

High-temperature correlation functions: Universality, extraction of exchange interactions, divergent correlation lengths, and generalized Debye length scales

Saurish Chakrabarty¹ and Zohar Nussinov^{1,2}¹*Department of Physics and Center for Materials Innovation, Washington University in St Louis, Missouri 63130, USA*²*Kavli Institute for Theoretical Physics, Santa Barbara, California 93106, USA*

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We derive a universal form for the correlation function of general n -component systems in the limit of high temperatures or weak coupling. This enables the extraction of effective microscopic interactions from measured high-temperature correlation functions. We find that in systems with long-range interactions, there exist diverging correlation lengths with amplitudes that tend to zero in the high-temperature limit. For general systems with disparate long-range interactions, we introduce the notion of generalized Debye length (and time) scales and further relate these to the divergence of the largest correlation length in the high-temperature (or weak-coupling) limit.

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I. INTRODUCTION

The study of correlation functions in systems with multicomponent fields is an extremely general problem having incarnations that range from systems in condensed matter physics to fundamental field theories. One of the cornerstones of field theories and the study of critical phenomena is the recognition of the universality that underlies general systems. This enables a unified understanding and potent tools of analysis.¹⁻³ Any system generally displays a disordered high-temperature (T) fixed point. Most of the research to date has focused on the behavior of myriad systems at and in the vicinity of various finite-temperature transitions. In this work, we will focus on high-temperature behavior and illustrate that a simple form of the two-point correlation function is universally exact for rather general systems. This enables us to make several striking observations. In particular, we will demonstrate that, in contrast to common intuition, general systems with long-range interactions have a correlation length that increases monotonically with temperature as $T \rightarrow \infty$. As they must, however, the correlations decay monotonically with temperature (as the corresponding amplitudes decay algebraically with temperature). There have been no earlier reports of diverging correlation lengths at high temperature to our knowledge. A thermally increasing length scale of a seemingly very different sort appears in plasmas.⁴ The Debye length, the distance over which screening occurs in a plasma, diverges, at high temperature, as $\lambda_D \propto \sqrt{T}$. We introduce the notion of a *generalized Debye length* associated with disparate long-range interactions (including confining interactions) and show that such screening lengths are rather general.

Many early works investigated the high-temperature disordered phase via a high-temperature series expansion⁵ with an eye toward systems with short-range interactions. In this paper, we report on our universal result for the Fourier-transformed correlation function for systems with general pair interactions. As it must, for nearest-neighbor interactions, our correlation function agrees with what is suggested by standard approximate methods [e.g., the Ornstein-Zernike (OZ) correlation function that may be derived by many approximate schemes⁶]. Our work places such approximate

results on a more rigorous footing and, perhaps most notably, enables us to go far beyond standard short-range interactions to find rather surprising results. Our derivations will be done for spin and other general lattice systems with multicomponent fields. However, as illustrated later, our results also pertain to continuum theories.

II. OUTLINE

In Sec. III, we introduce the systems we study (general multicomponent spin systems on a lattice; later sections generalize our result to other arenas—fluids, Bose and Fermi systems, and so on). Section IV contains a derivation of our main result about the universal form of the correlation function in the high-temperature limit. In Sec. V, we comment on how the correlation lengths in a system behave in the high-temperature limit. Section VI introduces a generalized Debye length. In Sec. VII, we present some generalizations of our result to systems which are not covered in Sec. III. Section VIII outlines standard approximate techniques used to obtain our result. We give our concluding remarks in Sec. IX.

In Appendix A, we show how to obtain a full high-temperature series expansion of the correlation function to arbitrary order. In Appendix B, we relate the generalized Debye length over which long-range interactions are screened to the diverging correlation length present in the high-temperature limit.

III. SYSTEMS OF STUDY

We consider a translationally invariant system with the Hamiltonian

$$H = \frac{1}{2} \sum_{\vec{x} \neq \vec{y}} V(|\vec{x} - \vec{y}|) \vec{S}(\vec{x}) \cdot \vec{S}(\vec{y}). \quad (1)$$

The sites \vec{x} and \vec{y} lie on a d -dimensional hypercubic lattice with N sites having unit lattice constant. The quantities $\{\vec{S}(\vec{x})\}$ portray n -component spins [“ $O(n)$ spins”] or general fields where $|\vec{S}(\vec{x})|^2 = n$ at all lattice sites \vec{x} . The normalization is adopted from Ref. 7. The case of $n = 1$ corresponds to Ising

spins, $n = 2$ to XY spins, and so on. We assume that whenever the interaction kernel $V(x)$ has a long-range component, that component (unless stated otherwise) will always have some *finite screening*, however small. This restriction is imposed to avoid well-known difficulties in taking thermodynamic limits in long-range systems. In what follows, $v(\vec{k})$ and $s_i(\vec{k})$ are the Fourier transforms of $V(|\vec{x} - \vec{y}|)$ and $S_i(\vec{x})$. With this, Eq. (1) reads $H = \frac{1}{2N} \sum_{\vec{k}} v(\vec{k}) \vec{s}(\vec{k}) \cdot \vec{s}(-\vec{k})$, up to an innocuous constant. Throughout, we employ the Fourier transform convention of $a(\vec{k}) = \sum_{\vec{x}} A(\vec{x}) e^{i\vec{k} \cdot \vec{x}}$ [and $A(\vec{x}) = \frac{1}{N} \sum_{\vec{k}} a(\vec{k}) e^{-i\vec{k} \cdot \vec{x}}$].

IV. THE UNIVERSAL FORM OF THE HIGH-TEMPERATURE CORRELATION FUNCTIONS

We now derive a universal form for the correlation function at high temperature. As in any other calculation with Boltzmann weights, the high-temperature limit is synonymous with weak coupling. Initially, we follow standard procedures and examine a continuous but exact dual theory. High T (or weak coupling) in the original theory corresponds to strong coupling in the dual theory. We will then proceed to examine the consequences of the dual theory at high temperature where the strong-coupling interaction term dominates over other nonuniversal terms that depend, e.g., on the number of components in the original theory. This enables an analysis with general results. Unlike most treatments that focus on the character of various phases and intervening transitions, our interest here is strictly in the *high-temperature limit of the correlation functions* in rather general theories of Eq. (1). Our aims are (i) to make conclusions concerning systems with long range interactions rigorous and (ii) to extract microscopic interactions from measurements. It is notable that due to convergence time constraints many numerical approaches, e.g., Ref. 8, compare candidate potentials with experimental data at high temperature (above the melting temperatures) where the approach that we will outline is most applicable. We will perform a transformation to a continuous but exact dual theory where the high-temperature character of the original theory can be directly examined.

