Critical behavior of the anisotropic n-vector model, self-avoiding rings, and polymerization

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We study the critical behavior of the m-anisotropic n-vector model with n and m both as continuous variables [$0 \leq n,m < 4-O(\epsilon)$, $\epsilon = 4-d$, d = dimensionality of space] to first order in ϵ. The limit $n \to 0$, $m > 0$ of the model is of interest as a model of self-avoiding rings and of polymerization. For $n \geq m,n,m$ integers, the critical behavior of the model is known to be that of the iostropic m-vector model, i.e., the $O(m)$ model. Here we prove that the critical behavior of the anisotropic model is *always* identical with that of the $O(m)$ model for real n,m regardless of whether $n \geq m$ or $n < m$. In particular, we prove that a single self-avoiding ring and a single self-avoiding walk belong to the *same* universality class of the $O(0)$ model, while polymerization belongs to the universality class of the $O(m)$ model, $m > 0$.

Recently, the m-anisotropic n-vector model in the formal limit $n \to 0$, keeping m fixed, has been used to describe self-avoiding rings (SAR's) and polymerization.[1] The analogy is established in *two* steps: (i) First, the *analytic continuation* in n for a fixed value of m is performed and the limit $n \to 0$ is taken. (ii) Then m is treated as a *continuous* variable and an analytic continuation in m is performed. The variable m is identified with the activity for a SAR. Such analytic continuations invariably violate convexity conditions,[2] but it is easily seen that they do not produce any anomalies for SAR's or for polymerization. Moreover, we will restrict ourselves to the high-temperature phase ($T \geq T_c$) where the above formal analogy can be demonstrated.

Since the above unphysical mapping ($m > n \to 0$) defines two *physically* realizable models,[3] it is important to understand the critical behvaior of the anisotropic model in this limit. For the physical situation of integer n and m, $n \geq m$, the critical behavior is determined by the isotropic m vector, i.e., the $O(m)$ model. Following renormalization-group calculations to first order in $\epsilon = 4-d$, we show here that the critical behavior of the m-anisotropic n-vector model is identical with that of the $O(m)$ model, regardless of the value of n. Our result agrees with the conjecture of Pfeuty and Wheeler for $n \to 0$ and $0 < m < 1$, but disagrees with their conjecture for $m > n \geq 1$. Our results also establish that a single self-avoiding walk and a single self-avoiding ring belong to the *same* universality class of the $O(0)$ model. However, the polymerization problem belongs to the universality class of the $O(m)$ model. Finally, we correct the error present in the derivations given in Ref. 1.

Let us consider the following m-anisotropic n-vector model on a lattice of N sites:

$$\mathcal{H}_n^{(m)} = K \sum_{\langle ij \rangle} \sum_{\alpha=1}^{m} S_i^{(\alpha)} S_j^{(\alpha)} + H \sum_i S_i^{(1)} , \qquad (1)$$

where $\vec{S}_i$ is an n-component ($n \geq m$) classical spin of length $\sqrt{n}$ located at the site i. The sum over $\langle ij \rangle$ is over all distinct nearest-neighbor pairs of sites and the sum over i is over all sites. A factor of $-1/kT$ is absorbed in the definition of $\mathcal{H}_n^{(m)}$, K is ferromagnetic in nature, and H is a magnetic field along the $\alpha = 1$ direction.

Following the derivation of the $n \to 0$ limit given in Ref. 4, we evaluate the $n \to 0$ limit $Z_0^{(m)}(K,H)$ of the partition function for the Hamiltonian $\mathcal{H}_n^{(m)}$ with fixed integer m. We have (see Fig. 1)

$$Z_0^{(m)}(K,H) = z^N \sum_{\Gamma} m^r \left[\frac{H^2}{z}\right]^p \left[\frac{K}{z}\right]^l \left[\frac{1}{2}\right]^{\bar{r}} \qquad (2)$$

with $z = 1 - H^2/2$. Here Γ represents some configuration with r self-avoiding rings (SAR's) and p self-

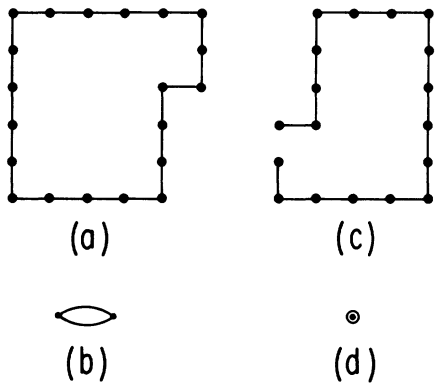

FIG. 1. Various possible disconnected parts of Γ: (a) A SAR of length $l > 2$ with weight $m(K/z)^l$; (b) A SAR between two nearest-neighbor sites of length $l = 2$, but with weight $(\frac{1}{2})m(K/z)^2$; (c) A SAW of nonzero length l weight $(H^2/z)(K/z)^l$; (d) A SAW of zero length with weight H^2/z.

