Renormalization Group, Entropy Optimization, and Nonextensivity at Criticality

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The scaling properties of pair correlations at criticality are reproduced through an equivalence between random walk distributions and order parameter correlations. The shift from Gaussian to fractal walks with self-similar clusters corresponds to the changeover from a Gaussian to a nontrivial fixed point with nonvanishing dimensional anomaly. We show that the renormalization group trajectories lead to fixed points of minimum entropy, and use the Tsallis entropy index q to measure nonextensivity as behavior departs from Gaussian.

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Our undertaking in this Letter is to demonstrate the connection that exists between the extremal properties of entropy expressions and the renormalization group (RG) approach when applied to systems with scaling symmetry.

Because of its central place in the foundation of statistical mechanics, the maximum entropy formalism is perhaps the most familiar procedure for obtaining distribution functions of both common and complex statistical problems [1]. Because of its power and elegance there has been considerable interest in identifying suitable constraints that would permit the application of the variational technique to a wider set of systems [2]. Among these stands out the class of problems involving sums of random independent variables that display long-tailed distributions and self-similarity under rescaling, i.e., those characterized by the Lévy distributions that have divergent integer moments of the order of 2 or higher. It has been noted [2] however that the auxiliary condition required to maximize the ordinary Boltzmann-Gibbs-Shannon (BGS) entropy expression to obtain these distributions has an inadequate complicated form. Yet, when the nonextensive generalized entropy [3] is considered, simpler constraints, similar to the familiar constancy of the second moment, yield distributions with the same large-argument asymptotic behavior of the Lévy distributions [4,5]. The departure of the Lévy distribution from the Gaussian can then be associated to a degree of nonextensivity of the random process as measured by the generalized entropy.

A random walk in continuum space with jump lengths governed by a Lévy distribution, a Lévy flight, is a prototypical example of self-similarity. And an admirable construction of the analog of this walk on a lattice [2,6,7] exhibits very evidently the scaling property since the trajectories are shown to consist of a hierarchy of self-similar clusters of visited sites. These sets of sites have a fractal dimension fixed by the strength of the power-law decay of the step distribution, and self-similar clustering and non-Gaussian behavior is seen to require the divergence of the second moment of this distribution. Interestingly, the design given to the walk assigns the form of the continuous nondifferentiable function of Weierstrass to the structure function or Fourier transform of the step distribution. And, remarkably, the nonanalytic features of this function, responsible for the non-Gaussian characteristics of the walk, have been shown [6,7] to be analogous to the singular behavior displayed by thermodynamic properties in ordinary critical phenomena. The structure function for the walk satisfies a functional equation with a scaling property equivalent to that of the transformation equation for the free energy of a spin system under the renormalization group.

The close relation between the concepts of renormalization and self-similarity has made the RG theory the leading application over the last decades of scaling symmetry in phase transitions and many other problems in statistical physics, in nonlinear dynamics, and in other fields [8]. There is a characteristic craft or adeptness element in the now ubiquitous RG theories, since for every chosen construction, the RG transformation can be suitably or unsuccessfully designed, and in practice a good implementation would be that which results in critical RG flow lines that terminate at a meaningful nontrivial fixed point [8]. In this theory the guiding quality of a variational approach is apparently lacking.

The three themes, extremal entropy, self-similarity, and RG theory were highlighted in Ref. [2] where one of the examples chosen as an illustration was the Lévy flight and its lattice random walk analog. Here we make use of the same lattice walk to describe the critical phenomena in a lattice gas or Ising model, a connection that can be exhibited through the existing analogy [9] between a random walk and the Ornstein-Zernike relation for the pair correlation functions in a fluid or magnet [10]. The main points in our analysis are (1) the RG method is applied to the random walk problem to obtain the fixed point scaling properties of the step distribution $p(l)$. (2) The relationship between $p(l)$ and the direct correlation function $c(l)$ of the statistical-mechanical model is used to associate the random walk properties with those of the pair correlations at criticality. (3) The anomalous dimension at criticality is identified with the index μ of the Lévy distribution, and the parameter q in the Tsallis entropy is used as a measure of the nonextensivity associated to the non-Gaussian fixed point. (4) The entropy function, for both its ordinary and generalized forms, is found to decrease monotonically as the RG transformation flow advances to the fixed point where it attains its minimum value.