We augment the right-hand side of Eq. (1) by $[-\sum_{\vec{x}} \vec{h}(\vec{x}) \cdot \vec{S}(\vec{x})]$ and differentiate in the limit $\vec{h} \rightarrow 0$ to obtain correlation functions in the usual way:

$$G(\vec{x} - \vec{y}) = \frac{1}{n} \langle \vec{S}(\vec{x}) \cdot \vec{S}(\vec{y}) \rangle = \lim_{h \rightarrow 0} \frac{1}{n\beta^2 Z} \sum_{i=1}^n \frac{\delta^2 Z}{\delta h_i(\vec{x}) \delta h_i(\vec{y})}, \quad (2)$$

with Z the partition function in the presence of the external field \vec{h} . By spin normalization, $G(\vec{x}) = 1$ for $\vec{x} = \vec{0}$. The index $i = 1, 2, \dots, n$ labels the n internal spin (or field) components. The partition function $Z = \text{Tr}_S[\exp(-\frac{\beta}{2N} \sum_{\vec{k}} v(\vec{k}) |\vec{s}(\vec{k})|^2 + \beta \sum_{\vec{x}} \vec{h}(\vec{x}) \cdot \vec{S}(\vec{x}))]$. The subscript S denotes the trace with respect to the spins. Using the Hubbard-Stratonovich (HS)

transformation,^{9,10} we introduce the dual variables $\{\vec{\eta}(\vec{x})\}$ and rewrite the partition function as

$$Z = \text{Tr}_S \left[\prod_{\vec{k}, i} \left(\{2\pi[-v(\vec{k})]\}^{-1/2} \times \int_{-\infty}^{\infty} d\eta_i(\vec{k}) e^{[N/2\beta v(\vec{k})] |\eta_i(\vec{k})|^2 + \eta_i(\vec{k}) s_i(-\vec{k})} \right) \prod_{\vec{x}} e^{\beta \vec{h}(\vec{x}) \cdot \vec{S}(\vec{x})} \right] \quad (3)$$

$$= \mathcal{N} \text{Tr}_S \left[\int d^{Nn} \eta \exp \left(\frac{N^2}{2\beta} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) + N \sum_{\vec{x}} \vec{\eta}(\vec{x}) \cdot \vec{S}(\vec{x}) + \beta \sum_{\vec{x}} \vec{h}(\vec{x}) \cdot \vec{S}(\vec{x}) \right) \right], \quad (4)$$

with $V^{-1}(\vec{x})$ the inverse Fourier transform of $1/v(\vec{k})$ and \mathcal{N} a numerical prefactor. The physical motivation in performing the duality to the HS variables is that we wish to retain the exact character of the theory [i.e., the exact form of the interactions and the $O(n)$ constraints concerning the spin normalization at all lattice sites]. It is for this reason that we do not resort to a continuum approximation (such as that of the canonical ϕ^4 theory that we will discuss for comparison later on) where normalization is not present. Another reason to choose to work in the dual space is the correspondence with field theories which, in the dual space, becomes clearer in the high-temperature limit (in which the quartic term of the ϕ^4 theories becomes irrelevant). Further details are in Ref. 11. For $O(n)$ spins,

$$Z = \mathcal{N}' \int d^{Nn} \eta \times \left[\exp \left(\frac{N^2}{2\beta} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) \right) \times \prod_{\vec{x}} \frac{I_{n/2-1}[\sqrt{n}|N\vec{\eta}(\vec{x}) + \beta\vec{h}(\vec{x})|]}{[\sqrt{n}|N\vec{\eta}(\vec{x}) + \beta\vec{h}(\vec{x})|]^{n/2-1}} \right]. \quad (5)$$

The second factor in Eq. (5) originates from the trace over the spins and as such embodies the $O(n)$ constraints (the trace in Eq. (4) is performed over all configurations with $[\vec{S}(\vec{x})]^2 = n$ at all sites \vec{x}). Here, $I_\nu(x)$ is the modified Bessel function of the first kind. In the Ising ($n = 1$) case, the argument of the product in Eq. (5) is a hyperbolic cosine. Up to an innocuous additive constant, Eq. (5) corresponds to the dual Hamiltonian

$$H_d = -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) - \frac{1}{\beta} \sum_{\vec{x}} \ln \left(\frac{I_{n/2-1}[\sqrt{n}|N\vec{\eta}(\vec{x}) + \beta\vec{h}(\vec{x})|]}{[\sqrt{n}|N\vec{\eta}(\vec{x}) + \beta\vec{h}(\vec{x})|]^{n/2-1}} \right). \quad (6)$$

Our interest is in the $h \rightarrow 0$ limit. The first term in Eq. (6) is the same for all n . This term dominates, at low β , over the (second) n -dependent term. As we will see, this dominance

will enable us to get universal results for all n . From Eq. (2) and the identity

$$\frac{d}{dx} \left[\frac{I_v(x)}{x^v} \right] = \frac{I_{v+1}(x)}{x^v},$$

we find that

$$G(\vec{x} - \vec{y}) = \delta_{\vec{x}, \vec{y}} + (1 - \delta_{\vec{x}, \vec{y}}) \left\langle \frac{\vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y})}{|\vec{\eta}(\vec{x})| |\vec{\eta}(\vec{y})|} \right\rangle_d \times \frac{I_{n/2}[N\sqrt{n}|\vec{\eta}(\vec{x})|] I_{n/2}[N\sqrt{n}|\vec{\eta}(\vec{y})|]}{I_{n/2-1}[N\sqrt{n}|\vec{\eta}(\vec{x})|] I_{n/2-1}[N\sqrt{n}|\vec{\eta}(\vec{y})|]} \Bigg|_d, \quad (7)$$

where the average ($\langle \cdot \rangle_d$) is performed with the weights $\exp(-\beta H_d)$. Now, here is a crucial idea regarding our exact dual forms. From Eq. (3), at high temperature, the variables $\eta_i(\vec{k})$ strictly have sharply peaked Gaussian distributions of variance,

$$\langle |\eta_i(\vec{k})|^2 \rangle_d \approx \frac{-\beta v(\vec{k})}{N} \quad \text{as } \beta \rightarrow 0. \quad (8)$$

Importantly, this variance tends to zero as $\beta \rightarrow 0$. By Parseval's theorem and translational invariance,

$$\begin{aligned} \langle [|\eta_i(\vec{x})|^2]_d \rangle &= \frac{1}{N} \sum_{\vec{x}} \langle [|\eta_i(\vec{x})|^2]_d \rangle \\ &= \frac{1}{N^2} \sum_{\vec{k}} \langle |\eta_i(\vec{k})|^2 \rangle_d \approx -\beta V(0)/N^2. \end{aligned}$$

Thus, at high temperature, $\langle [|\eta_i(\vec{x})|^2] \rangle \ll 1$. It is therefore useful to perform a series expansion in the dual variables η and this will give rise to a high-temperature series expansion in the correlation function. The Hamiltonian in dual space is given by,

$$\begin{aligned} H_d &= -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) - \frac{N^2}{2\beta} \sum_{\vec{x}, i} \eta_i(\vec{x})^2, \\ &= -\frac{N}{2\beta^2} \sum_{\vec{k}, i} \frac{1}{v(\vec{k})} |\eta_i(\vec{k})|^2 - \frac{N}{2\beta} \sum_{\vec{k}, i} |\eta_i(\vec{k})|^2, \end{aligned} \quad (9)$$

with errors of $\mathcal{O}(1/T)$. Expanding Eq. (7) to $\mathcal{O}(1/T^2)$,

$$G(\vec{k}) = \frac{k_B T}{v(\vec{k}) + k_B T} + \frac{1}{N} \sum_{\vec{k}'} \frac{v(\vec{k}')} {v(\vec{k}') + k_B T}. \quad (10)$$

Equation (10) leads to counterintuitive consequences for systems with long-range interactions. The second term in Eq. (10) is independent of \vec{k} and ensures that $G(\vec{x}) = 1$ for $\vec{x} = \vec{0}$. Inverting this result enables us to find the microscopic (spin exchange or other) interactions from the knowledge of the high-temperature correlation function. We thus flesh out (and further generalize for multicomponent systems such as spins) the mathematical uniqueness theorem of Henderson for fluids,¹² for which a known correlation function $G(\vec{x})$ leads to a known pair potential function $V(\vec{x})$ up to an innocuous constant. Equation (10) leads to a correlation function which is independent of $V(0)$. Therefore, we can shift $v(\vec{k})$ for all \vec{k} 's

by an arbitrary constant or equivalently set $V(0)$ to an arbitrary constant. To $\mathcal{O}(1/T)$, for $V(0) = 0$, we have

$$v(\vec{k}) = \frac{k_B T}{G(\vec{k})} - \frac{1}{N} \sum_{\vec{k}'} \frac{k_B T}{G(\vec{k}')}. \quad (11)$$

