Statistical Models on Spherical Geometries

S. Boettcher* and M. Moshe
Physics Department
Technion – Israel Institute of Technology, Haifa 32000, ISRAEL

Abstract

We use a one-dimensional random walk on $D$-dimensional hyper-spheres to determine the critical behavior of statistical systems in hyper-spherical geometries. First, we demonstrate the properties of such a walk by studying the phase diagram of a percolation problem. We find a line of second and first order phase transitions separated by a tricritical point. Then, we analyze the adsorption-desorption transition for a polymer growing near the attractive boundary of a cylindrical cell membrane. We find that the fraction of adsorbed monomers on the boundary vanishes exponentially when the adsorption energy decreases towards its critical value.

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* Permanent Address: Department of Physics, Brookhaven National Laboratory, Upton, NY 11973, USA.
The study of random walk models in statistical mechanics has led to a variety of practical applications\cite{1} and illuminating analytical results.\cite{2} They provide many insights into the nature of critical phenomena observed in more complicated systems. For instance, in statistical field theory, the success of random walk models is best epitomized by its application to the triviality problem.\cite{3, 4} A fruitful area of application closer to the subject of this letter concerns the study of polymers using self-avoiding walks.\cite{5}

In this letter we propose a new model of random walks that substantially simplifies the study of statistical systems in arbitrary dimensions. In general, in systems with spherical symmetry we can decouple radial and angular motion. For such systems it is often found that many of the qualitative features of the dynamics are determined by the radial component alone. We show that nontrivial critical properties of physical quantities depending only on a radial separation are obtained with our model of random walks on concentric hyper-spheres.

With this model we also extend the powerful techniques developed for random walk models to access the plethora of phenomena that spatial boundary conditions induce.\cite{6} It is well known that the introduction of a boundary can alter the physical character of a statistical system.\cite{7} As an example of the subtle effects that our method reveals for statistical systems near curved boundaries, we discuss the adsorption-desorption transition of polymers growing near an attractive boundary.\cite{8} In the limit of an infinitely extended polymer, a finite fraction $P(\kappa)$ of monomers gets adsorbed on the boundary as soon as the attractive potential $\kappa$ on the boundary increases above a critical value. For planar boundaries one generically finds that $P(\kappa)$ vanishes linearly when $\kappa$ approaches $\kappa_c$ in the adsorbed phase. With our model we can study such a system near a curved boundary like a cylindrical cell membrane.\cite{9} Here, the configurational entropy due to the “open space” available to the polymer chain is bigger than that in the neighborhood of a flat boundary. Accordingly, one would expect that the transition is weaker. In fact, with our model we show that for a cylinder of radius $m \geq 0$ in monomer units and for $\Delta \kappa \equiv \kappa - \kappa_c \to 0_+$, the asymptotic behavior of $P(\kappa)$ is given by

$$P(\kappa) \sim \frac{4}{81} e^{-\frac{8}{8(m+1)\Delta \kappa}} \left( m+1 \right)^{-\Delta \kappa^2}. \tag{1}$$

This asymptotic expression ceases to be valid when $\Delta \kappa \sim 0.188/(m+1)$ where we observe a crossover to linear growth in the exact expression of $P(\kappa)$.

In this letter we first describe our model of random walks on a hyper-spherical geometry. We calculate the phase diagram for a simple percolation model to demonstrate the effects that random walks in such a geometry bring about. Then, we present our calculation of the adsorption transition for the case of a cylindrical geometry which leads to Eq. (1).

