vec{x}) = \vec{\phi}(0, \vec{x}) - W(T)\vec{J}$. Therefore, from Eq. (28), it follows that

$$P_{\vec{\phi}(0)}(\vec{u};\vec{J},T) = \frac{1}{\sqrt{(2\pi)^N \det \Sigma(\vec{J},T)}} e^{-\frac{1}{2}(\vec{u}-W(T)\vec{J})^T \Sigma(\vec{J},T)^{-1}(\vec{u}-W(T)\vec{J})}, \quad (40)$$

where $P_{\vec{\phi}(0)}(\vec{u}; \vec{J}, T)$ is the probability that $\vec{\phi}(0)$ is equal to \vec{u} in the presence of source \vec{J} which is inserted at time T.

The matrix $\Sigma(\vec{J}, T)$ transforms in the adjoint representation of O(N),

$$\Sigma(R\vec{J},T) = R\Sigma(\vec{J},T)R^T, \qquad (41)$$

and consequently, the linear term in the expansion of $\Sigma(\vec{J}, T)$ in \vec{J} vanishes [the only invariant tensor of the O(N) group with two indices is δ_{ab}]. It follows that, to first order in \vec{J} , one can replace $\Sigma(\vec{J}, T)$ by $\Sigma = \sigma^2 I$ where σ is defined by Eq. (31). Therefore, $P_{\vec{\phi}(0)}(\vec{u}; \vec{J}, T)$ can be expanded in \vec{J} as

$$P_{\vec{\phi}(0)}(\vec{u};\vec{J},T) = P_{\vec{\phi}(0)}^{(0)}(\vec{u}) - \rho(T)(\vec{J}\cdot\nabla_{\vec{u}})P_{\vec{\phi}(0)}^{(0)}(\vec{u}) + \mathcal{O}(J^2)$$

$$= P_{\vec{\phi}(0)}^{(0)}(\vec{u})(1 + \rho(T)(\vec{J}\cdot\Sigma^{-1}\vec{u})) + \mathcal{O}(J^2)$$

$$= P_{\vec{\phi}(0)}^{(0)}(\vec{u})\left(1 + \frac{\rho(T)}{\sigma^2}\vec{J}\cdot\vec{u}\right) + \mathcal{O}(J^2). \quad (42)$$

Defining $\rho = \lim_{T \to -\infty} e^{-mT} \rho(T)$ [which is finite since $\rho(T) \propto e^{mT}$ for $T \to -\infty$], from Eqs. (37) and (38), one obtains

$$\langle \Omega | \delta(\vec{\bar{\phi}}(0) - \vec{u}) | m, a \rangle = \frac{\rho}{\sigma^2} P^{(0)}_{\vec{\phi}(0)}(\vec{u}) u_a.$$
(43)

It follows that the first order correction to the joint distribution function (arising from the lowest energy excited multiplet of states) is

$$P^{(1)}_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = e^{-mt} \Delta \vec{u} \cdot \vec{v} P^{(0)}_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}), \quad (44)$$

⁷For $N \neq 2$, SO(N) invariance is enough to arrive at this conclusion. For N = 2, invariance under reflection needs to be assumed as otherwise $W_{ab}(T) \propto \epsilon_{ab}$ is also a valid possibility where ϵ_{ab} is the two-dimensional (2D) Levi-Civita symbol.

where $\Delta = \frac{\rho^2}{\sigma^4} > 0$. Therefore, including the first order correction, the full joint distribution is given by

$$P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = \frac{1}{(2\pi)^N \sigma^{2N}} e^{-\frac{1}{2\sigma^2}(\vec{u}\cdot\vec{u}+\vec{v}\cdot\vec{v})} (1+e^{-mt}\Delta\vec{u}\cdot\vec{v}) + \mathcal{O}(e^{-m't})$$
$$= \frac{1}{(2\pi)^N \sigma^{2N}} e^{-\frac{1}{2\sigma^2}(\vec{u}\cdot\vec{u}+\vec{v}\cdot\vec{v})+e^{-mt}\Delta\vec{u}\cdot\vec{v}} + \mathcal{O}(e^{-m't}), \tag{45}$$

where $2m \ge m' > m$ and in the second line the correction term has been exponentiated. It follows that for N = 2, the results of the Sec. II are valid up to the first order in $K_f(t)$ with the identification $K_f(t) \equiv e^{-mt}\Delta\sigma^4$.