The leading term of this expression for $v(\vec{k})$ does not scale with T . This is so as $[1 - G(\vec{k})] \propto 1/T$ at high temperatures. Correlation functions obtained from experimental data can be plugged into the right-hand side to obtain the effective pair potentials. Alternatively, in real space, for $\vec{x} \neq \vec{0}$,

$$V(\vec{x}) = -k_B T G(\vec{x}) + k_B T \sum_{\vec{x}' \neq \vec{0}, \vec{x}} G(\vec{x}') G(\vec{x} - \vec{x}'). \quad (12)$$

Note that the two terms in Eq. (12) are $\mathcal{O}(1)$ and $\mathcal{O}(1/T)$, respectively, since $G(\vec{x})$ is proportional to $1/T$ at high temperature for $\vec{x} \neq \vec{0}$. Extension to higher orders may enable better comparison to experimental or numerical data. Our expansion is analytic in the high-temperature phase (i.e., so long as no transitions are encountered as $1/T$ is increased from zero). The Gaussian form of Eq. (9) similarly leads to the free energy density,

$$F = \frac{k_B T}{2N} \sum_{\vec{k}} \ln \left| \frac{k_B T}{v(\vec{k})} + 1 \right| + \mathcal{O}(1/T). \quad (13)$$

Armed with Eqs. (9) and (10), we can compute any correlation function with the aid of Wick's theorem. For example, for unequal \vec{k}_i 's, we have $\langle [\vec{s}(k_1) \cdot \vec{s}(-k_1)] \cdots [\vec{s}(k_m) \cdot \vec{s}(-k_m)] \rangle = (Nn)^m \prod_{i=1}^m G(\vec{k}_i)$.

It is straightforward to carry out a full high-temperature series expansion of the correlation function to arbitrary order. This is outlined in Appendix A. For example, when $V(\vec{x} = 0) = 0$, the real space correlation function for separations $\vec{x} \neq 0$ is, to order $\mathcal{O}(1/T^3)$, given by

$$\begin{aligned} G(\vec{x}) &= -\frac{V(\vec{x})}{k_B T} + \frac{1}{(k_B T)^2} \sum_{\vec{z}} V(\vec{z}) V(\vec{x} - \vec{z}) \\ &\quad - \frac{1}{(k_B T)^3} \left[\sum_{\vec{y}, \vec{z}} V(\vec{y}) V(\vec{z}) V(\vec{x} - \vec{y} - \vec{z}) \right. \\ &\quad \left. - 2V(\vec{x}) \sum_{\vec{z}} V(\vec{z}) V(-\vec{z}) + 2 \frac{[V(\vec{x})]^3}{n+2} \right]. \end{aligned} \quad (14)$$

V. HIGH-TEMPERATURE CORRELATION LENGTHS

We now illustrate that (i) in systems with short- (or finite-) range interactions, the correlation length tends to zero in the high-temperature limit and (ii) in systems with long-range interactions¹³ the high-temperature correlation length tends to the screening length and diverges in the absence of screening.

A. Decaying length scales

We consider first the standard case of short-range interactions. On a hypercubic lattice in d spatial dimensions, nearest-neighbor interactions have the lattice Laplacian $\Delta(\vec{k}) = 2 \sum_{l=1}^d (1 - \cos k_l)$, with k_l the l th Cartesian component of the wave vector \vec{k} as their Fourier transform. In

the continuum (small- k) limit, $\Delta \sim |\vec{k}|^2$. Generally, in the continuum, arbitrary finite-range interactions of spatial range p have $v(\vec{k}) \sim |\vec{k}|^{2p}$ with $p > 0$ (and superpositions of such terms) as their Fourier transforms. In general finite-range interactions, similar multinomials in $(1 - \cos k_i)$ and in k_j^2 appear on the lattice and the continuum, respectively. For simplicity, we consider $v(\vec{k}) \sim |\vec{k}|^{2p}$. Correlation lengths are determined by the reciprocal of the imaginary part of the poles of Eq. (10), $|\text{Im}\{k_*\}|^{-1}$. We then find that in the complex k plane $(k_*)^{2p} \sim -k_B T$. Poles are given by $k_* \sim (k_B T)^{1/(2p)} \exp[(2m+1)\pi i/(2p)]$ with $m = 0, 1, \dots, 2p-1$. Correlation lengths then tend to zero in the high-temperature limit as $\xi \sim T^{-1/(2p)} / |\sin(2m+1)\pi/(2p)|$ —there are p such correlation lengths. Similarly, there are p periodic modulation lengths scaling as $L_D \sim 2\pi T^{-1/(2p)} / |\cos(2m+1)\pi/(2p)|$. The usual case of $p = 1$ corresponds to an infinite L_D [i.e., spatially uniform (nonperiodic) correlations] and $\xi \sim T^{-1/2}$.

B. Diverging length scales

An unusual feature arises in the high-temperature limit of systems with long-range interactions where $v(\vec{k})$ diverges in the small- k limit. Such a divergence enables the correlator of Eq. (10) to have a pole at low k and consequently, on Fourier transforming to real space, to have a divergent correlation length. In the presence of screening $v(\vec{k})$ diverges and $G(k)$ has a pole when the imaginary part of k is equal to the reciprocal of the screening length. The correlation length then tends to the screening length at high temperature. For concreteness, we consider generic screened interactions where the Fourier-transformed interaction kernel $v_L(k) \sim \frac{1}{(k^2 + \lambda^{-2})^{p'}}$ with $p' > 0$ and λ the screening length. Perusing the poles of Eq. (10), we find that, for all p' , the correlation lengths tend to the screening length in the high-temperature limit,

$$\lim_{T \rightarrow \infty} \xi(T) = \lambda. \quad (15)$$

From Eq. (15), when λ becomes arbitrarily large, the *correlation length diverges*. Physically, such correlations enable global “charge neutrality”¹⁴ for the corresponding long-range interactions (Coulomb or other). This general divergence of high-temperature correlation lengths in systems with long-range interactions is related to the effective range of the interactions. At high temperature, the correlation function matches the “direct” contribution, $e^{-\beta V_{\text{eff}}(\vec{r})} - 1 \sim -\beta V_{\text{eff}}(\vec{r})$. If the effective interactions between two fields have a range λ , then that is reflected in the correlation length. In Coulomb systems, the Debye length λ_D sets the range of the interactions (for large distances, the interactions are screened). As stated earlier, at high temperature, λ_D diverges. As we see by Fourier-transforming Eq. (10), although the imaginary part of the poles tends to zero (and thus the correlation lengths diverge), the prefactor multiplying $e^{-|\vec{x}|/\xi}$ is a monotonically decaying function of T . Thus in the high-temperature limit the real space correlator $G(\vec{x})$ monotonically decays with temperature (as it must). For instance, for $p' = 1$ in $d = 3$ dimensions, the pair correlator $G(x) \sim e^{-x/\lambda}/(Tx)$ tends, for any non-zero x , to zero as $T \rightarrow \infty$.¹⁵ That is, *the amplitude vanishes* in the high-temperature limit as $(1/T)$. We find similar results when we have more than one interaction. For