Consider an infinite set of concentric and equally spaced spheres in arbitrary spatial dimension $D$. $S_n$, $n = 0$, 1, 2, 3, \ldots, designates the surface of the $n$th sphere from the center with area $2\pi^{D/2}n^{D-1}/\Gamma(D/2)$. We define a random walk on such a configuration in the following way:\cite{10} Let $c_{n,t}$, $t \geq 0$, $n \geq 1$, be the probability for a random walker to be located anywhere between $S_{n-1}$ and $S_n$ at time step $t$. In this way, the angular position of the walker with respect to the origin is completely averaged away. The walker may have the choice to stay inside the region between $S_{n-1}$ and $S_n$ with probability $P_{stay}(n)$, walk
outward with a probability proportional to the total surface area of the sphere just outward, $P_{\text{out}}(n) = n^{D-1}/N(n)$, and similarly inward with $P_{\text{in}}(n) = (n-1)^{D-1}/N(n)$, $n \geq 2$, where the norm $N$ is defined through $P_{\text{out}} + P_{\text{in}} + P_{\text{stay}} \equiv 1$. Thus, we find a $1+1$-dimensional evolution equation to describe the behavior of the walker in this $D$-dimensional geometry:

$$c_{n,t} = P_{\text{out}}(n-1) c_{n-1,t-1} + P_{\text{stay}}(n) c_{n,t-1} + P_{\text{in}}(n+1) c_{n+1,t-1}. \quad (2)$$

To be consistent with Ref. 10, we designate $n = 1$ to be the innermost region, leading to the boundary condition $P_{\text{in}}(1) = 0$ (which is implicit for $D > 1$). In Ref. 10, the properties of Eq. (2) were analyzed for the initial condition $c_{n,0} = \delta_{n,0}$ and arbitrary $P_{\text{out}}$ and $P_{\text{in}}$ with $P_{\text{stay}} \equiv 0$. For example, for the case of concentric spheres it was found that the probability of ever returning to the origin for a random walker starting at the origin is given by $\Pi D = 1 - 1/\zeta(D-1)$ for $D > 2$ and unity for $D \leq 2$. This result is in qualitative agreement with $\Pi D$ for a hyper-cubic lattice.\[10\] In fact, it has been shown that one-dimensional random walks on a hyper-spherical lattice have the same scaling behavior as $D$-dimensional random walks on a hyper-cubic lattice.\[12\]

These ideas can be extend to the following directed percolation problem: For $t = 0$, there is one “wet” site on an infinitely extended line of “dry” sites with unit spacing. At even times $t$, sites take on only integer values, at odd times $t$, sites take on only half-integer values, $\pm 1/2$, $\pm 3/2$,..... If at time $t-1$ two neighboring sites at $i$ and $i+1$ are “dry”, then at time $t$ the site at $i + 1/2$ is also “dry”. Furthermore, we assume that two “wet” sites at $i$ and $i+1$ at time $t-1$ always produce a “wet” site at $i+1/2$ at time $t$. The latter assumption makes the percolation cluster, i. e. the region of all “wet” sites at any time $t$, compact and there are only two interfaces between the compact “wet” cluster in the middle and the two surrounding “dry” regions. Thus, we merely have to specify the following three situations: On the next time step the gap between the interfaces either makes a unit step outward with a probability $P_{\text{out}}$, or it makes a unit step inward with a probability $P_{\text{in}}$, or both interfaces shift to the right or to the left without widening the gap with a total probability $P_{\text{stay}}$. The behavior of such a compact percolation cluster can be mapped into the one-dimensional random walk in Eq. (2) by defining $c_{n,t}$ to be the probability that the gap between both interfaces at time $t \geq 0$ is of width $n \geq 0$.\[13\] Note that $c_{n,t}$ is now defined for all $n \geq 0$, implying the boundary condition $P_{\text{in}}(0) = 0$ here. The percolation probability $P$ is then defined as the probability of the cluster to persist for all times $t$, i. e. $n > 0$ for all $t$. Thus, $P$ is the complement of the probability of ever returning to the origin for a random walker in Eq. (2). Essam\[14\] has analyzed this problem in depth for the case $P_{\text{out}} = q^2$, $P_{\text{in}} = (1-q)^2$, and $P_{\text{stay}} = 2q(1-q)$ where $q$, $0 \leq q \leq 1$, is a constant independent of the width of the cluster. Generally, we find the percolation probability [see also Eq. (3.16) in Ref. 10]

$$P = \left[ \sum_{n=1}^{\infty} \prod_{i=1}^{n-1} \frac{P_{\text{in}}(i)}{P_{\text{out}}(i)} \right]^{-1}, \quad (3)$$

reducing to Essam’s result: $P(q) = (2q - 1)/q^2$ for $q > 1/2$, and $P(q) \equiv 0$ for $q \leq 1/2$.