In a similar fashion, one obtains the first order correction to $P_{C_{\bullet}}(t)$ in Eq. (33) as

$$P_{C_{\bullet}(t)}^{(1)}(x) = \frac{e^{-mt}\Delta}{2\pi} \int d\omega e^{i\omega x} \int d\vec{u} d\vec{v} e^{-i\omega \vec{u} \cdot \vec{v}} \vec{u} \cdot \vec{v} P_{\vec{\phi}(t),\vec{\phi}(0)}^{(0)}(\vec{u},\vec{v})$$
$$= \frac{e^{-mt}\Delta}{2\pi} \int d\omega e^{i\omega x} \left(i\frac{\partial}{\partial\omega}\right) \int d\vec{u} d\vec{v} e^{-i\omega \vec{u} \cdot \vec{v}} P_{\vec{\phi}(t),\vec{\phi}(0)}^{(0)}(\vec{u},\vec{v})$$
$$= \frac{1}{2\pi} \int d\omega e^{i\omega x} \left(ie^{-mt}\Delta \frac{\partial}{\partial\omega}\right) \Phi_{C_{\bullet}(T)}^{0}(\omega).$$
(46)

From the above relation, up to the first order correction, it is seen that $\Phi_{C,(t)}(\omega)$ is given as

$$\Phi_{C,(t)}(\omega) = \Phi_{C,(t)}^{(0)}(\omega) + ie^{-mt}\Delta \frac{\partial}{\partial \omega} \Phi_{C,(t)}^{(0)}(\omega) + \mathcal{O}(e^{-m't})$$
$$= \Phi_{C,(t)}^{(0)}(\omega + ie^{-mt}\Delta) + \mathcal{O}(e^{-m't}).$$
(47)

From this expression, it is clear that including the first order correction to the characteristic function $\Phi_{C,(t)}(\omega)$ is equivalent to a shift in the argument in the imaginary direction that decreases as $t \to \infty$.

C. All times

It has been shown in Eqs. (30) and (45) that both in the large-time limit and even including its first correction, the joint probability density $P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v})$ is given by a coupled Gaussian probability density, in the infinite volume limit. In this subsection, it will be shown that this fact is valid including all corrections in the infinite volume limit.

Consider a division of the spatial volume into boxes of sizes $l > \xi$, where ξ is the correlation length in lattice units. Boxes are enumerated by I = 1, ..., K with each box having $E = \frac{L^d}{K}$ sites. For each box, box-averaged fields are defined as

$$\bar{\phi}_{a,I}(t) = \frac{1}{\sqrt{E}} \sum_{\vec{x} \sim I} \phi_a(t, \vec{x}), \qquad (48)$$

where the summation over $\vec{x} \sim I$ is over all sites in the *I*th box. One notes immediately that

$$\bar{\phi}_a(t) = \frac{1}{\sqrt{K}} \sum_I \bar{\phi}_{a,I}(t).$$
(49)

For $I \neq J$, $\bar{\phi}_{a,I}(t)$ can be considered independent of $\bar{\phi}_{b,J}(t')$ up to the corrections proportional to $e^{-\sqrt{l_{IJ}^2 + (t-t')^2}/\xi}$, where l_{IJ} is the distance between centers of the boxes *I* and *J* in lattice units.

For each box I, a 2N-tuple of fields,

$$\vec{Q}_{I}(t) = \begin{pmatrix} \bar{\phi}_{1,I}(t) \\ \cdots \\ \bar{\phi}_{N,I}(t) \\ \bar{\phi}_{1,I}(0) \\ \cdots \\ \bar{\phi}_{N,I}(0) \end{pmatrix},$$
(50)

will be considered. The joint distribution of $\vec{\phi}(t)$ and $\vec{\phi}(0)$ is then equivalent to the distribution of $\vec{Q}(t)$, where $\vec{Q}(t)$ is defined by

$$\vec{Q}(t) = \frac{1}{\sqrt{K}} \sum_{I=1}^{K} \vec{Q}_I(t).$$
 (51)

The goal here is to show that this vector follows a Gaussian probability distribution. The main assumption needed to show this is the independence of $\vec{Q}_I(t)$ and $\vec{Q}_J(t)$ for $I \neq J$. The errors due to this approximation can be made arbitrarily small in the infinite volume limit by taking $l, K \rightarrow \infty$. Therefore, in the infinite volume limit, one may write

$$\begin{split} \lim_{V \to \infty} P_{\vec{Q}(t)}(\vec{z}) &= \lim_{K \to \infty} \int \prod_{I=1}^{K} d\vec{z}_{I} \delta\left(\vec{z} - \frac{1}{\sqrt{K}} \sum_{J=1}^{Z} \vec{z}_{J}\right) P_{\vec{Q}_{I}(t)}(\vec{z}_{I}) \\ &= \frac{1}{(2\pi)^{2N}} \lim_{K \to \infty} \frac{1}{(2\pi)^{2NK}} \int d\vec{w} e^{i(\vec{z} - \frac{1}{\sqrt{K}} \sum_{J=1}^{Z} \vec{z}_{J}) \cdot \vec{w}} \prod_{I=1}^{K} d\vec{z}_{I} d\vec{w}_{I} \Phi_{\vec{Q}_{1}(t)}(\vec{w}_{I}) e^{i\vec{w}_{I} \cdot \vec{z}_{I}} \\ &= \frac{1}{(2\pi)^{2N}} \int d\vec{w} e^{i\vec{w} \cdot \vec{z}} \lim_{K \to \infty} \prod_{I=1}^{K} \Phi_{\vec{Q}_{1}(t)}\left(\frac{\vec{w}}{\sqrt{K}}\right) \\ &= \frac{1}{(2\pi)^{2N}} \int d\vec{w} e^{i\vec{w} \cdot \vec{z}} \lim_{K \to \infty} \exp\left(-\frac{1}{2K} \vec{w}^{T} \hat{\Sigma}(t) \vec{w} + \mathcal{O}\left(\frac{1}{K\sqrt{K}}\right)\right)^{K} \\ &= \frac{1}{(2\pi)^{2N}} \int d\vec{w} e^{i\vec{w} \cdot \vec{z}} e^{-\frac{1}{2}\vec{w}^{T} \hat{\Sigma}(t) \vec{w}} \\ &= \frac{1}{(2\pi)^{2N}} \int d\vec{w} e^{i\vec{w} \cdot \vec{z}} e^{-\frac{1}{2}\vec{w}^{T} \hat{\Sigma}(t) \vec{w}} \end{split}$$
(52)