instance, in the presence of both a short- and a long-range interaction, (at least) two correlation lengths are found. One correlation length (or, generally, set of correlation lengths) tends to zero in the high-temperature limit (as for systems with short-range interactions) while the other correlation length (or such set) tends to the screening length (as we find for systems with long-range interactions). An example of a system where this can be observed is the screened “Coulomb frustrated ferromagnet,”^{15–17} given by the Hamiltonian $H = [-J \sum_{\langle \vec{x}, \vec{y} \rangle} S(\vec{x})S(\vec{y}) + Q \sum_{\vec{x} \neq \vec{y}} V_L(|\vec{x} - \vec{y}|)S(\vec{x})S(\vec{y})]$, with $J, Q > 0$ and the long-range interaction $V_L(x) = \frac{e^{-x/\lambda}}{x}$ in $d = 3$ dimensions and $V_L(x) = K_0(x/\lambda)$ in $d = 2$, with λ the screening length and K_0 a modified Bessel function of the second kind. Similar dipolar systems^{18–20} have been considered. Apart from the usual correlation length that vanishes in the high-temperature limit, we find an additional correlation length that tends to the screening length λ .

VI. GENERALIZED DEBYE LENGTH (AND TIME) SCALES

We now introduce the notion of generalized Debye length (and time) scales that are applicable to general systems with effective or exact long-range interactions. These extend the notion of a Debye length from Coulomb-type system where it was first found. If the Fourier space interaction kernel $v(k)$ in a system with long-range interactions is such that $\frac{1}{v(k)}$ is analytic at $k = 0$, then the system has a diverging correlation length ξ_{long} at high temperature. To get the characteristic diverging length scales, we consider the self-consistent small- k solutions to $k_B T/v(k) = -1$ for high temperature (which gives the poles in the correlation function). Thus, as $T \rightarrow \infty$, ξ_{long} diverges as $\sqrt[p]{k_B T}$, where p is the order of the first nonzero term in the Taylor series expansion of $\frac{1}{v(k)}$ around $k = 0$. This divergent length scale could be called the generalized Debye length. If the long-range interactions in the system are of Coulomb type, then this corresponds to the usual Debye length λ_D where $p = 2$. A more common way to obtain this result is as follows. Suppose we have our translationally invariant system which interacts via pairwise couplings as in Eq. (1). We can define a potential function for this system as

$$\phi(\vec{x}) = \sum_{\vec{y}, \vec{y} \neq \vec{x}} V(|\vec{x} - \vec{y}|)S(\vec{y}). \quad (16)$$

The “charge” $S(\vec{x})$ in the system is perturbed by an amount $\hat{S}(\vec{x})$, and we observe the response $\hat{\phi}(\vec{x})$ in the potential function $\phi(\vec{x})$, assuming that we stay within the regime of linear response. We assume that $S(\vec{x})$ follows a Boltzmann distribution, i.e., $S(\vec{x}) = A \exp[-\beta C \phi(\vec{x})]$, where C is a constant depending on the system. It follows that $\hat{S}(\vec{x}) = -\beta C S(\vec{x}) \hat{\phi}(\vec{x})$. At this point, we can ignore the fluctuation in $S(\vec{x})$ as it does not contribute to the leading-order term. Thus, $\hat{S}(\vec{x}) = -\beta C S_0 \hat{\phi}(\vec{x})$, where $S_0 = \langle S(\vec{x}) \rangle$. In Fourier space, this leads to the relation

$$\hat{\phi}(\vec{k}) = -\beta C S_0 v(\vec{k}) \hat{\phi}(\vec{k}). \quad (17)$$

The modes with nonzero response are therefore given by

$$-v(\vec{k}) \propto k_B T. \quad (18)$$

For a Coulomb system, these modes are given by $(-k^{-2}) \propto k_B T$, yielding a correlation length $\lambda_D \propto \sqrt{k_B T}$.

As a brief aside, we discuss what occurs when the above considerations (and also those to be detailed anew in Sec. VIII A) are applied to an imaginary time action of a complex field ψ that has the form,

$$S_{\text{action}} = \frac{1}{2} \int d\tau d\tau' d^d x d^d x' \times [\psi(x, \tau) K(x - x', \tau - \tau') \psi(x', \tau')] + \dots \quad (19)$$

In the above, the imaginary time coordinates $0 \leq \tau, \tau' \leq \beta$ with a kernel K that is long range in space or imaginary time and the ellipsis denoting higher-order terms (e.g., generic $|\psi|^4$ -type terms) or imposing additional constraints on the fields ψ [such as normalization, which we have applied thus far for $O(n)$ systems]. In such a case, the associated Debye length (or imaginary time) scale may diverge in the weak-coupling (i.e., $K \rightarrow aK$ with $a \rightarrow 0^+$) limit. In an analogous way, repeating all of the earlier calculations done thus far for spatial correlations, we find divergent correlation times in the low-coupling limit for systems with a kernel K that is long range in $|\tau - \tau'|$. An action such as that of Eq. (19) may also describe a system at the zero-temperature limit (whence $\beta \rightarrow \infty$) and the (imaginary) time scale is unbounded.

In Appendix B, we will relate the divergence of the *generalized Debye-type length scales* in the high-temperature limit to a similar divergence in the largest correlation length in systems with long-range interactions.

A. Confining potentials

We discussed long-range interactions (with, in general, a screening which may be set to be arbitrarily small) such as those that arise in plasma, dipolar systems, and other systems in condensed matter physics. In all of these systems, the long-range potentials dropped monotonically with increasing distance. Formally, we may consider generalizations which further encompass confining potentials such as those that capture the effective confining potentials in between quarks in quantum chromodynamics (QCD) as well as those between charges in one-dimensional Coulomb systems (where the effective potentials associated with the electric flux tubes in one dimension lead to linear potentials). The derivations that we carried through also hold in such cases. For instance, in a one-dimensional Coulomb system, the associated linear potential $V(x) \sim |x|$ leads to the usual Coulomb Fourier space kernel $v(k) \sim k^{-2}$. In general, for a potential $V(x) \sim |\vec{x}|^{-a}$ in d spatial dimensions, the corresponding Fourier space kernel is, as in the earlier case, $v(k) \sim |k|^{-p}$, where $p = d - a$. Following the earlier discussion, this leads, at asymptotically high temperatures (and for infinitesimal screening), to correlation lengths that scale as $\xi \sim \sqrt[p]{T}$. In the presence of screening, the correlation length at infinite temperature saturates and is equal to the screening length. Similarly, as seen by Eq. (18), the generalized Debye screening length scales in precisely the same manner. In Eq. (B2), we comment on the relation between the two scales.

VII. GENERALIZATIONS

Here we illustrate how our results can be generalized to systems which do not fall into the class of systems introduced in Sec. III.

A. Disorder

When Eq. (1) is replaced by a system with non-translationally-invariant exchange couplings $V(\vec{x}, \vec{y}) \equiv \langle \vec{x} | V | \vec{y} \rangle$, then V will be diagonal in an orthonormal basis ($|\vec{u}\rangle$) different from the momentum space eigenstates, i.e., $V|\vec{u}\rangle = v(\vec{u})|\vec{u}\rangle$. Our derivation will be identical in the $|\vec{u}\rangle$ basis. In particular, Eq. (10) will be the same with $v(\vec{k})$ replaced by $v(\vec{u})$.