More interesting results can be generated from Eq. (3) by choosing distance-dependent coefficient functions $P_{\text{out}}$ and $P_{\text{in}}$. [Note that Eq. (3) does not depend on $P_{\text{stay}}$.] For instance,
for $P_{\text{out}}(n) = q^2(n+1)^\delta/\mathcal{N}(n)$ and $P_{\text{in}}(n) = (1-q)^2n^\delta/\mathcal{N}(n)$, $n \geq 1$, with $P_{\text{out}}(0) = 1$, we obtain $\delta$-dependent critical coefficients. We compute the percolation probability\footnote{For $\delta = 2$ we can study the case of a spherical boundary while for $\delta = 0$ or $m \to \infty$ we recover the case of a planar boundary. Negative $\delta$ would correspond to a polymer growing in a cavity.}

$$P(q, \delta) = \left[\sum_{n=0}^{\infty} \left(\frac{1-q}{q}\right)^{2n} (n+1)^{-\delta}\right]^{-1} = \Phi\left[\left(\frac{1-q}{q}\right)^2, \delta, 1\right]^{-1}. \tag{4}$$

Again, for $\delta = 0$ we return to Essam’s result. In Fig. 1 we plot Eq. (4). For all $\delta$ we obtain $q_c = 1/2$. But while for $\delta < 1$ the transition to percolation is second order, we find a tricritical point at $\delta = 1$ and a first order transition for $\delta > 1$. The discontinuity is equal to $1/\zeta(\delta)$. Such a model can be interpreted as directed compact percolation in a spherical configuration where $n$ refers to the radius of the percolating bubble in dimension $D = \delta + 1$. Other choices of $P_{\text{out}}$, $P_{\text{in}}$, and $P_{\text{stay}}$ might lead to further interesting interpretations.

As an application of the ideas presented in the previous paragraphs, we discuss the adsorption fraction for an extended polymer growing near an attractive cylindrical boundary.\footnote{This restriction on the directed walk will have no impact on the scaling behavior for $L \to \infty$.} It highlights the profound impact of a curved boundary on the critical behavior of physical quantities that a planar approximation could not reveal.

In outlining the theory we extend on the beautiful treatment in Refs. 2 and 17. Consider a lattice consisting of an infinite set of concentric cylinders of unit spacing. Let the innermost cylinder - the surface of the boundary - be of integer radius $m \geq 0$, the next innermost of radius $m + 1$, and so on. Each cylinder is labeled by its radius. Now consider a random walk in unit steps either parallel to the length or perpendicular to these cylinders, starting on the boundary. A parallel step is taken with a relative weight of $P_{\text{stay}} \equiv 1$, steps outward and inward are taken with relative weights of $P_{\text{out}}(n) = 2(n+1)^\delta/[n^\delta + (n+1)^\delta]$ and $P_{\text{in}}(n) = 2n^\delta/[n^\delta + (n+1)^\delta]$, respectively, for $\delta = 1$ and $n > m\footnote{This restriction on the directed walk will have no impact on the scaling behavior for $L \to \infty$.}$ while on the boundary $P_{\text{out}}(m) = 1$, $P_{\text{in}}(m) = 0$. At each step the walker picks up a statistical weight $z$, while for each step on the boundary the walker also acquires an additional weight of $\kappa \geq 1$. For simplicity, we neglect self-interaction and excluded-volume effects.