where translational invariance has been used to set $\Phi_{\vec{Q}_I(t)} = \Phi_{\vec{Q}_1(t)}$ for all *I*. Note also that $\Phi_{\vec{Q}_1(t)}(0) = 1$ and $\Phi'_{\vec{Q}_1(t)}(0) = 0$, which permits one to write $\Phi_{\vec{Q}_1(t)}(\vec{w}) = \exp(-\frac{1}{2}(\vec{w})^T \hat{\Sigma}(t) \vec{w} + \mathcal{O}(w^3))$. Here,

$$\hat{\Sigma}(t) = \begin{pmatrix} \Sigma & \tilde{\Sigma}(t) \\ \tilde{\Sigma}(t) & \Sigma \end{pmatrix},$$
(53)

where $\Sigma_{ab} = \sigma^2 \delta_{ab}$ was introduced in Sec. III A and $\tilde{\Sigma}_{ab}(t) = \langle \bar{\phi}_{a,1}(t) \bar{\phi}_{b,1}(0) \rangle = \langle \bar{\phi}_a(t) \bar{\phi}_b(0) \rangle$. From O(N) invariance, it follows that $\tilde{\Sigma}_{ab}(t) = K(t) \delta_{ab}$ for some K(t). Therefore, $\hat{\Sigma}(t)$ can be written in the form $\hat{\Sigma}_{(\tau a)(\tau' b)}(t) = \delta_{ab} \bar{\Sigma}_{\tau\tau'}$ where $\tau \in \{1, 2\}$ with different τ corresponding to different times ($\tau = 1$, 2 correspond to 0 and *t*, respectively) and $\bar{\Sigma}_{\tau\tau'}(t)$ is given by

$$\bar{\Sigma}(t) = \begin{pmatrix} \sigma^2 & K(t) \\ K(t) & \sigma^2 \end{pmatrix}.$$
(54)

It follows that $\hat{\Sigma}_{(\tau a)(\tau' b)}^{-1}(t) = \delta_{ab} \bar{\Sigma}_{\tau\tau'}^{-1}$, where $\bar{\Sigma}_{\tau\tau'}^{-1}$ is given as

$$\bar{\Sigma}^{-1}(t) = \frac{1}{\sigma^4 - K(t)^2} \begin{pmatrix} \sigma^2 & -K(t) \\ -K(t) & \sigma^2 \end{pmatrix}.$$
 (55)

Therefore, the joint probability distribution of $\vec{\phi}(t)$ and $\vec{\phi}(0)$ in the limit $L \to \infty$ is given from Eq. (52) as

$$P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v}) = \frac{1}{(2\pi)^N (\sigma^4 - K(t)^2)^{\frac{N}{2}}} \\ \times \exp\left(-\frac{\sigma^2(|\vec{u}|^2 + |\vec{v}|^2)}{2(\sigma^4 - K(t)^2)} + \frac{K(t)(\vec{u}\cdot\vec{v})}{\sigma^4 - K(t)^2}\right).$$
(56)

Note that this expression has been derived without taking $t \to \infty$ and reduces to Eq. (6) for N = 2.

D. Distribution of $C_{\bullet}(t)$

For arbitrary t and β , it follows from Eq. (56) that $P_{C_{\bullet}}(x)$ is given by

$$P_{C_{\bullet}(t)}(x;\omega_{+},\omega_{-},N) = \int du dv \delta(x-\vec{u}\cdot\vec{v}) P_{\vec{\phi}(t),\vec{\phi}(0)}(\vec{u},\vec{v})$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega x} \frac{(\omega_{+}\omega_{-})^{\frac{N}{2}}}{(\omega-i\omega_{+})^{\frac{N}{2}}(\omega+i\omega_{-})^{\frac{N}{2}}},$$

(57)

where the poles ω_{\pm} are given by

$$\omega_{\pm} = \frac{1}{\sigma^2 \pm K(t)},\tag{58}$$

and the dependence on N is made explicit. Note that Eq. (57) defines

$$\Phi_{C,(t)}(\omega) = \frac{(\omega_{+}\omega_{-})^{\frac{N}{2}}}{(\omega - i\omega_{+})^{\frac{N}{2}}(\omega + i\omega_{-})^{\frac{N}{2}}}.$$
 (59)