B. Fluids

Our results can be directly applied to fluids. In this case the spin at each site in Eq. (1) may be replaced by the local mass density. The pair structure factor $S(k)$ is the same as the Fourier space correlation function $G(k)$.²¹ For $r \neq 0$, the pair distribution function $g(r)$ is related to the correlation function $G(r)$ defined above as

$$g(r) = G(r) + 1. \quad (20)$$

For $r = 0$, $g(r) = 0$.

C. General multicomponent interactions

In the case of systems with multiple interacting degrees of freedom at each lattice site, we have a similar result. We consider, for instance, the non-rotationally-invariant $O(n)$ Hamiltonian

$$H = \frac{1}{2} \sum_{\vec{x} \neq \vec{y}} \sum_{a, b} V_{ab}(\vec{x}, \vec{y}) S_a(\vec{x}) S_b(\vec{y}), \quad (21)$$

where the interactions $V_{ab}(\vec{x}, \vec{y})$ depend on the spin components $1 \leq a, b \leq n$ as well as the locations \vec{x} and \vec{y} . By fiat, in Eq. (21), $V_{ab}(\vec{x} = \vec{y}) = 0$. Non-rotationally-symmetric interactions such as those of Eq. (21) with a kernel V_{ab} which is not proportional to the identity matrix in the internal spin space $1 \leq a, b \leq n$ appear in, e.g., Dzyaloshinsky-Moriya interactions,²² isotropic²³ and nonisotropic compasses,²⁴ and Kugel-Khomskii^{23,25} and Kitaev-type²⁶ models. Such interactions also appear in continuous and discretized non-Abelian-gauge backgrounds (and scalar products associated with metrics of curved surfaces) used to describe metallic glasses and cholesteric systems.²⁷⁻³⁶ The lattice ‘‘soccer ball’’ spin model²⁷ is precisely of the form of Eq. (21). Replicating the calculations leading to Eq. (A6), for $\vec{x} \neq \vec{y}$, to $\mathcal{O}(1/T^2)$, we find that

$$G_{ab}(\vec{x}, \vec{y}) = \langle S_a(\vec{x}) S_b(\vec{y}) \rangle = -\frac{V_{ab}(\vec{x}, \vec{y})}{k_B T} + \frac{1}{(k_B T)^2} \sum_{c, \vec{z}} V_{ac}(\vec{x}, \vec{z}) V_{cb}(\vec{z}, \vec{y}). \quad (22)$$

Correspondingly, in Fourier space, this explicitly takes the form

$$G_{ab}(\vec{k}) = \delta_{ab} - \frac{v_{ab}(\vec{k})}{k_B T} + \frac{1}{(k_B T)^2} \sum_c v_{ac}(\vec{k}) v_{cb}(\vec{k}). \quad (23)$$

D. Bose and Fermi gases

Here we discuss Bose and Fermi systems to illustrate the generality of our result from Eq. (10). We consider the Hamiltonian given by

$$H = H_0 + H_I,$$

where

$$\begin{aligned} H_0 &= \sum_{\vec{x}} \hat{\psi}^\dagger(\vec{x}) \frac{\mathbf{p}^2}{2m} \hat{\psi}(\vec{x}), \\ H_I &= \frac{1}{2} \sum_{\vec{x}, \vec{x}'} \hat{\rho}(\vec{x}) V(\vec{x} - \vec{x}') \hat{\rho}(\vec{x}'), \end{aligned} \quad (24)$$

with $\hat{\rho}(\vec{x}) = \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x}) - \langle \hat{\psi}^\dagger \hat{\psi} \rangle_0$.

Here and throughout, $\langle \cdot \rangle_0$ denotes an average with respect to H_0 (the ideal gas Hamiltonian). The fields ψ obey appropriate statistics (Bose-Einstein or Fermi-Dirac) depending on the system being studied. The standard partition function is

$$Z = Z_0 \int D\eta(\vec{x}, \tau) e^{-\beta\Phi}. \quad (25)$$

Here, τ is the standard imaginary time coordinate ($0 \leq \tau \leq \beta$). Z_0 is the partition function of the noninteracting system described by H_0 and the η 's are the dual fields after performing the HS transformation. We can express Φ as

$$\begin{aligned} \Phi &= -\frac{N^2}{2\beta^3} \int_0^\beta d\tau \sum_{\vec{x}, \vec{x}'} \eta(\vec{x}, \tau) V^{-1}(\vec{x} - \vec{x}') \eta(\vec{x}', \tau) \\ &\quad - \frac{N}{\beta} \ln \left\langle T_\tau \exp \left(\frac{1}{\beta} \int_0^\beta d\tau \sum_{\vec{x}} \eta(\vec{x}, \tau) \hat{\rho}(\vec{x}, \tau) \right) \right\rangle, \end{aligned} \quad (26)$$

where T_τ is the (imaginary) time-ordering operator. It is clear that the factor of the partition function which controls high-temperature behavior comes from the first term in Φ . Thus, for small β (high temperature), Φ of Eq. (26) results in a distribution of the values of η which is sharply peaked around $\eta = 0$. Also, for small β , the integrands of Eq. (27) have little dependence on τ . Therefore, at high temperature,

$$\Phi = -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{x}'} \eta(\vec{x}) [V^{-1}(\vec{x} - \vec{x}') + \beta A(\vec{x} - \vec{x}')] \eta(\vec{x}'), \quad (27)$$

where $A(\vec{x} - \vec{x}') = \langle \rho(\vec{x}) \rho(\vec{x}') \rangle_0 = C \delta_{\vec{x}, \vec{x}'}$, with $C = \rho_0^2$ being a constant. The correlation function for this system is defined as $G(\vec{x} - \vec{y}) = \langle \rho(\vec{x}) \rho(\vec{y}) \rangle$. It is easy to show that, written in terms of the dual variables,

$$G(\vec{x} - \vec{y}) = \left\langle \frac{f'(N\eta(\vec{x}))}{f(N\eta(\vec{x}))} \frac{f'(N\eta(\vec{y}))}{f(N\eta(\vec{y}))} \right\rangle_d, \quad (28)$$

where $f(a) = \text{Tr}_{\rho(\vec{x})} e^{a\rho(\vec{x})}$ and, as before, $\langle \cdot \rangle_d$ denotes the average with respect to the dual fields η . For small values of the η variables (high temperature), we have, in general,

$G(\vec{x} - \vec{y}) = C_0 + C_1 \langle \eta(\vec{x}) \eta(\vec{y}) \rangle_d$, with C_0 chosen such that $G(\vec{x}) = C$ for $\vec{x} = \vec{0}$ and C_1 defined by the statistics of ρ and the form of the pair interaction V . Therefore, we have

$$G(\vec{k}) = C + \frac{C_1 k_B T}{C[Cv(\vec{k}) + k_B T]} - \frac{1}{N} \sum_{\vec{k}} \frac{C_1 k_B T}{C[Cv(\vec{k}) + k_B T]}. \quad (29)$$

This is similar to the classical $O(n)$ correlation function in Fourier space [Eq. (10)]. We can easily generalize Eq. (29) for multicomponent or polyatomic systems as in Eq. (22). Applied to *scattering data* from such systems, our results may enable the determination of effective unknown microscopic interactions that underlie the system. Similarly, replication of the same derivation, *mutatis mutandis*, for quantum SU(2) spins $\vec{S} = (S_x, S_y, S_z)$ in the coherent spin representation leads to the high-temperature result of three-component [$O(n=3)$] classical spins. This illustrates the well-known maxim that at high temperature, details may become irrelevant and systems “become classical.” In a similar manner, at high T , the details underlying the classical $O(n)$ model [the $O(n)$ normalization constraints concerning a fixed value of $|\vec{S}(\vec{x})|$ for n -component vectors $\vec{S}(\vec{x})$ at all sites \vec{x}] effectively became irrelevant at high temperature—the behavior for all n was similar.