A walk with $L > 0$ parallel steps has reached $L$ levels, $\{h_i\}_{i=1}^{L+1}$, $h_i \geq m$, above or on the boundary. We want to restrict these walks such that $|h_{i+1} - h_i| \leq 1$, $0 \leq i \leq L\footnote{This restriction on the directed walk will have no impact on the scaling behavior for $L \to \infty$.}$ The transfer matrix $T_{h_{i+1},h_i}$ that describes the transition of the walker from the $i$th to the $(i+1)$st level is given by

$$T_{j,i} = z^{|j-i|\kappa^m} \left[P_{\text{stay}}\delta_{j,i} + P_{\text{out}}(i)\delta_{j-1,i} + P_{\text{in}}(i)\delta_{j+1,i}\right]. \tag{5}$$

The partition function $Z_L$ for walks extending $L$ parallel steps is given by

$$Z_L = z^L \sum_{h_i} \delta_{m,h_0} T_{h_1,h_0} T_{h_2,h_1} \ldots T_{h_L,h_{L-1}} = z^L \tilde{\mathcal{B}}(L) T^L \tilde{e}. \tag{6}$$

The total partition function for walks of all length, $Z = \sum_{L=1}^\infty Z_L$, then evaluates to

$$Z(z, \kappa) = z\tilde{\mathcal{B}}(L) T(1 - zT)^{-1} \tilde{e}. \tag{7}$$
If $\lambda_{\text{max}}$ is the largest eigenvalue of $T$, then $Z$ diverges for $z \nearrow z_{\infty}(\kappa) = 1/\lambda_{\text{max}}$.

The average length of a walk and the average number of steps taken on the surface of the boundary are usually defined to be

$$< N(z, \kappa) > = z \partial_z \ln Z(z, \kappa), \quad < N_s(z, \kappa) > = \kappa \partial_\kappa \ln Z(z, \kappa),$$

respectively. Both, $< N >$ and $< N_s >$, diverge for $z \nearrow z_{\infty}(\kappa)$, defining an infinitely long walk. We want to interpret such walks with the infinite chain limit of polymers stretched out along a cylindrical boundary. Then, $< N_s >$ refers to the number of monomers which are adsorbed on the boundary as a function of the attractive potential $\kappa$. The fraction of adsorbed monomers $P(\kappa)$ is given by

$$P(\kappa) = \lim_{z \nearrow z_{\infty}(\kappa)} \frac{< N_s(z, \kappa) >}{< N(z, \kappa) >} = -\frac{\kappa}{z_{\infty}(\kappa)} \frac{dz_{\infty}(\kappa)}{d\kappa}.$$  

Thus, $z_{\infty}(\kappa)$ marks a line in the $(\kappa, z)$-plane for which $P(\kappa)$ is defined. To obtain a non-vanishing adsorption fraction it is necessary that the attractive potential $\kappa$ is larger than some critical value, $\kappa_c$. In terms of the eigenvalues $\lambda = \lambda(z, \kappa)$ of the transfer matrix $T$, $\kappa_c$ is found to be the smallest value of $\kappa$ for which $T$ has a bound state on the line $z = z_{\infty}(\kappa)$.

The spectrum $\lambda$ of the transfer matrix $T$ is determined by the eigenvalue problem

$$\lambda g_n = \sum_{i=m+1}^{\infty} T_{n,i} g_i = \begin{cases} g_n + z \frac{2n}{2n-1} g_{n-1} + \frac{2(n+1)}{2n+3} g_{n+1}, & n \geq m + 2; \\ g_{m+1} + zg_m + \frac{2(m+2)}{2m+5} g_{m+2}, & n = m + 1; \\ \kappa g_m + \kappa z \frac{2(m+1)}{2m+3} g_{m+1}, & n = m. \end{cases}$$