To begin, we consider a generalization of a symmetric one-dimensional random walk [2,6,7] where the probability $P_n(l)$ of occupancy of site l after n steps is generated from the initial condition $P_0(l)$ via the recursion relation $P_n(l) = \sum_{l'=-\infty}^{\infty} p_r(l - l')P_{n-1}(l')$, and choose the step distribution $p_r(l)$ to be

$$p_r(l) = \frac{A_r}{2} \sum_{n=0}^{r} a_n(\delta_{l,-b^n} + \delta_{l,b^n}). \qquad (1)$$

The walks are made out of sets of unevenly spaced step lengths b^n, $b > 1$, with probabilities proportional to a_n, the range of the step lengths is b^r, and A_r normalizes $p_r(l)$, i.e., $A_r^{-1} = \sum_{n=0}^{r} a_n$. The structure function $\lambda_r(k) = \sum_l p_r(l) \exp(ikl)$ for these walks is

$$\lambda_r(k) = A_r \sum_{n=0}^{r} a_n \cos(b^n k). \qquad (2)$$

The special case $a_n = a^{-n}$, $a > 1$, in the limit $r \to \infty$, denoted here $p_\infty^{\mu}(l)$, was analyzed in Refs. [6] and [7]. With this choice the step distribution acquires a power-law decay, $p_\infty^{\mu}(l) = A_\infty l^{-\mu}$, $A_\infty = 1 - a^{-1}$, $\mu \equiv \ln a / \ln b$, and when this is sufficiently slow, i.e., $\mu < 2$, the mean-squared displacement per jump diverges. As mentioned, the structure function $\lambda_\infty^{\mu}(k)$ becomes the continuous nondifferentiable function of Weierstrass, and its nonanalytic small-k behavior was demonstrated to arise from an infinite sum of regular terms obtained by iteration of the scaling equation

$$\lambda_\infty^{\mu}(k) = a^{-1}\lambda_\infty^{\mu}(bk) + A_\infty \cos k. \qquad (3)$$

When $\mu \leq 2$ the singular part of $\lambda_\infty^{\mu}(k)$ is of the form $Q(k)\,|k|^{\mu}$ with $Q(k)$ periodic in $\ln|k|$ with period $\ln b$. The connection with the Lévy distributions was exhibited and the fractal dimension of the walks was determined to be given by $\mu \leq 2$ [6,7]. To illustrate these features it is sufficient to define the model in one dimension although a multidimensional space lattice can be equally used, while the spacing between step lengths given by b^n is convenient when describing the power law $l^{-\mu}$. It has been shown [6] that in the continuum limit of this walk a Lévy flight of dimension μ^* is recovered, where $\mu^* = \lim_{\Delta \to 0} \ln a / \ln b$ with $a = 1 + \alpha\Delta + o(\Delta)$, $b = 1 + \beta\Delta + o(\Delta)$, and where Δ is the lattice spacing. Thus, while a Lévy distribution decays for large distances $x = \lim_{\Delta \to 0} \Delta l$ as $|x|^{-\mu^*-1}$ its discrete analog behaves as $|l|^{-\mu}$.

We introduce next the RG transformation $a_n' \equiv R[a_n] = a a_{n+1}$ for our family of walks. This transformation maps the sites $l = b^{n+1}$ into the sites $l' = b^n$ (therefore eliminating intermediate lattice space between allowed step lengths) and then renormalizes the step probability by a restoring factor a. It is clear that the Weierstrass walk $p_\infty^{\mu}(l)$ and the simple nearest-neighbor step walk $p_0(l)$ are both fixed points of R. The first one is nontrivial in the sense that it is associated to an infinite-ranged step distribution that can be reached via the RG transformation only from other infinite-ranged step distributions $p_\infty(l)$ required to approach asymptotically the condition $a_n = a^{-n}$, $n \to \infty$. The distributions $p_\infty(l)$ span the "critical hypersurface" and the quantities $\alpha_n \equiv a_n - a^{-n}$ are the irrelevant variables that vanish as R is repeatedly applied. The other fixed point $p_0(l)$ is trivial since it is generated by the application of the RG transformation to any "noncritical" finite-ranged $p_r(l)$, $r < \infty$.