VIII. APPROXIMATE METHODS

The exact high-temperature results that we obtained for lattice spin systems and the generalizations that we discussed in Sec. VII are, as we will show below, similar to those attained by several approximate methods. This coincidence of our exact results with the more standard and intuitive approximations enables a better understanding from different approaches. A corollary of what we discuss below is that the divergence of the correlation lengths in systems with long-range interactions in the high-temperature limit (as in Sec. V) appears in all of these standard approximations. However, as we illustrated earlier in our work, and in Sec. V in particular, this divergence is not a consequence of a certain approximation but is an exact feature of all of these systems in their high-temperature limits.

In what follows, we will specifically discuss (i) ϕ^4 field theories, (ii) the large- n limit, and (iii) the OZ approach for fluids invoking the mean-spherical approximation (MSA).³⁷

A. Ginzburg-Landau ϕ^4 -type theories

In the canonical case, the free energy density of the ϕ^4 theory is given by

$$\mathcal{F} = \frac{1}{2} [\nabla\phi(\vec{x})]^2 + \frac{1}{2} r \phi^2(\vec{x}) + \frac{a}{4!} \phi^4(\vec{x}). \quad (30)$$

A finite value of a corresponds to the “soft-spin” approximation where the norm is not constrained, $\langle \phi^2(\vec{x}) \rangle \neq 1$. Here, $r = c(T - T_0)$, with c a positive constant. The partition function³⁸ is $Z = \int D\phi e^{-F}$ where $F = \int \mathcal{F} d^d x$ with d the spatial dimension. At high temperature, the correlator behaves in a standard way (the OZ form) $\langle |\phi(\vec{k})|^2 \rangle = \frac{1}{k^2 + r}$. The irrelevance of the ϕ^4 term may, e.g., be seen by effectively setting $\phi^4(\vec{x}) \rightarrow 6\langle \phi^2(\vec{x}) \rangle \phi^2(\vec{x})$ in the computation of the partition function. As $\langle \phi^2(\vec{x}) \rangle$ is small [in fact, from Fourier transforming the above,

$\langle \phi^2(\vec{x}) \rangle = \mathcal{O}(1/T)$], the ϕ^4 term is smaller than the $(\nabla\phi)^2$ term in Eq. (30) by a factor of a/T and therefore can be neglected. When general two-body interactions with an interaction kernel $v(\vec{k})$ are present, we similarly have $\langle |\phi(\vec{k})|^2 \rangle = \frac{1}{v(\vec{k}) + \mu}$. Our result of Eq. (10) for interactions of arbitrary spatial range illustrates that suggestive results for the correlation lengths attained by soft-spin approximations are not far off the mark for general systems in the high-temperature limit. As far as we are aware, the high-temperature correlation length of general theories was not known to be similar to that suggested by various perturbative schemes [including the $1/n$ (Ref. 39) and ϵ (Ref. 40) expansions].

B. Correlation functions in the large- n limit

We now provide a derivation of Eq. (10) as it applies in the large- n limit. Long ago, Stanley⁷ demonstrated that the large- n limit of the $O(n)$ spins is identical to the spherical model first introduced by Berlin and Kac.⁴¹

The single-component spherical model is given by the Hamiltonian

$$H = \frac{1}{2} \sum_{\vec{x} \neq \vec{y}} V(|\vec{x} - \vec{y}|) S(\vec{x}) S(\vec{y}). \quad (31)$$

The spins in Eq. (31) satisfy a single global (“spherical”) constraint,

$$\sum_{\vec{x}} S^2(\vec{x}) = N, \quad (32)$$

enforced (as an ensemble average³⁷) by a Lagrange multiplier μ . This leads to the functional $H' = H + \mu N$ which renders the model quadratic [as both Eqs. (31) and (32) are quadratic] and thus exactly solvable; see, e.g., Ref. 16.

From the equipartition theorem, in the higher temperature region of $T \geq T_c$ [when no order onsets and no Fourier mode is macroscopically occupied to form “a condensate” (i.e., $\langle |s(\vec{k})|^2 \rangle / N^2 \rightarrow 0$ for all \vec{k} in the thermodynamic ($N \rightarrow \infty$) limit)], the Fourier space correlator

$$G(\vec{k}) = \frac{1}{N} \langle |s(\vec{k})|^2 \rangle = \frac{k_B T}{v(\vec{k}) + \mu}. \quad (33)$$

The real space two-point correlator is given by

$$G(\vec{x}) \equiv \langle S(0) S(\vec{x}) \rangle = \frac{k_B T}{N} \sum_{\vec{k}} \frac{e^{i\vec{k} \cdot \vec{x}}}{v(\vec{k}) + \mu}. \quad (34)$$

To complete the characterization of the correlation functions at different temperatures, we note that the Lagrange multiplier $\mu(T)$ is given by the implicit equation $1 = G(\vec{x} = \vec{0})$. Thus,

$$\frac{k_B T}{N} \sum_{\vec{k}} \frac{1}{v(\vec{k}) + \mu} = 1. \quad (35)$$

This implies that the temperature T is a monotonically increasing function of μ . Equation (34) also implies that, in the high-temperature limit,

$$\mu = k_B T. \quad (36)$$

Taken together, Eqs. (33) and (36) yield Eq. (10) in the asymptotic high-temperature limit. For completeness, we

briefly note what happens at low T ($T < T_c$). In the spherical model, at the critical temperature (T_c), the Lagrange multiplier μ takes the value

$$\mu_{\min} = -\min_{\vec{k}} \{v(\vec{k})\}. \quad (37)$$

For $T < T_c$, (at least) one mode \vec{q} is macroscopically occupied; the mode(s) \vec{q} being occupied is one for which $v(\vec{k})$ is minimum. The “condensate fraction” $\langle |s(\vec{q})|^2 \rangle / N^2 > 0$.

C. Ornstein-Zernike equation

As noted earlier, application of the MSA to the OZ equation for fluids reproduces similar results for the “total correlation function” $h(\vec{r})$. This is defined as $h(\vec{r}) = g(\vec{r}) - 1$, where $g(\vec{r})$ is the standard radial distribution function. The OZ equation for a fluid with particle density ρ is given by

$$h(\vec{r}) = C(\vec{r}) + \rho \int dr' C(\vec{r} - \vec{r}') h(\vec{r}'), \quad (38)$$

where $C(\vec{r})$ is the “direct correlation function.” Using the MSA, $C(\vec{r}) = -\beta V(\vec{r})$,³⁷ we get in Fourier space

$$S(\vec{k}) = \frac{k_B T}{\rho v(\vec{k}) + k_B T}. \quad (39)$$

This is similar to our result for $G(\vec{k})$. However, it is valid only for systems in which the MSA is a good approximation.

IX. CONCLUSIONS

(i) We derived a universal form for high-temperature correlators in general $O(n)$ theories as well as Bose and Fermi gases and quantum spin systems. This enables the *extraction of unknown microscopic interactions* from measurements of the high-temperature correlation functions. Similar considerations may also be enacted for general Potts and other systems.

(ii) We discovered *divergent* correlation lengths in systems with long-range interactions in the high-temperature limit. This divergence is replaced by a saturation when the long-range interactions are screened.