This system of equations is most conveniently examined with generating function techniques: Defining $H(x) = \sum_{m=0}^{\infty} x^m g_n/(2n+1)$, we obtain a first order linear, inhomogeneous differential equation for $H$. Bound states of $T$ are determined by requiring both, that $g_n \to 0$ for $n \to \infty$ and that $g_n$ fulfills the boundary condition at $n = m$. This eigenvalue condition is equivalent to requiring that $H(x)$ may have no singularity for $|x| < 1$. Writing $\epsilon = 2z/(\lambda - 1)$ and $\gamma = (1 - \sqrt{1 - \epsilon^2})/\epsilon$, we find

$$\frac{z\kappa \epsilon}{\gamma} = \left[ (2z + \epsilon)(\kappa - 1) - \frac{z\kappa}{m+1} \right] \frac{m+1}{m+1/2} F \left( \frac{1}{2}, m+1; m+\frac{3}{2}; \gamma \right),$$

where $F$ is a hypergeometric function. We obtain $z_{\infty}(\kappa)$ implicitly from Eq. (11) by replacing $\lambda = 1/z_{\infty}(\kappa)$. If $\lambda \geq 1+2z$, or equivalently $\kappa \geq \kappa^*(z) = (1+2z)/(1+z)$, there is one solution of Eq. (11) for $\lambda = \lambda_{\text{max}}$ such that both conditions on the eigenvectors $g$ are met. We obtain $\kappa_c = 4/3$, $z_c = 1/2$ at the intersection of $\kappa^*(z)$ and $z_{\infty}(\kappa)$. Inserting $z_{\infty}(\kappa) = z_c - \Delta z(\kappa)$ and $\kappa = \kappa_c + \Delta \kappa$ into the equation for $z_{\infty}$, we get in the limit $\Delta z \to 0_+$, $\Delta \kappa \to 0_+$:

$$\Delta z(\kappa) \sim \frac{1}{48} \exp \frac{-8}{3(m+1)} \Delta \kappa, \quad \Delta \kappa \ll 1/(m+1),$$

neglecting exponentially smaller corrections. Using Eq. (9), we arrive at Eq. (1). In Fig. 2 we plot the exact values of $P(\kappa)$ for $m = 0, 1, 2, 3$ and $m = \infty$ for $\kappa \geq \kappa_c = 4/3$. Note
the substantial error in estimating $\kappa_c$ for small $m$ using an extrapolation from values where $P(\kappa)$ appears to be linear. A measure of the overestimate on $\kappa_c$ is given by the inflection point of $P(\kappa)$ in Eq. (1) at $\Delta\kappa = 0.188/(m+1)$, beyond which the approximation in Eq. (1) ceases to be valid and $P(\kappa)$ grows linearly.

The simplicity of the dynamics in this new random walk model, and the nontrivial scaling obtained from it, raise interesting questions regrading the universal properties of this lattice. At the critical transition only a few fundamental properties of the system determine its behavior. In this model, the critical behavior arises from the balance between a short-range attractive potential and the spatial entropy. We argue that these features are sufficiently well represented by a random walk on a hyper-spherical lattice. It has been shown that such a lattice reproduces all the universal scaling properties expected of lattices.\[12\] The critical behavior obtained on this lattice for rotationally symmetric systems should therefore reflect the universal critical behavior of the system. The advantage of random walks on hyper-spheres is to describe the critical behavior in a minimal and tractable way in comparison, for example, to a far more structured hyper-cubic lattice.

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FIGURE CAPTIONS

FIGURE 1: The percolation probability $P(q, \delta)$ for directed compact percolation in a curved geometry. For any $\delta$, the percolation threshold occurs at $q_c = 1/2$, but for $\delta < 1$ the transition is second order, while for $\delta > 1$ the transition is first order with a discontinuity of $P(q_c, \delta > 1) = 1/\zeta(\delta)$, indicated by a darkened wedge.

FIGURE 2: The exact adsorption fraction $P(\kappa)$ plotted for $m = 0, 1, 2, 3$ and $m = \infty$ and $\kappa \geq \kappa_c = 4/3$. For finite $m$, $P(\kappa)$ vanishes exponentially for $\kappa - \kappa_c \rightarrow 0^+$ while it crosses over to a linear increase when $\kappa - \kappa_c > 0.188/(m + 1)$. For $m = \infty$ we recover the linear scaling for $P(\kappa)$ that was found in Ref. 17.
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Figure 1
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