The integral in Eq. (57) will be calculated explicitly for x > 0; the result for x < 0 can be obtained using the relation $P_{C,(t)}(x; \omega_+, \omega_-, N) = P_{C,(t)}(-x; \omega_-, \omega_+, N)$. The calculation begins with the observation that

 $P_{C,(t)}(x; \omega_+, \omega_-, N)$ is an analytic function of *N* for $\operatorname{Re}(N) > 0$. This can be seen by using the relation $e^{i\omega x} = -\frac{i}{x}\partial_{\omega}e^{i\omega x}$ to find another expression for $P_{C,(t)}(x; \omega_+, \omega_-, N)$ through integration by parts:

$$P_{C,(t)}(x;\omega_{+},\omega_{-},N) = \frac{-i(\omega_{+}\omega_{-})^{\frac{N}{2}}}{2\pi x} \left[\frac{e^{i\omega x}}{(\omega - i\omega_{+})^{\frac{N}{2}}(\omega + i\omega_{-})^{\frac{N}{2}}} \right]_{\omega=-\infty}^{\omega=\infty} + \frac{iN(\omega_{+}\omega_{-})^{\frac{N}{2}}}{4\pi x} \int_{-\infty}^{\infty} d\omega \frac{(2\omega - i(\omega_{+} - \omega_{-}))e^{i\omega x}}{(\omega - i\omega_{+})^{1+\frac{N}{2}}(\omega + i\omega_{-})^{1+\frac{N}{2}}}.$$
(60)

The analyticity of $P_{C,(t)}(x; \omega_+, \omega_-, N)$ for $\operatorname{Re}(N) > 0$ then follows because the first term above vanishes for $\operatorname{Re}(N > 0)$ and the integral in the second term is absolutely convergent for $\operatorname{Re}(N) > 0$.

Assuming x > 0, one can deform the integration contour of the integral given in Eq. (57) to the upper complex plane; see Fig. 1. For 0 < Re(N) < 2, the contribution of the integral over the semicircle below ω_+ vanishes as the radius of the semicircle goes to 0. Therefore, for 0 < Re(N) < 2,

$$P_{C_{\bullet}(t)}(x > 0; \omega_{+}, \omega_{-}, N) = \frac{(\omega_{+}\omega_{-})^{\frac{N}{2}}}{2\pi} 2 \sin\left(\frac{\pi N}{2}\right) \int_{\omega_{+}}^{\infty} dy \frac{\exp(-yx)}{(y - \omega_{+})^{\frac{N}{2}}(y + \omega_{-})^{\frac{N}{2}}} \\ = e^{\frac{1}{2}(\omega_{-} - \omega_{+})x} \left(\frac{\omega_{+}\omega_{-}}{\omega_{+} + \omega_{-}}\right)^{\frac{N}{2}} \frac{\sqrt{\omega_{+} + \omega_{-}}}{\sqrt{\pi}\Gamma(\frac{N}{2})} x^{\frac{N-1}{2}} K_{\frac{N-1}{2}} \left(\frac{1}{2}(\omega_{+} + \omega_{-})x\right),$$
(61)

where as before $K_n(x)$ is a modified Bessel function. Since this expression is analytic for Re(N) > 0, it can be continued to all Re(N) > 0.

Imposing the above relation between x > 0 and x < 0, the full distribution can be expressed compactly as

$$P_{C_{\bullet}(t)}(x;\omega_{+},\omega_{-},N) = e^{\frac{1}{2}(\omega_{-}-\omega_{+})x} \left(\frac{\omega_{+}\omega_{-}}{\omega_{+}+\omega_{-}}\right)^{\frac{N}{2}} \frac{\sqrt{\omega_{+}+\omega_{-}}}{\sqrt{\pi}\Gamma\left(\frac{N}{2}\right)} |x|^{\frac{N-1}{2}} K_{\frac{N-1}{2}}\left(\frac{1}{2}(\omega_{+}+\omega_{-})|x|\right).$$
(62)

For large times $K(t) \to 0$ and $\omega_{\pm} \to \frac{1}{\sigma^2}$ in Eq. (62), so it follows that



$$P_{C,(t)}^{(0)}(x;\sigma,N) = \lim_{t\to\infty,\beta\to\infty} P_{C,(t)}(x;\sigma^2)$$
$$= \frac{2^{\frac{1-N}{2}}\sigma^{-N-1}}{\Gamma\left(\frac{N}{2}\right)\sqrt{\pi}} |x|^{\frac{N-1}{2}} K_{\frac{N-1}{2}}\left(\frac{|x|}{\sigma^2}\right). \quad (63)$$

For N = 1, Eq. (63) reduces to the result found previously in Ref. [24], and more generally, this case is referred to as the Matérn covariance [29].

IV. NUMERICAL ANALYSIS FOR THE O(2) MODEL

In this section, the relations derived in Sec. III will be tested numerically for the case N = 2 in two dimensions. The action of the theory is given⁸ by

FIG. 1. The integration contour used to evaluate $P_{C_{\bullet}}(x;\omega_+, \omega_-, N)$ for x > 0.