Now consider the order-parameter fluctuation $\delta\rho(l) = \rho(l) - \rho$ about a uniform state ρ, again on a one-dimensional lattice of site positions l, and an effective Hamiltonian (divided by $k_B T$) of the form $H = (1/2) \times \sum_{l',l''} C(l)\delta\rho(l')\delta\rho(l'')$, where $C(l) \equiv \delta H / \delta\rho(l')\delta\rho(l'')$ depends only on $l = |l' - l''|$ when evaluated at $\rho(l') = \rho(l'') = \rho$. The kernel $C(l)$ is simply related to the so-called direct correlation function $c(l)$ via $C(l) = \delta_{l,0}\rho^{-1} - c(l)$. We write $c(l)$ as

$$c(l) = c_0\delta_{l,0} + c_1 A_r \sum_{n=0}^{r} a_n(\delta_{l,-b^n} + \delta_{l,b^n}). \qquad (4)$$

In this way H has the lattice analog form for a Landau free energy where the nearest-neighbor term $n = 0$ corresponds to the square-gradient term for a coarse-grained fluctuation $\delta\rho(l) = \rho\zeta(l)$. In terms of the Fourier component $\rho\tilde{\zeta}(k)$ of $\delta\rho(l)$ one has $H = (1/2)\rho^2 \times \int dk\, \tilde{C}(k)\tilde{\zeta}(k)\tilde{\zeta}(-k)$, where $\tilde{C}(k) = w[1 - z\lambda_r(k)]$ with $w = \rho^{-1}(1 - \rho c_0)$, $z = 2\rho c_1(1 - \rho c_0)^{-1}$. The consideration of the limit $r \to \infty$ of an infinite-ranged $c(l)$ with a power-law decay introduces a critical point behavior in the system. We have chosen a one-dimensional lattice in order to match the statistical-mechanical system with the random walk model. The customary RG methods can be applied to H, however we can readily recognize that this model for the critical state of a simple fluid or spin system can be related to the random walks with self-similar clusters described above and studied in Refs. [6] and [7].

The Ornstein-Zernike equation $h(l) = c(l) + \rho\sum_{l'} \times c(l')h(l - l')$ relating the total pair correlation $h(l)$ with $c(l)$ can be put into correspondence [9] with the equation for the generating function $P(l;z) = \sum_n P_n(l)z^n$ of a lattice random walk $P(l;z) - z\sum_{l'} p(l')P(l - l';z) = \delta_{l,0}$, [11]. The equivalence requires that the weight factor z is given as above and that $w = \rho^{-1}(1 - \rho)^{-1}P(0;z)$. The correlations for $l \neq 0$ are given by $c(l) = wzp(l)$ and $\rho^2 h(l) = w^{-1}P(l;z)$. The divergence of the susceptibility [9] $\chi = (1 - \rho)[\rho P(0;z)(1 - z)]^{-1}$ indicates that the critical point is attained when $z = 1$, and one can easily establish through the equivalence between $h(l)$ and $P(l;z)$ that the anomalous dimension exponent η is $\eta = 2 - \mu$.

In Fourier space $\tilde{h}(k) \sim [1 - z\lambda_r(k)]^{-1}$ and at the critical fixed point $\tilde{h}(k) \sim |k|^{-\mu}$ when $z = 1$ and $k \to 0$. The convolution between $p(l)$ and $P(l;z)$ in the generating function equation indicates that $P(l;z)$ is built from terms containing all multiplefold convolution products of $p(l)$, and implies that the fixed point $h(l)$ is closely associated to the particular form of the Lévy distributions in the continuum limit of space and time obtained from the generalized central limit theorem [12]. It should be kept in mind that the formal equivalence here employed is between the correlations of nonindependent degrees of freedom in a statistical-mechanical system and the distributions of random independent variables of a stochastic process.

