Random Walks as Critical Systems

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(Dated: May 21, 2021)

We provide an overview of the theory of random walks and how this can be viewed as a theory of a critical system. We introduce the self avoiding walk and argue that it is in a different universality class from the unrestricted walk. We then go on to perform a renormalization group transformation both on a lattice and a field theory in order to estimate the critical exponents, before generating numerical estimates of the critical exponent on a simple two dimensional lattice.

I. INTRODUCTION

Polymer science is among the most important components of modern biophysics. Some of the earliest models of polymers describe the polymer as a collection of connected links in a d dimensional space, with the first link attached to the origin. Each link is oriented in a random direction uniformly over the d-dimensional sphere. This model, commonly referred to as a freely jointed chain, describes the polymer as an unristricted random walk. It thus predicts that the ensemble average position of the end of the polymer is $\langle \boldsymbol{r} \rangle = 0$, while the average distance of the end from the origin is given as $\langle \boldsymbol{r}^2 \rangle^{1/2} = aN^{1/2}$ where a is the length of any individual link and N is the number of links in the chain. As the number of links $N \to \infty$, the mean distance from the origin diverges as N^ν with $\nu = 1/2$. In this light, it is natural to view the random walk as a critical system [1] with the "temperature" being $1/N$ and ν being a critical exponent. As with most critical exponents, ν is a universal quantity which does not depend strongly on the microscopic model in question, this is essentially the statement of the Central Limit Theorem. As this scaling is universal, different implementations of this polymer model (such as on a lattice) give the same scaling with N.

All of these models mentioned assume that the monomers of our polymer have no physical size and can thus overlap without issue. Clearly, this is an unrealistic assumption and we should consider excluded volume effects due to the size of monomers. It is actually easiest to implement this idea on a lattice, where the walk cannot return to the same site more than once. Such a description is known as a self-avoiding walk (SAW). Much work has been done to study the critical properties of the SAW, and it has been known for many years now that in dimensions $d \leq 4$ the SAW has a distinct critical exponent ν from the unrestricted case. A very clever argument first presented by Flory actually proposes that for dimensions less than four, $\nu = \frac{3}{2+d}$. This turns out to be exact in both one and two dimensions. With the invention of the Renormalization Group (RG) and the insights of Kadanoff and Wilson [2], it then became possible to examine the SAW in 3 dimensions analytically [3, 4], as well as numerically [5]. In this project, we will review some RG approaches to studying the SAW as both a lattice model and a field theory. We will also present some numerical findings using Monte Carlo simulation methods.

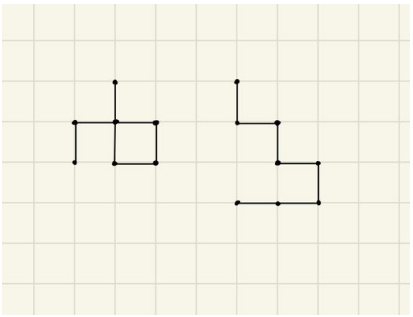

FIG. 1. On the left is an example of an unrestricted random walk, on the right is an example of a SAW. These walks are drawn on a lattice for simplicity, each taking seven steps.

II. POSITION SPACE RG AND THE SAW UNIVERSALITY CLASS

The unrestricted random walk (RW) has a universality class described in full by the Central Limit Theorem. In particular, a lattice random walk of N steps has a mean end-to-end distance $\sqrt{\langle R^2 \rangle} \sim N^\nu$ where $\nu = 1/2$. One may naturally wonder whether or not the SAW falls into the same universality class as the RW in d spatial dimensions. Here, we will carry out a real space RG procedure [6] in order to calculate the critical exponent ν for a SAW in $d = 2$ dimensions [7]. From this calculation, we will see that the SAW actually falls into a *different* universality class for $d \leq 4$. For a fixed walk length N, we take all SAWs to be equally likely. Knowing this, we can construct the grand partition function for the SAW as

$$Z(y) = \sum_N y^N \Omega_N \tag{1}$$

where Ω_N is the number of SAWs of length N, and y is a fugacity dual to the walk length N. Here, y serves as a coupling constant which will flow under our RG scheme. We will implement our scheme on a square lattice in 2 dimensions. We will rescale by a factor $b = 2$, and map SAWs from the fine lattice onto those of the coarser lat-