⁸For these calculations, an adaptation of the publicly available code in Ref. [30] is used, where periodic boundary conditions are assumed and a heat bath algorithm is used to generate configurations.

$$S = \sum_{i} \left[\left(2 - \frac{\theta}{2} \right) |\psi_i|^2 + \frac{\chi}{4} |\psi_i|^4 \right] - \frac{1}{2} \sum_{\langle ij \rangle} \psi_i^* \psi_j + \psi_j^* \psi_i,$$
(64)

where *i* labels the sites, $\sum_{\langle ij \rangle}$ indicates summation over all pairs of neighboring points, θ and χ are the couplings, and ψ_i is a complex field [equivalent to the O(2) model]. The simulations are performed for various geometries $L \times \beta$ and for various sets of couplings that are parametrized by a single parameter *s* through the relations

$$\chi = -\ln s,$$

$$\theta = -\ln (1 - s).$$
(65)

To demonstrate the validity of the various results introduced in Secs. II and III, and in particular to test the assumptions made in deriving them, it is useful to consider the total variation \mathcal{T} between the empirical distribution E(q) determined from the numerical calculations and any proposed probability distribution P(q):

$$\mathcal{T} = \frac{1}{2} \int dq |E(q) - P(q)|. \tag{66}$$

This quantity is unity if the distributions have support on disjoint domains and vanishes when the distributions are identical. Results will be presented for $C_{\bullet}(t)$, so comparisons are made to the distributions $P_{C_{\bullet}}^{(0)}(t)$ valid at asymptotically large times [Eq. (63)] and to the improved distribution $P_{C_{\bullet}}(t)$ [Eq. (62)] that incorporates corrections to the asymptotic case. The asymptotic distribution depends on a single parameter (σ), and the improved distribution depends on two parameters (ω_{\pm}). In comparing the empirical distributions to these analytic forms, the following estimators for ω_{\pm} and σ are used. Assume that one has \mathcal{N} samples x_i of $C_{\bullet}(t)$, where $i \in \{1, ..., \mathcal{N}\}$. Then, estimators for ω_{\pm} and σ are given⁹ as

$$\hat{\omega}_{+} = \frac{1 - \sqrt{\frac{|\hat{x}| - \hat{x}}{|\hat{x}| + \hat{x}}}}{\hat{x}},$$
$$\hat{\omega}_{-} = \frac{\sqrt{\frac{|\hat{x}| + \hat{x}}{|\hat{x}| - \hat{x}}} - 1}{\hat{x}},$$
$$\hat{\sigma} = \sqrt{|\hat{x}|},$$
(67)

where \hat{x} and $|\hat{x}|$ are defined by

$$\hat{x} = \frac{1}{\mathcal{N}} \sum_{i} x_{i},$$
$$|\hat{x}| = \frac{1}{\mathcal{N}} \sum_{i} |x_{i}|.$$
(68)

In Fig. 2, the total variation is shown for a fixed geometry and couplings as a function of the temporal separation of the operators in the correlation function for various values of the number of samples used in the numerical calculations. Comparisons to both the asymptotic and improved distributions are shown. Since periodic temporal boundary conditions are used, the results are approximately symmetric around the midpoint of the



FIG. 2. The logarithm of the total variation as a function of temporal separation for three different sample sizes, \mathcal{N} , for s = 0.56, L = 100, $\beta = 40$ for the large-time limit in (a) and with the corrections in (b).

⁹The validity of these estimators, in the infinite sample size limit, follows from Eq. (11), noting that $P_{C,(t)}^{(0)}(x)$ is equivalent to $P_{C_{\rm Im}(t)}(x)$ with the identification $\omega_I(t) = \frac{1}{\sigma^2(t)}$.



FIG. 3. The logarithm of the total variation as a function of correlation function time for two choices of the temporal extent, β , with fixed values of s = 0.56, L = 100, $\mathcal{N} = 10^6$ for the large-time limit in (a) and with the corrections in (b).

temporal extent. As can be seen, the sample size sets a lower floor on the total variation in both cases, but results for $\mathcal{N} = 10^6$ samples are sufficient to cleanly resolve deviations from the asymptotic distribution, with that deviation achieving its minimum around the temporal midpoint. For the improved distribution, the total variation has not saturated even at $\mathcal{N} = 10^6$ and should be viewed as an upper bound on the true total variation.