avoiding walks (SAW's), and the sum over Γ is over all such configurations. There are $\bar{r}$ out of r SAR's that represent loops of length two between two nearest-neighbor sites (see Fig. 1) and come from $(K^2/2) \times (S_i^{(\alpha)} S_j^{(\alpha)})^2$ in the expansion of $\exp(K S_i^{(\alpha)} S_j^{(\alpha)})$. There are m such loops for $\alpha = 1, 2, \ldots, m$ that remain even in the limit $n \to 0$. These contributions have not been taken into account in the derivations given in Ref. 1. The weight of any of these $\bar{r}$ SAR's is $m(K^2/2z^2)$. The weight of any of the remaining r-$\bar{r}$ SAR's of length λ is, on the other hand, $m(K/z)^\lambda$. Thus we observe that each of the $\bar{r}$ SAR's contributes an extra factor of $(\frac{1}{2})$ which appears in Eq. (2). The presence of such SAR's of length two is a *deficiency* of the above correspondence for two reasons: (i) The activity for any one of these is $(m/2)(K/z)^2$ and not $m(K/z)^2$, and (ii) there are no such polymer rings of length two that are allowed in the corresponding partition function for SAR's or for polymerization. The origin of such SAR's is identical to that of single-site filled circles as explained in Ref. 4(a). Because of the extra factor of $\frac{1}{2}$, such SAR's *cannot* be truly regarded as SAR's with K/z as the bond activity. There does not apear to be any way to get rid of these unwanted SAR's as was possible with filled circle sites in Ref. 4(a). However, it is expected that the presence of such SAR's is not going to modify the critical behavior of the model, and our main interest here is to study the critical behavior. Thus we will not attempt to make any distinction between the two kinds of SAR's present in Eq. (2).

A generalized version of Eq. (2) in which SAR and SAW bonds have separate activities can be obtained from the following Hamiltonian defined for $2n$-component spins $\vec{S}_i'$ ($|\vec{S}_i'| = \sqrt{2n}$):

$$\mathcal{H}_{2n}'^{(m)} = \sum_{\langle ij \rangle} \left[K \sum_{\alpha=1}^{n} S_i'^{(\alpha)} S_j'^{(\alpha)} + K' \sum_{\alpha=n+1}^{n+m} S_i'^{(\alpha)} S_j'^{(\alpha)} \right] + H \sum_i S_i'^{(1)} ,$$

with n, m integers and $n \geq m$. For fixed m, as $n \to 0$, the corresponding partition function is given by

$$Z_0'^{(m)}(K, K', H) = z^N \sum_{\Gamma} m^r \left(\frac{K'}{z} \right)^{l_r} \left(\frac{H^2}{z} \right)^{p} \left(\frac{K}{z} \right)^{l_p} (\tfrac{1}{2})^{\bar{r}} .$$

Here l_r denotes the number of SAR bonds and l_p the number of SAW bonds. For $K = K'$, $\mathcal{H}_n^{(m)}$ and $\mathcal{H}_{2n}'^{(m)}$ become "identical" in the limit $n \to 0$ in that any quantity calculated from them in this limit, for example, $Z_0^{(m)}(K, H)$ and $Z_0'^{(m)}(K, K, H)$, become identical. The correspondence between $Z_0^{(m)}(K, H)$ and polymerization has been clearly expressed in Ref. 1(a). This model of polymerization is different from other models of polymerization obtained through $n \to 0$ trick but which do not contain SAR's.[4(b),5] In what follows, we will not consider $\mathcal{H}_0'^{(m)}$ and its consequences any further, but instead focus our attention on $\mathcal{H}_0^{(m)}$ given in Eq. (1).