We proceed to evaluate the entropy of the step distribution $p_r(l)$ along two representative types of RG trajectories: (i) A noncritical trajectory starting with a truncated power-law distribution

$$p_r^{(1)}(l) = (A_r/2) \sum_{n=0}^{r} a^{-n}(\delta_{l,-b^n} + \delta_{l,b^n}) \tag{5}$$

that flows under R into the trivial fixed point $p_0(l)$. And (ii) a critical trajectory with a starting infinite-ranged distribution

$$p_m^{(2)}(l) = (A_m/2) \sum_{n=0}^{m} a_n(\delta_{l,-b^n} + \delta_{l,b^n}) + (A_m/2) \sum_{n=m+1}^{\infty} a^{-n}(\delta_{l,-b^n} + \delta_{l,b^n}) \tag{6}$$

that flows under R into the nontrivial fixed point $p_\infty^\mu(l)$. For $p_r^{(1)}(l)$ the BGS expression $S_1 \equiv -k_B \sum_{|l|} p(l) \ln p(l)$ (for lattice coordination number independence we chose the entropy sums to be over $|l|$) yields

$$k_B^{-1} S_1^r[p^{(1)}] = \ln\frac{1 - \epsilon^{r+1}}{1 - \epsilon} - \frac{\epsilon \ln\epsilon}{1 - \epsilon} + \frac{(r+1)\epsilon^{r+1} \ln\epsilon}{1 - \epsilon^{r+1}}, \tag{7}$$

for all μ with $\epsilon = a^{-1}$. Whereas the generalized Tsallis entropy [3] $S_q \equiv k_B(q-1)^{-1}\{1 - \sum_{|l|}[p(l)]^q\}$, that is nonextensive for $q \neq 1$ but reduces to the customary extensive expression when $q = 1$, [3] gives

$$S_q^r[p^{(1)}] = \frac{k_B}{q-1}\left[1 - \frac{(1-\epsilon)^q}{1-\epsilon^q} \frac{1 - \epsilon^{q(r+1)}}{(1 - \epsilon^{r+1})^q}\right], \tag{8}$$

again for all μ. The fixed point $p_0(l)$ has a vanishing entropy $S_q^0 = 0$ for all q, and by taking the limit $S_q^\infty = \lim_{r\to\infty} S_q^r$ we obtain for the nontrivial fixed point

$$S_q^\infty = \frac{k_B}{q-1}\left[1 - \frac{(1-\epsilon)^q}{1-\epsilon^q}\right] \tag{9}$$

with

$$S_1^\infty = k_B\left[\ln\frac{1}{1-\epsilon} - \frac{\epsilon \ln\epsilon}{1-\epsilon}\right]. \tag{10}$$

For all $q \geq 1$ and all $r > 0$ we find (since $\epsilon^{q(r+1)} < q\epsilon^{r+1}$, $0 < \epsilon < 1$) that $S_q^0 < S_q^r < S_q^\infty$, therefore the entropy along the RG flow is monotonously decreasing and vanishes at the trivial fixed point.

The case for $p_m^{(2)}(l)$ is a little more complicated and we present results when the deviation from $p_\infty^\mu(l)$, $\delta p_m(l) \equiv (A_m/2)\sum_{n=0}^m \alpha_n(\delta_{l,-b^n} + \delta_{l,b^n})$, is small. The expression $S_1 \equiv -k_B \sum_{|l|} p(l) \ln p(l)$ yields

$$k_B^{-1} S_1^m[p^{(2)}] = \ln\frac{1-\delta_m}{1-\epsilon} - \left[\frac{\epsilon(1-\delta_m)}{1-\epsilon} - \gamma_m\right]\ln\epsilon - \delta_m, \tag{11}$$