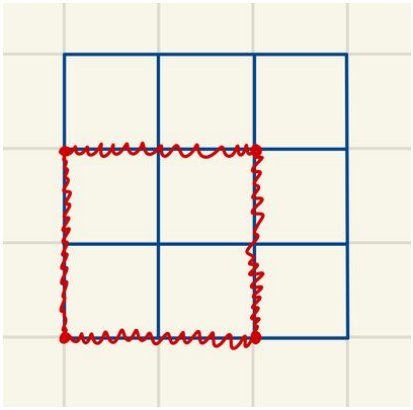

FIG. 2. Schematic representation of our real space coarse-graining procedure. The blue is our original lattice, while the red, squiggly lines represent our new coarse-grained lattice with $b = 2$.

tice. By coarse graining our walks, the fugacity y is altered according to

$$y' = 2y^2 + 4y^3 + 2y^4 \tag{2}$$

which has a non-trivial fixed point at $y^* = 0.297$ which gives a value for $\nu = \frac{\log b}{\log \frac{dy'}{dy}|_{y^*}} = 0.771$. The exact value of ν on the $d = 2$ square lattice is known to be $\nu = 3/4$, we see our RG scheme is in good agreement with this result. This discrepancy can be accounted for by noting that when we coarse grain our walks onto this new lattice, there are some walks that are lost in this process. This is in the same spirit as a moving bond approximation used to study the $d = 2$ Ising model. This simple RG scheme has also allowed us to show that the SAW in two dimensions is in a different universality class from the RW.

III. FIELD THEORIES OF THE SAW

A. SAWs as a theory of $n \to 0$ magnets

The critical properties of the SAW can be examined by studying the $O(n)$ magnetization model. We begin with n-component spins on some lattice, allowed to interact with their neighbors according to

$$-\beta H = K \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \tag{3}$$

We will perfrom a high-temperature expansion in terms of graphs as we did in lecture. The partition function is

$$Z = \mathrm{Tr}\ \exp\left(K \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j\right) = \sum_{\text{Graphs}} \frac{K^l}{l!} \mathrm{Tr} \prod_{\langle i,j \rangle \in G} \vec{s}_i \cdot \vec{s}_j \tag{4}$$

Where l is the number of bonds in each graph and Tr tells us to trace over each spin degree of freedom. One can show that in the limit $n \to 0$, the only graphs that contribute to the correlation function $\langle \vec{s}_0 \cdot \vec{s}_r \rangle$ are those in which describe self avoiding walks from 0 to r [8]. This provides a mapping between the Landau theory magnets and SAWs, allowing us to estimate the critical properties of the SAW by looking at the $O(n \to 0)$ magnet. In particular, we can formalize our previous estimate that the upper critical dimension is $d_c = 4$ and in dimensions $d > d_c$ the critical properties of the SAW are those of the unrestricted RW. In $d = 4$ dimensions, we actually see logarithmic corrections [9] to our scaling, while in $d = 4 - \epsilon$ dimensions we can import our results for the $O(n)$ magnet in the limit $n \to 0$ to find

$$\nu = \frac{1}{2} + \frac{\epsilon}{16} + O(\epsilon^2) \tag{5}$$

B. Perturbative Renormalization of a Worldsheet

One could also hope to study the SAW as a perturbation to a free Hamiltonian describing an unrestricted RW. At sufficiently large scales, the random walk can be viewed as a curve $\boldsymbol{r}(s) \in \mathbb{R}^d$ where s parameterizes the length along the curve. Symmetry considerations demand that the Hamiltonian for this curve be invariant under all rotations and translations $\boldsymbol{r} \to \boldsymbol{R}\boldsymbol{r} + \boldsymbol{c}$. To lowest order in a gradient expansion, the most general Hamiltonian we can write down is

$$\beta H = \frac{K}{2} \int_0^L ds (\partial_s \boldsymbol{r})^2 \tag{6}$$

Here, L is the length of the curve we are considering, it should be viewed analogously to the number of steps in the discrete random walk case. This Hamiltonian defines our free theory which describes the unrestricted random walk. We can insist the walk be self-avoiding by penalizing configurations that intersect themselves. We do this by including an infinite range interaction

$$\mathcal{U} = u \int_0^L ds \int_{s+a}^L ds'\ \delta^d(\boldsymbol{r}(s) - \boldsymbol{r}(s')) \tag{7}$$