Figure 3 shows the dependence of the total variation on the temporal extent of the lattice geometry for fixed spatial extent and a single choice of the couplings. Similarly, Fig. 4 shows the dependence of the total variation on the spatial lattice extent for a fixed set of couplings and temporal extent. In both figures, the total variation is shown in



FIG. 4. The logarithm of the total variation as a function of correlation function time for four values of the spatial extent, L, with a fixed choice of s = 0.56, $\beta = 40$, $\mathcal{N} = 10^6$ for the large-time limit in (a) and with the corrections in (b).

comparison to the asymptotic and improved probability distributions. As can be seen in Fig. 3, the temporal extent of the lattice geometry significantly affects the total variation, with the periodicity requirement competing against the approach of the correlation function to the asymptotic distribution. Even for the improved distribution, deviations of the total variation are statistically resolved when the correlation function is measured for short time separations (including the effects of periodicity). The behavior of the total variation with respect to the spatial volume seen in Fig. 4 is in agreement with the discussions in the previous sections. As the spatial volume increases for a fixed t, the empirical distributions of the correlation function approach the analytic forms derived above assuming the infinite volume limit. For the couplings chosen in Fig. 4,



FIG. 5. The logarithm of the total variation as a function of the temporal separation for various values of the parameter *s* that determines the couplings. Fixed values of L = 100, $\beta = 40$, and $\mathcal{N} = 10^6$ are used and results are shown for the large-time limit in (a) and with the corrections in (b).

L = 100 is sufficient to see agreement with the asymptotic result, at least to the precision allowed by the finite sample size.

Figure 5 show the variation of the total variation with respect to the parameter *s* that determines the couplings through Eq. (65). As *s* increases from s = 0 toward $s \sim 0.6$, the theory moves toward the critical surface that separates the quasiordered and disordered phases. As this surface is approached, the correlation length diverges, and as a consequence, the temporal separation of the correlation function and the spatial and temporal extents of the lattice geometry necessary to see agreement with the results in Secs. II and III (to a given accuracy) are correspondingly larger. As seen in Fig. 5, for larger values of *s*, corresponding to larger correlation lengths, the contamination from



FIG. 6. The logarithm of the total variation with respect to the improved distribution as a function of the temporal separation in the correlation function for various different spatial extents *L*, for $\beta = 40$, $\mathcal{N} = 10^6$, and s = 0.59.

nonasymptotic contributions is more significant. This is particularly apparent for the total variation with respect to the asymptotic distribution, Eq. (63), but the trend is also seen in the deviation from the improved distribution, Eq. (62). A similar effect is seen comparing Figs. 6 and 4(b), which only differ in the value of *s* that is used; clearly, for the case with the larger correlation length, larger deviations from the improved distribution are seen.

The numerical results above summarized through calculations of the total variation with respect to the asymptotic and improved distributions provide strong evidence for the validity of the assumptions that have been used to derive the results of the previous sections. To provide further support, Figs. 7–9 show histograms of the empirical probability distributions for the real part of the correlation function $P_{C.(t)}$ obtained for various couplings and geometries at representative temporal separations. As has been seen in studies of correlation function distributions in other contexts [8–10,16,19,23], the distributions are strongly asymmetric under reflection about x = 0 at small times but become increasingly symmetric as *t* increases. Note that in all cases, the distributions have support for x < 0 and so are not describable by log-normal distributions [19].

Figures 7–9 also show the best fits for the asymptotic and improved analytic distributions in each case. As can be seen from the figures, for large enough spatial volume, the improved distribution accurately describes the histograms for all of the temporal separations that are presented. The asymptotic distribution (necessarily symmetric about x = 0) provides a poor description at small times, but the disagreement decreases as *t* increases.

Finally, in Fig. 10, histograms of the phase differences between the spatially averaged fields at 0 and t are





FIG. 7. Probability distribution of $C_{\bullet}(t)$ for s = 0.52, $L = 40, \beta = 40$, and $\mathcal{N} = 10^6$ for t = 1 in (a), for t = 10 in (b), and for t = 19 in (c). Improved and asymptotic (asym) distributions are as described in the text.

FIG. 8. Probability distribution of $C_{\bullet}(t)$ for s = 0.59, $L = 40, \beta = 40$, and $\mathcal{N} = 10^6$ for t = 1 in (a), for t = 10 in (b), and for t = 19 in (c). Improved and asymptotic (asym) distributions are as described in the text.





FIG. 9. Probability distribution of $C_{\bullet}(t)$ for s = 0.59, $L = 130, \beta = 40$, and $\mathcal{N} = 10^6$ for t = 1 in (a), for t = 10 in (b), and for t = 19 in (c). Improved and asymptotic (asym) distributions are as described in the text.

FIG. 10. Probability distribution of the phase difference for s = 0.56, L = 130, $\beta = 40$, and $\mathcal{N} = 10^6$ for t = 1 in (a), for t = 10 in (b), and for t = 19 in (c).

presented for various times for s = 0.56. As seen in previous studies [8,9,23], these phase distributions become increasingly broad as *t* increases. The figure also shows fits of the asymptotic phase distribution given in Eq. (15) to these histograms; in all cases, this form provides an accurate description of the histograms, significantly improving on an assumption of wrapped normality made in previous studies [10].