Let us consider a SAR of length l and let ξ_R denote a measure of its linear dimension. As $l \to \infty$, we expect ξ_R to behave like $\xi_R \sim l^{\nu_R}$. The linear dimension ξ_w of a SAW of length l in the same limit behaves as $\xi_W \sim l^{\nu_W}$. The exponent ν_W is given by the $O(0)$ model.[6] From the topological constraint that the two points of a SAR must be identical, we expect physically that $\xi_R \leq \xi_W$. Thus, heuristically, we expect the following inequality to be obeyed:

$$\nu_R \leq \nu_W . \tag{3}$$

From Eq. (2), we observe that a single SAR, or more precisely, a dilute solution of SAR's, is obtained in the following limit: $H = 0$, $K \to K_c^-$ (K_c is the critical value of K), and $m \to 0+$ (m *cannot* be set identically equal to zero because this would mean that there is *no* SAR in $Z_0^{(0)}$). This limit implies $l \to \infty$. Thus ν_R should be identified with the correlation length exponent of $\mathcal{H}_0^{(m)}$ as $m \to 0+$. As we will show here, the critical behavior of the theory is that of the $O(m)$ model regardless of the value of n. This will imply that $\nu_R = \nu(m)$, $m \to 0+$, the correlation length exponent for the $O(m)$ model. Thus we conclude that[7] $\nu_R = \nu(m \to 0+) = \nu_w$, thereby satisfying the above equality in (3). This is also confirmed by direct renormalization-group calculations.[8] It should also be evident from above that a single SAW and a single SAR belong to the *same* universality class of the $O(0)$ model.

To study the effect of the anisotropy, it is convenient to study the following related Hamiltonian for small g:

$$\mathcal{H}_n^{(m)}(g) = \mathcal{H}_n + \mathcal{H}(g) ,$$

$$\mathcal{H}_n = K \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j ,$$

$$\mathcal{H}(g) = \frac{g}{2n} \sum_{\langle ij \rangle} [(n-m) \vec{S}_{iL} \cdot \vec{S}_{jL} - m \vec{S}_{iT} \cdot \vec{S}_{jT}] .$$

Here

$$\vec{S}_{iL} = \{ S_i^{(\alpha)} | \alpha = 1, 2, \ldots, m \}$$

and

$$\vec{S}_{iT} = \{ S_i^{(\beta)} | \beta = m+1, m+2, \ldots, n \} .$$

The above choice of $\mathcal{H}(g)$ ensures that it is orthogonal to $\mathcal{H}_n$.[9] The perturbation $\mathcal{H}(g)$ shows that the critical behavior of $\mathcal{H}_n^{(m)}(g)$ is described by that of the $O(m)$ model for $g > 0$ and that of the $O(n-m)$ model for $g < 0$. For $g = 0$, the behavior is that of the $O(n)$ model as expected. The corresponding contin-

uum version of $\mathcal{H}_n^{(m)}(g)$ is described by

$$\mathcal{H}_n^{(m)}(g)=\frac{1}{2}[(\partial\vec{S}_L)^2+(\partial\vec{S}_T)^2+r_L\vec{S}_L^2+r_T\vec{S}_T^2] + \left(\frac{1}{4!}\right)[u(\vec{S}_L^2)^2+2v\vec{S}_L^2\vec{S}_T^2+w(\vec{S}_T^2)^2] \ ,$$

with $r_L=r_0-(n-m)g/n$ and $r_T=r_0+mg/n$. From now on, we will restrict ourselves to the case of $g>0$. The results for $g<0$ are easily obtained by the transformation $m\rightarrow(n-m)$ and $g\rightarrow -g$.

Let us rewrite $\mathcal{H}_n^{(m)}(g)$ as follows:

$$\mathcal{H}_n^{(m)}(g)=\left(K-\frac{mg}{2n}\right)\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j+\left(\frac{g}{2}\right)\sum_{\langle ij\rangle}\vec{S}_{iL}\cdot\vec{S}_{jL} \ .$$

The analytic continuation in n *should* be defined so as not to change the nature of the ferromagnetic interaction. Thus K must be of the form $K=K_0+mg/2n$ with $K_0>0$ and independent of n. It is easily seen that as $n\rightarrow 0$, the above Hamiltonian indeed gives rise to SAR's. This choice of K implies that r_0 must be of the form $r_0=\bar{r}_0-mg/n$, with $\bar{r}_0$ independent of n. Therefore $r_L=\bar{r}_0-g$ and $r_T=\bar{r}_0$ and that $r_T>r_L$ for $g>0$. We identify r_0 with the temperature variable: $r_0=[T-T_c(0)]/nT$, where $T_c(0)$ is the critical temperature of the model for $g=0$ and the factor of n in the denominator is included for convenience so that the critical temperature remains finite as $n\rightarrow 0$, as will be seen below.