(iii) We introduced *generalized Debye lengths* (and times) associated with such divergent correlation lengths (and decay times).

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APPENDIX A: HIGH-TEMPERATURE SERIES EXPANSION OF THE CORRELATION FUNCTION

We now outline in detail how we may obtain a high-temperature (T) series expansion of the correlation function to arbitrary order for a general system with translational invariance. The results we present below are valid in the high-temperature phase of general lattice (spin or other) and continuum systems. However, these may hold at low temperatures provided we can analytically continue to low temperatures from the high-temperature phase, i.e., arrive

at these without having a phase transition. We should emphasize that as we set the temperature to be arbitrarily high, the density does not have to be small, as is assumed in methods derived from Mayer's cluster expansion for fluids. Our result is therefore valid for the high-temperature phase of any system. Albeit trivial, we should remark that, formally, for any finite size system of N sites (or of finite volume for a continuum theory), no matter how large yet still finite, there are no phase transitions [instead there might be progressively sharp (as N increases), yet analytic, crossovers]. Thus, in finite size systems, the radius of convergence of the high T expansion is infinite. In general, the long-range character of the interactions will not enable us to invoke many of the simplifying elegant tricks presented elsewhere. For instance, the counting of connected contours and loops^{42,43} that appear in high-temperature series expansions involving nearest-neighbor interactions cannot be applied here.

We can perform the high-temperature series expansion directly in the original spin space. However, we find it easier to make a transformation to a dual space where our Boltzmann weights become Gaussian in the high-temperature limit.

The correlation function of the original theory can be expressed in terms of the correlation function (and higher moments) of the dual theory—we employ that in our calculation. The dual theory to a nearest-neighbor ferromagnetic system is a Coulomb gas. A nearest-neighbor ferromagnetic system in dimensions $d > 2$ at low T has an ordered phase and a small correlation length (the correlation length diverges at $T = T_c$). This does *not* imply that the Coulomb system has a small correlation length at high temperature. $O(n)$ constraints become faint at high T in the dual theory whereas, in the exact Coulomb gas at high T , the $O(n)$ constraints are there. The same also applies for a soft-spin realization of the Coulomb gas, where $\exp[-\beta u(S^2 - 1)^2]$, which is zero as $\beta \rightarrow \infty$ (or $T \rightarrow 0$) unless $S^2 = 1$ everywhere. By contrast, in the exact dual theory at high temperature, the relative strength of the $O(n)$ constraints becomes negligible relative to the “interaction” term containing $(\beta V)^{-1}$. Even though we can ignore β prefactors when $\beta = \mathcal{O}(1)$ and consider dual theories and soft-spin realization, we cannot ignore the T dependence at high T about the infinite- T disordered limit. Otherwise we get a contradiction, as our exact calculation with the exact dual theory (containing the T -dependent prefactors) shows.

We will keep things general and perform the simple series expansion of the dual Hamiltonian H_d in Eq. (6):

$$\begin{aligned} H_d &= -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) \\ &\quad - \frac{1}{\beta} \sum_{\vec{x}} \ln \left(\frac{I_{n/2-1}[\sqrt{n}N|\vec{\eta}(\vec{x})|]}{[\sqrt{n}N|\vec{\eta}(\vec{x})|]^{n/2-1}} \right) \\ &= -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) - \frac{N^2}{2\beta} \sum_{\vec{x}} \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{x}) \\ &\quad + \frac{N^4}{4(n+2)\beta} \sum_{\vec{x}} [\vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{x})]^2 + \dots \end{aligned} \quad (\text{A1})$$

In Eq. (A1), the interaction V should be thought of as a translationally invariant matrix. That is, in a Dirac-type notation,

$\langle \vec{x} | V | \vec{y} \rangle = V(\vec{x} - \vec{y})$. In Eq. (A1), V^{-1} is the inverse Fourier transform of $1/v(k)$, where $v(k)$ is the Fourier transform of $V(\vec{x})$.⁴⁴

Next, we separate H_d into a quadratic part H_{d0} and higher-order (interaction-type) terms which we denote by ΔH . That is,

$$\begin{aligned} H_{d0} &= -\frac{N^2}{2\beta^2} \sum_{\vec{x}, \vec{y}} V^{-1}(\vec{x} - \vec{y}) \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{y}) \\ &\quad - \frac{N^2}{2\beta} \sum_{\vec{x}} \vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{x}), \end{aligned} \quad (\text{A2})$$

$$\Delta H = \frac{N^4}{4(n+2)\beta} \sum_{\vec{x}} [\vec{\eta}(\vec{x}) \cdot \vec{\eta}(\vec{x})]^2 + \dots \quad (\text{A3})$$

The expectation value of any quantity X may be computed by

$$\begin{aligned} \langle X \rangle_d &= \frac{\langle X e^{-\beta \Delta H} \rangle_{d0}}{\langle e^{-\beta \Delta H} \rangle_{d0}} \\ &= \langle X \rangle_{d0} - \beta [\langle X \Delta H \rangle_{d0} - \langle X \rangle_{d0} \langle \Delta H \rangle_{d0}] \\ &\quad + \frac{\beta^2}{2!} [\langle X (\Delta H)^2 \rangle_{d0} - 2 \langle X \Delta H \rangle_{d0} \langle \Delta H \rangle_{d0} \\ &\quad + 2 \langle X \rangle_{d0} \langle \Delta H \rangle_{d0}^2 - \langle X \rangle_{d0} \langle (\Delta H)^2 \rangle_{d0}] + \dots, \end{aligned} \quad (\text{A4})$$

where $\langle \cdot \rangle_{d0}$ represents the expectation value calculated with the Boltzmann weight associated with the Hamiltonian H_{d0} . We may retain terms to arbitrary order in η^2 (or corresponding order in $1/T$). Equation (7) can be expanded to arbitrary order in η^2 , where we rewrite all expectation values with respect to the Hamiltonian H_{d0} . The terms become expectation values of a product of an even number of η fields with respect to the quadratic Hamiltonian H_{d0} . We can then use Wick's theorem to compute the expectations with respect to H_{d0} to all orders. To order $1/T^3$ we obtain for $\vec{x} \neq \vec{0}$,

$$\begin{aligned} G(\vec{x}) &= -\frac{V(\vec{x})}{k_B T} \\ &\quad + \frac{1}{(k_B T)^2} \left[\sum_{\vec{z}} V(\vec{z}) V(\vec{x} - \vec{z}) - 2V(0)V(\vec{x}) \right] \\ &\quad + \frac{1}{(k_B T)^3} \left[-\sum_{\vec{y}, \vec{z}} V(\vec{y}) V(\vec{z}) V(\vec{x} - \vec{y} - \vec{z}) \right. \\ &\quad \left. + 2V(\vec{x}) \sum_{\vec{z}} V(\vec{z}) V(-\vec{z}) + 3V(0) \sum_{\vec{z}} V(\vec{z}) V(\vec{x} - \vec{z}) \right. \\ &\quad \left. - 5[V(0)]^2 V(\vec{x}) - 2 \frac{[V(\vec{x})]^3}{n+2} \right]. \end{aligned} \quad (\text{A6})$$