for all μ, where we have kept only the linear terms $\delta_m \equiv \sum_l \delta p_m(l) = A_m \sum_{n=0}^m \alpha_n$ and $\gamma_m \equiv A_m \sum_{n=0}^m n\alpha_n$. The generalized expression $S_q \equiv k_B(q-1)^{-1}\{1 - \sum_{|l|}[p(l)]^q\}$ under the same condition gives

$$S_q^m[p^{(2)}] = \frac{k_B}{q-1}\left[1 - \frac{(1-\epsilon)^q}{1-\epsilon^q}(1-\delta_m)^q - q(1-\epsilon)^{q-1}(1-\delta_m)^{q-1}\gamma_m\right], \tag{12}$$

again for all μ, where now $\gamma_m \equiv A_m \sum_{n=0}^m \epsilon^{(q-1)n}\alpha_n$. Under the constraint $\sum_{n=0}^m n\alpha_n = \sum_{n=0}^m (n+1)a^{-1}\alpha_n$, that contains as a special case the fixed point condition $a_n = a a_{n+1}$, we find for all $q \geq 1$ and all $m > 0$ that $S_q^m > S_q^\infty$. Therefore the entropy along the RG flow is monotonously decreasing and attains a minimum at the nontrivial fixed point.

Finally, the moments $\langle l^\nu \rangle_q^r \equiv \sum_{|l|} l^\nu [p_r^{(1)}(l)]^q$ are given by

$$\langle l^\nu \rangle_q^r = \left[\frac{1-\epsilon}{1-\epsilon^r}\right]^q \frac{1 - \epsilon^{(q-\nu/\mu)r}}{1 - \epsilon^{q-\nu/\mu}}, \tag{13}$$

so that $\langle l^\nu \rangle_q^\infty$ is finite and given by $\langle l^\nu \rangle_q^\infty = (1-\epsilon)^q(1 - \epsilon^{q-\nu/\mu})^{-1}$ provided $q > \nu/\mu$, but diverges otherwise. In particular, the mean-square displacement $\langle l^2 \rangle_1^\infty$ diverges when $\mu \leq 2$, but $\langle l^2 \rangle_q^\infty$ is finite when $\mu \leq 2$ with $q > 1$. The limiting value of q for the convergence of $\langle l^2 \rangle_q^\infty$ is $q = 1$ for $\mu > 2$, and $q = 2/\mu$ for $\mu \leq 2$ and this choice of the parameter q provides a convenient measure of nonextensivity at the critical point. Thus, the Gaussian nonfractal behavior obtained when $\mu > 2$ is extensive, whereas the Lévy-type fractal behavior for $\mu \leq 2$ is increasingly nonextensive as the anomalous dimension exponent $\eta = 2 - \mu$ departs from zero. Interestingly, $\langle l^2 \rangle_1^\infty = A_\infty \sum_l l^{2-\mu}$, $\mu > 2$ and $\langle l^\mu \rangle_{2/\mu}^\infty = A_\infty^{2/\mu} \sum_l l^{\mu-2}$, $\mu \leq 2$.

In summary, we have shown that an RG transformation applicable to a random walk process with cluster formation but also to criticality in a simple fluid or spin system is associated to a monotonously decreasing entropy function that becomes minimum under an appropriate constraint at the fixed point. This result might be anticipated in view of the structureless power-law character of the fixed point distribution as compared with other infinite-ranged distributions with nonvanishing irrelevant variables. We have identified the fixed point step distribution $p_{\infty}^{\mu}(l) = A_{\infty} l^{-\mu}$ with that employed before [6,7] to obtain walks with self-similar clusters and the fractal behavior of Lévy-type distributions. The departure of this distribution from Gaussian behavior when $\mu < 2$ gives rise in the equivalent direct correlation function of the statistical-mechanical model to a nonvanishing dimensional anomaly η and to nonextensivity at criticality, the latter measured by the generalized Tsallis entropy index q. The links we have exhibited among the various properties of scaling symmetry suggest that the variational technique of optimal entropy may be of practical importance to the RG applications.

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