V. IMPROVED ESTIMATORS

In this section, an improved estimator for the mean of $C_{\text{Re}}(t)$ will be presented. A detailed discussion of the concepts and examples considered in this section can be found in Ref. [31]. According to the Cramér-Rao bound, a classical result in estimation theory, if $\hat{\theta}$ is an unbiased estimator¹⁰ of a parameter θ , its variance $\text{Var}(\hat{\theta})$ satisfies the bound,

$$\operatorname{Var}(\hat{\theta}) \ge \frac{1}{\mathcal{N}I(\theta)},$$
 (69)

where \mathcal{N} is the sample size and $I(\theta)$ is the Fisher information defined by

$$I(\theta) = \int_{-\infty}^{\infty} dx P(x;\theta) \left(\frac{d\log P(x;\theta)}{d\theta}\right)^2, \quad (70)$$

where $P(x;\theta)$ is the distribution of the samples, parametrized by θ . Asymptotically, when the maximum likelihood estimator exists, it saturates the Cramér-Rao bound and therefore has the least variance among all unbiased estimators. However, in some cases, there are other examples of minimum-variance unbiased estimators for finite sample size. As a simple example,¹¹ if one considers the uniform distribution supported on the interval $[0, \theta]$, the minimum-variance unbiased estimator of the mean of θ is given by

$$\hat{\mu}_{U,mvue} = \frac{\mathcal{N}+1}{2\mathcal{N}} \max_{i} x_{i}.$$
(71)

In fact, for this example, the ratio of the variance of the minimum-variance unbiased estimator defined above to the variance of the sample mean $\hat{\mu}_{U,sm}$ can be calculated easily and is found to be

$$\frac{\operatorname{Var}(\hat{\mu}_{U,mvue})}{\operatorname{Var}(\hat{\mu}_{U,sm})} = \frac{3}{\mathcal{N}+2},$$
(72)

which vanishes as the sample size goes to infinity. In certain cases, an estimator with smaller mean squared error¹² (MSE) can be constructed if a bias is accepted. For example, for the example considered above, a biased estimator $\hat{\mu}_{U,b}$ can be constructed as

$$\hat{\mu}_{U,b} = \frac{\mathcal{N} + 2}{2(\mathcal{N} + 1)} \max_{i} x_i, \tag{73}$$

whose MSE is less than that of $\hat{\mu}_{U,mvue}$.

In the context of the O(2) model correlation functions, using the analytic form of the PDF in Eq. (11) for the real part of the correlation function, it can be shown that the sample mean $\hat{\mu}_{\text{Re},sm}$ is efficient within the class of unbiased estimators of μ_{Re} . According to the bivariate generalization of the Cramér-Rao bound, given the parameters $\vec{\theta} = \{\theta_1, \theta_2\}$, the variance of the an unbiased estimator \hat{T} of a quantity $T = T(\theta_1, \theta_2)$ is given by

$$\operatorname{Var}(\hat{T}) \ge \frac{1}{\mathcal{N}} \sum_{i,j=1}^{2} \frac{\partial T}{\partial \theta_i} \frac{\partial T}{\partial \theta_j} I_{ij}^{-1}, \tag{74}$$

where I_{ij} is defined by

$$I_{ij} = \int_{-\infty}^{\infty} dx P(x; \vec{\theta}) \frac{\partial \log P(x; \vec{\theta})}{\partial \theta_i} \frac{\partial \log P(x; \vec{\theta})}{\partial \theta_j}.$$
 (75)

It is convenient to choose the parameters as $\theta_1 = \omega_{\text{Re},+}$, $\theta_2 = \omega_{\text{Re},-}$. From Eq. (11), it follows that

$$\mu_{\rm Re} = \frac{1}{\omega_{R,+}} - \frac{1}{\omega_{R,-}},$$

$$\sigma_{\rm Re}^2 = \frac{1}{\omega_{R,+}^2} + \frac{1}{\omega_{R,-}^2}.$$
 (76)

Choosing $T = \mu_{\text{Re}}$, it is found from Eqs. (74) and (76) that $\operatorname{Var}(\hat{T}) \geq \frac{1}{N} \sigma_{\text{Re}}^2$ for all unbiased estimators \hat{T} of T. For the sample mean $\hat{\mu}_{\text{Re},sm} = \frac{1}{N} \sum_{i=1}^{N} x_i$, the variance is $\operatorname{Var}(\hat{\mu}_{\text{Re},sm}) = \frac{1}{N} \sigma_{\text{Re}}^2$, so the sample mean is the minimum variance unbiased estimator in this case.

The PDF of $C_{\text{Re}}(t)$ given in Eq. (11) also allows for the construction of improved estimators that outperform the sample mean of $C_{\text{Re}}(t)$. In particular, a biased estimator for μ_{Re} can be defined as

$$\hat{\mu}_{\text{Re},b} = \frac{1}{\mathcal{N}+1} \sum_{i=1}^{\mathcal{N}} x_i.$$
 (77)

The mean squared error for $\hat{\mu}_{\text{Re},b}$ is given by

¹⁰In what follows, "hats" will be used to denote estimators, which depend on the given sample and therefore are random variables.

¹¹In this case, the Fisher information $I(\theta)$ is divergent, and therefore the Cramér-Rao bound is not available.