For $n\geq m,n,m$ integers, the behavior of $\mathcal{H}_n^{(m)}(g)$ or $\bar{\mathcal{H}}_n^{(m)}(g)$ has been studied extensively.[9,10] We will assume in the following that $0\leq n,m\leq 4-O(\epsilon)$, $\epsilon=4-d$, so that for $g=0$, the isotropic $O(n)$ fixed point is the only stable fixed point.[11] Also, since we are interested in the renormalization-group (RG) calculations, we will consider only $\bar{\mathcal{H}}_n^{(m)}(g)$ below. The analytic continuation for $\bar{\mathcal{H}}_n^{(m)}(g)$ is obtained in a perturbation expansion.[6] Since the RG recursion relations[9,10] are also derived in a perturbation expansion, we will consider the analytic continuation of these relations to define the continuation of the theory.

To be definite, let us consider the susceptibility $\chi(t,g)$ in zero field. It is described by

$$\chi(t,g)=At^{-\gamma(n)}X(x), \quad x=Bg/|t|^{\phi},$$

$$t=[T-T_c(0)]/T_c(0) \ ,$$

where ϕ is the crossover exponent, $\gamma(n)$ is the susceptibility exponent for the $O(n)$ model, and A and B are unimportant constants. The function $X(x)$ is normalized so that $X(0)=1$. Thus at $g=0$, $\chi(t,0)\sim At^{-\gamma(n)}$ as expected.

We will follow the scheme of Ref. 10 step by step to carry out our RG calculations to first order in ϵ for all real n,m in the above range. In this range of n and m, the recursion relations of Ref. 10 remain valid. We will set from the start $u=v=w=u_n^*$, where u_n^* is the isotropic $O(n)$ fixed point: $u_n^*=\epsilon/(n+8)+O(\epsilon^2)$. The scheme is as follows. Since $r_L(l)<r_T(l)$ (the argument l will be used to denote the value of a quantity after a rescaling by e^l and the initial value will be denoted by the symbol without the argument), $r_T(l)$ becomes of order unity before $r_L(l)$ does:

$$r_T(l)=r_0(l)+(m/n)g(l)=1 \ . \tag{4}$$

We cut off the renormalizations at this stage. The $\vec{S}_T$ fields are integrated out of the problem for fixed values of $\vec{S}_L$ which may still be close to criticality. The criticality of $\vec{S}_L$ is determined by the zero of $r_L(l)$, which is the effective temperature for the $\vec{S}_L$ field[10]:

$$r_L(l)=r_0(l)-[(n-m)/n]g(l)=0 \ . \tag{5}$$

For Eqs. (4) and (5) to be consistent, l should be chosen so that $g(l)=1$. At this l, $r_0(l)=(n-m)/n$. By defining $r_0(l)=t(l)/n$, so that the limit $n\rightarrow 0$ can be taken conveniently (compare with the initial value correspondence $r_0=t/n$), we find that $t(l)=(n-m)$. For $n>m$, $t(l)>0$ and $\vec{S}_L$ become critical at $T_c(g)>T_c(0)$. For $t(l)>0$, t must be chosen positive. For $n<m$, $t(l)<0$ and $\vec{S}_L$ become critical at $T_c(g)<T_c(0)$. For $t(l)<0$, t must be negative. It should be evident from this discussion that $\vec{S}_L$ can always be close to criticality, *regardless* of whether $n>m$ or $n<m$.

From $g(l)=1$ and $t(l)=n-m$, it is easily seen that $t_c=(n-m)g^{1/\phi}$, where $t_c=[T_c(g)-T_c(0)]/T_c(g)$ and $\phi=1+\epsilon n/2(n+8)+O(\epsilon^2)$. The zero of $X(x)$ is determined by the zero of $r_L(l)$: $X(x)\sim[r_L(l)]^{-\gamma(m)}$, where $\gamma(m)$ is the susceptibility exponent for the $O(m)$ model. It should now be evident from above that the critical behavior of the theory is that of the $O(m)$ model, regardless of whether $n>m$ or $n<m$, with $T_c(g)\neq T_c(0)$. For $n=m$, $T_c(g)=T_c(0)$. This should not be surprising as for $n=m$, the anisotropy parameter g is meaningless, and the behavior of the theory must be that of the $O(n)$ model.

Thus we have shown, to first order in ϵ, that the critical behavior of the m-anisotropic n-vector model is that of the $O(m)$ model for all n, where $0\leq n,m\leq 4-O(\epsilon)$.[11] Therefore a single self-avoiding ring ($n\rightarrow 0, m\rightarrow 0+$) belongs to the same universality class as that of a single self-avoiding walk: They are both governed by the $O(0)$ symmetry. On the other hand, the problem of polymerization belongs to a different universality class which is determined by the $O(m)$ symmetry, for a given m.

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