Here, a is some short distance cutoff analogous to the step size in the discrete model. Combining our two Hamiltonians gives us what is known as the Edwards Hamiltonian [10, 11]. Ignoring for the time being the first step of the RG, we can rescale space and our field as $s \to bs, \boldsymbol{r} \to \zeta \boldsymbol{r}$ to find

$$K' = b^{-1}\zeta^2 K \tag{8}$$

$$u' = b^2 \zeta^{-d} u \tag{9}$$

Around the fixed point where $K' = K$ we take $\zeta = b^{1/2}$ and our perturbation scales as $u' = b^{2-d/2}u$. From this, we can see that for $d > 4$, u is an irrelevant operator and we flow towards our Gaussian fixed point where we have an unrestricted random walk. For $d < 4$, the inclusion of

a self-avoiding interaction changes the universality class and brings the theory to a new fixed point of the RG. Further, we notice that our field $\boldsymbol{r}$ has units $[\boldsymbol{r}] = 1/2$ (where length has units $[s] = 1$). The scaling of $\boldsymbol{r}$ about the fixed point defines the critical exponent ν. Here, we will demonstrate how to renormalize this theory to $O(u)$. We begin by examining the free theory defined by Equation 6. This theory is Gaussian, so we have

$$\langle \partial_s r_\alpha(s) \partial_s r_\beta(s') \rangle_0 = \frac{\delta(s-s')\delta_{\alpha\beta}}{K} \tag{10}$$

Which implies

$$\langle (\boldsymbol{r}(L) - \boldsymbol{r}(0))^2 \rangle_0 = \frac{dL}{K} \tag{11}$$

This confirms that the free theory does in fact describe the simple random walk we expect with $\nu = 1/2$. We proceed as usual, breaking up our field into slow and fast modes, $\boldsymbol{r}(s) = \boldsymbol{r}_s^< + \boldsymbol{r}_s^>$, where we remain in real space and have moved the spatial index to a subscript for brevity. To first order in u, we are left to calculate

$$\langle \mathcal{U} \rangle_0^> \sim \langle \delta^d(\boldsymbol{r}_s - \boldsymbol{r}_{s'}) \rangle_0^> \tag{12}$$

$$= \int \frac{d^d q}{(2\pi)^d} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_s^< - \boldsymbol{r}_{s'}^<)} \times \langle e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_s^> - \boldsymbol{r}_{s'}^>)} \rangle_0^> \tag{13}$$

$$= \int \frac{d^d q}{(2\pi)^d} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_s^< - \boldsymbol{r}_{s'}^<)} e^{-\frac{q^2}{2}\langle (\boldsymbol{r}_s^> - \boldsymbol{r}_{s'}^>)^2 \rangle_0^>} \tag{14}$$

$$= \int \frac{d^d q}{(2\pi)^d} e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_s^< - \boldsymbol{r}_{s'}^<)} e^{-\frac{q^2}{2}\frac{(s'-s)}{K}} \tag{15}$$

Where all that is left to do is the gaussian integrals over $\boldsymbol{q}$. Upon integrating out our fast modes, we have shifted our cutoff $a \to ba$. Keeping ba as a lower cutoff in 7, we have a new contribution to the energy in the form

$$\Delta\beta H = u \int_0^L ds \int_{s+a}^{s+ba} ds' \Big(\frac{K}{2\pi(s'-s)}\Big)^{d/2} e^{-\frac{K(\boldsymbol{r}_s^< - \boldsymbol{r}_{s'}^<)^2}{2(s'-s)}} \tag{16}$$

Because s is close to s', we can expand $\boldsymbol{r}_{s'}^< - \boldsymbol{r}_s^< = (s'-s)\partial_s \boldsymbol{r}_s^<$, and further expand the exponential. The upshot is that we have a term $\sim (\partial_s \boldsymbol{r})^2$ which renormalizes K. We will also generate all other terms consistent with symmetry in this gradient expansion, but these will be irrelevant as we flow towards the IR.

$$\widetilde{K} = K - uK\Big(\frac{K}{2\pi}\Big)^{d/2} \int_a^{ba} x^{1-d/2} dx \tag{17}$$