¹²The MSE of an estimator $\hat{\mu}$ of μ is defined by $MSE(\hat{\mu}) = \langle (\hat{\mu} - \mu)^2 \rangle$.

$$MSE(\hat{\mu}_{Re,b}) = \langle (\hat{\mu}_{Re,b} - \mu_{Re})^2 \rangle \\ = \left\langle \frac{1}{(\mathcal{N}+1)^2} \left(\sum_{i=1}^{\mathcal{N}} x_i \right)^2 - \frac{2}{\mathcal{N}+1} \mu_{Re} \sum_{i=1}^{\mathcal{N}} x_i + \mu_{Re}^2 \right\rangle \\ = \frac{1}{(\mathcal{N}+1)^2} (\mathcal{N}(\sigma_{Re}^2 + \mu_{Re}^2) + \mathcal{N}(\mathcal{N}-1)\mu_{Re}^2) - \frac{\mathcal{N}-1}{\mathcal{N}+1} \mu_{Re}^2 \\ = \frac{\mathcal{N}\sigma_{Re}^2 + \mu_{Re}^2}{(\mathcal{N}+1)^2}.$$
(78)

From Eq. (76) and the form of the PDF, it follows that $\sigma_{\text{Re}}^2 > \mu_{\text{Re}}^2$. Therefore, $\text{MSE}(\hat{\mu}_{\text{Re},b}) < \frac{\sigma_{\text{Re}}^2}{N+1}$, and

$$\frac{\text{MSE}(\hat{\mu}_{\text{Re},b})}{\text{MSE}(\hat{\mu}_{\text{Re},sm})} < \frac{\mathcal{N}}{\mathcal{N}+1},$$
(79)

showing that $\hat{\mu}_{\text{Re},b}$ is a marginally more efficient estimator of the mean than the sample mean, albeit a biased one. The bias of $\hat{\mu}_{\text{Re},b}$ can be calculated easily and is found to be

$$\operatorname{Bias}(\hat{\mu}_{\operatorname{Re},b}) = -\frac{\mu_{\operatorname{Re}}}{\mathcal{N}+1},\tag{80}$$

which vanishes as $\mathcal{N} \to \infty$. While $\hat{\mu}_{\text{Re},b}$ is only marginally more efficient than the sample mean for $\mathcal{N} \to \infty$, other biased estimators may exist that improve on this behavior. With recent interest in so-called "master field" Monte Carlo calculations [32], where a small number of samples of large volume lattice geometries are envisioned, even improvements that are only significant at finite sample sizes are of interest.

The validity of improved estimators such as $\hat{\mu}_{\text{Re},b}$ rests on the use of data that arise from asymptotically large volumes such that the distributions derived in Sec. III apply. Before such estimators are used, it is important to assess whether deviations from the predicted distributions are empirically apparent.

VI. CONCLUSIONS

In the present work, the exact probability distributions of the two-point correlation functions of the O(N) model in the disordered phase at vanishing spatial momentum and infinite volume have been derived. Numerical tests have been performed for the N = 2 case and are found to support the assumptions needed in the analytic derivations. Note that the results presented here fundamentally rest on the basic principles of (three-dimensional) volume averaging and the Gaussian nature of fluctuations; the key results in this work are the applications of these concepts to correlations between these fluctuations as relevant for the particular statistical questions being investigated. While the theories discussed in the present work are relatively simple, the insights gained from having an analytic description of the PDF of correlation functions are quite far reaching. They provide a means of assessing the reliability of numerical Monte Carlo calculations and an alternative method whereby the spectrum of a theory can be accessed from a single time slice [24]. As shown in Sec. V for the case of the O(2) model, knowledge of the PDF allows better estimators of the expectation value of a correlation function than the sample mean. If such estimators could be found for the expectation values of correlation functions in lattice quantum field theories in general, it would provide an interesting path toward addressing the commonly occurring signal-to-noise problem.

As discussed earlier, the arguments presented here generalize readily to correlation functions of bosonic theories without an O(N) symmetry, although the expressions for the PDFs become more complicated. For N = 1, the discussion above can be¹³ extended to the case of the broken phase by expressing the probability distributions as a superposition of correlation function distributions associated with the multiple different vacua. For N > 1, the broken phase has Goldstone bosons and therefore has infinite correlation length in the absence of explicit symmetry breaking. Consequently, the arguments presented here do not immediately generalize to this case. In principle, the arguments used in this study can be applied to higher-point correlation functions, although the resulting expressions for PDFs are expected to be more complicated. Finally, it is likely that the framework developed here can be adapted to correlation functions of glueball interpolating operators and of large Wilson loops in pure gauge theories. These directions will be explored in subsequent work.

¹³Except when d = 1. In this case, solitonic vacua also appear, and as these vacua do not have a mass gap, further discussion is needed.

ACKNOWLEDGMENTS

We are grateful to M. L. Wagman for discussions and E. T. Neil for comments. This work is supported by the National Science Foundation under Cooperative Agreement PHY-2019786 (the NSF AI Institute for Artificial Intelligence and Fundamental Interactions and by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Contract No. DE-SC0011090. W. D. is also supported by the SciDAC5 Grant No. DE-SC0023116.

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