As a brief aside, we note that from the fluctuation dissipation theorem the susceptibility $\chi = \beta \sum_{\vec{x}} G(\vec{x})$. At asymptotically high temperature, $G(\vec{x}) \simeq \delta_{\vec{x},0}$, giving rise to Curie's law, $\chi \propto 1/T$. The terms in Eq. (A6) lead to higher-order corrections. To next order, $\chi = \frac{1}{k_B(T-\theta_C)}$ with the Curie temperature $\theta_C = \sum_{\vec{x} \neq 0} V(\vec{x})$ in the weak-coupling limit. Thus far, in the literature, the Curie-Weiss form has been invoked to ascertain

whether a given system has dominantly ferromagnetic or antiferromagnetic interactions (by examining the sign of θ_C) and their strength ($|\theta_C|$). We see that by not focusing solely on $\chi = \beta G(\vec{k} = \vec{0})$ but rather on the scattering function $G(\vec{k})$ for all \vec{k} , we can in principle deduce the interaction $v(\vec{k})$ and hence $V(\vec{x})$. We further note, in passing, that for ferromagnetic systems (ones with $V(\vec{x}) \leq 0$), all terms in $G(\vec{x})$ are positive and the correlation functions are monotonically decreasing with T (or increasing with the inverse temperature β). This and similar relations are consequences of extensions of the standard Griffiths inequalities⁴⁵ to general $O(n)$ systems with arbitrary range (ferromagnetic) interactions. The extension of these relations to the $O(n)$ systems discussed here follows from, e.g., an explicit Feynman type diagrammatic expansion (e.g., Ref. 46) that represents the high temperature series expansion and noting that each diagram is trivially positive. Replacing the sums for the clock model of Ref. 46, in e.g., $O(2)$ systems, all angular integrals reduce to products of the type $\int_0^{2\pi} d\theta \exp(in\theta) = 2\pi \delta_{n,0} \geq 0$.

In Fourier space, the real space convolutions become momentum space products and vice versa. Equation (A6) then reads

$$\begin{aligned} G(\vec{k}) = & 1 - \frac{v(\vec{k})}{k_B T} + \frac{1}{(k_B T)^2} [v(\vec{k})]^2 - 2V(\vec{x} = \vec{0})v(\vec{k}) \\ & + \frac{1}{(k_B T)^3} \left[-[v(\vec{k})]^3 + \frac{2v(\vec{k})}{N} \sum_{\vec{k}_1} [v(\vec{k}_1)]^2 \right. \\ & + 3V(\vec{x} = \vec{0})[v(\vec{k})]^2 - 5[V(\vec{x} = \vec{0})]^2 v(\vec{k}) - \frac{2}{N^2(n+2)} \\ & \left. \times \sum_{\vec{k}_1, \vec{k}_2} v(\vec{k}_1)v(\vec{k}_2)v(\vec{k} - \vec{k}_1 - \vec{k}_2) \right] - G_1(0), \quad (\text{A7}) \end{aligned}$$

where $G_1(0)$ is the value obtained by inserting $\vec{x} = \vec{0}$ in Eq. (A6). It should be noted that the real space correlation function cannot change if we shift the on-site interaction $V(\vec{x} = \vec{0})$, which is equivalent to a uniform shift to $v(\vec{k})$ for all \vec{k} . This is because the $O(n)$ spin is normalized— $|\vec{S}(\vec{x})|^2 = n$ at all sites \vec{x} . This invariance to a constant shift holds for all T and consequently, to any order in $1/T$, the coefficients must be invariant to a global shift in $v(k)$. Among other things, we earlier invoked this invariance¹¹ to the shift $v(\vec{k})$ to enable a HS transformation in the cases for which initially $v(\vec{k}) > 0$ for some values of \vec{k} . We can, of course, invoke this invariance here also to obtain the above high-temperature series expansion with a well-defined HS dual. The final results, as we reiterated above, are invariant under this shift, as is also manifest in our series expansion in powers of $1/T$. Although obvious, we note that the expansion in Eq. (A7) is performed in powers of $1/T$ involving $v(k)$ for real vectors \vec{k} . In examining the correlation lengths via contour integration in the complex k plane, the corresponding $v(k)$ may be extended for complex k .

We see from the expansion in Eq. (A7) that already to $\mathcal{O}(1/T)$ it is also clear that the length scales of the system (which are determined by the poles of the Fourier space correlation function) are governed by the poles of $v(\vec{k})$ in the complex \vec{k} space. Thus, if, e.g., $v(\vec{k}) = 1/(k^2 + \lambda^{-2})$, the

correlation length tends to λ at high temperature. It therefore must diverge for a system with no screening.

In cases where the correlation function is known from some experimental technique or otherwise, the series expansion for the correlation function can be inverted to arbitrary order to obtain the pairwise interactions. To $\mathcal{O}(1/T^2)$, for nonzero separation \vec{x} , the potential function is given by

$$\begin{aligned} V(\vec{x}) = & -k_B T \left[G(\vec{x}) - \sum'_{\vec{z}} G(\vec{z})G(\vec{x} - \vec{z}) \right. \\ & + \sum'_{\vec{y}, \vec{z}} G(\vec{y})G(\vec{z})G(\vec{x} - \vec{y} - \vec{z}) \\ & \left. + 2G(\vec{x}) \sum'_{\vec{z}} G(\vec{z})G(-\vec{z}) - \frac{2(G(\vec{x}))^3}{n+2} \right]. \quad (\text{A8}) \end{aligned}$$

The prime indicates that the sum excludes terms containing $G(0)$. As is evident from our earlier results and discussion, in Eq. (A8), each correlation function $G(\vec{x})$ is of order $(1/T)$.

We reiterate that, as in our discussion in Sec. VIII, our results for lattice $O(n)$ spin models match with the leading-order behavior at high temperature obtained from several standard approximate theories based on Mayer's cluster expansion derived for liquid systems, e.g., Born-Green theory⁴⁷ and OZ theory with the Percus-Yevick approximation⁴⁸ or MSA.³⁷ As implicit above, our $1/T$ expansion can indeed be extended to systems in which the liquid and the gas phases are not separated by a phase transition, e.g., for pressures larger than the pressure at the liquid-vapor critical point. As further noted in Sec. VIII, various approximations also suggest that at high temperature the correlation length may match the length scale characterizing the interaction potential and, in particular, will diverge in systems having long-range interactions (as we have established).

APPENDIX B: RELATION BETWEEN THE GENERALIZED DEBYE LENGTHS AND DIVERGENCE OF THE HIGH-TEMPERATURE CORRELATION LENGTHS

An intuitive approximate approach for the understanding of the rigorous yet seemingly paradoxical result that we report in this work—that of the divergence of the correlation lengths in the high-temperature limit of systems with long-range interactions—is afforded by the OZ framework. Specifically, in the language of OZ approximations, the “total” high-temperature correlation function is the same as the “direct” correlation function [see, e.g., Ref. 21 (Sec. 2.6) for the definition of the direct OZ correlation functions] and behaves as

$$G(\vec{x}) \sim -\beta V(\vec{x}) \quad (\text{B1})$$

for $\vec{x} \neq \vec{0}$. Thus, if the potential is screened beyond a distance λ , the correlation length approaches λ at high temperature. That is, if we have an effective interaction resulting, e.g., from higher-order effects in $1/T$, such as that leading to the Debye screening length (λ_D) in Coulomb systems [and

generalizations introduced earlier in Eq. (18)], then at high temperature, the correlation length

$$\xi \xrightarrow{T \rightarrow \infty} \lambda_D. \quad (\text{B2})$$

This is a particular case of Eq. (15).

To $\mathcal{O}(1/T^2)$, Eq. (A7) is identical to Eq. (10). The poles of G in the complex k plane can, of course, be computed by finding those of Eq. (10) or considering directly those of Eq. (A7): both give rise to the same answer as they must.

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