Going to $O(u^2)$ renormalizes our interaction to $\widetilde{u} = u - 2u^2\Big(\frac{K}{2\pi}\Big)^{d/2} \int_a^{ba} x^{1-d/2} dx$ [12]. Performing the final steps of the RG, we rescale $s \to bs$ and $\boldsymbol{r} \to \zeta \boldsymbol{r}$ and expand $b \approx 1 + \ell$, $d = 4 - \epsilon$. We find to $O(\epsilon)$

$$K' = b^{-1}\zeta^2 (K - uK\Big(\frac{K}{2\pi}\Big)^{d/2} \int_a^{ba} x^{1-d/2} dx) \tag{18}$$

$$\approx b^{-1}\zeta^2 K(1 - u\Big(\frac{K}{2\pi}\Big)^{d/2} \ell) + O(\epsilon^2, \ell^2, \epsilon\ell) \tag{19}$$

$$u' \approx b^2 \zeta^{-d} u(1 - 2u\Big(\frac{K}{2\pi}\Big)^{d/2} \ell) + O(\epsilon^2, \ell^2, \epsilon\ell) \tag{20}$$

Defining $\alpha = u\Big(\frac{K}{2\pi}\Big)^{d/2}$, we can examine a fixed point where $K = K'$ by taking

$$\zeta = \sqrt{\frac{b}{1-\alpha\ell}} = b^{1/2+\alpha/2} + O(\ell^2) \tag{21}$$

Similarly, at the fixed point $u' = u + O(\ell^2, \epsilon^2)$. Solving gives

$$\alpha = \frac{\epsilon}{8-\epsilon} = \frac{\epsilon}{8} + O(\epsilon^2) \tag{22}$$

and

$$\nu = \frac{1}{2} + \frac{\epsilon}{16} \tag{23}$$

which is exactly what we saw for the $O(n \to 0)$ model.

IV. NUMERICAL SIMULATION

There has also been extensive work to probe the critical properties of the SAW numerically. With the onset of modern computing, this allows us to generate high fidelity estimates of ν through simple Monte-Carlo simulations. Perhaps unsurprisingly, one of the main difficulties in sampling the distribution of SAWs is consistently generating valid walk configurations. There have been many approaches to alleviate this problem. We will describe one especially simple approach here, the *pivot* algorithm [13, 14]. The pivot algorithm allows one to generate configurations on any lattice with symmetry group G, as has been done in the literature. The steps of the algorithm are as follows

1. Initialize a valid SAW of length N, denoted $\boldsymbol{\omega} = (\omega_1, \omega_2, ..., \omega_N)$. It is simplest to have this initialization just be a walk along one of the axes, and is the most common choice.

2. Select an index $k = 2, ..., N-1$ uniformly at random. This index will serve as our pivot. Additionally, choose an element $g \in G$ of the symmetry group of the lattice. For example, on the two dimensional square lattice $\mathbb{Z}^2$, g would be a rotation matrix by some multiple of $\pi/2$

3. generate a proposal walk defined as $\boldsymbol{\omega}_p = (\omega_1, ..., \omega_k, \widetilde{\omega}_{k+1}, ..., \widetilde{\omega}_N)$ where

$$\widetilde{\omega}_j = \omega_k + g(\omega_j - \omega_k) \tag{24}$$

4. if $\boldsymbol{\omega}_p$ is a SAW, accept it with probability $1/2$. This preserves detailed balance and reflects the fact that the distribution of configurations should be uniform across all SAWs of fixed length.

5. repeat steps 2-4 to generate a suitable number of sample configurations.

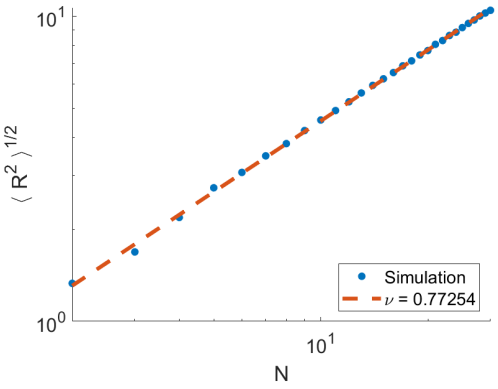

FIG. 3. Estimation of the critical exponent ν using the pivot algorithm to sample the configuration space of SAWs on the square lattice $\mathbb{Z}^2$.

As seen in Figure 3, our simulations give an estimate of $\nu = 0.77$, which is accurate to about 3%! The algorithm presented is very general, and can be implemented on many lattice structures. Since the critical exponents are universal properties, the choice of lattice should not matter and it suffices to choose simple (hyper)cubic lattices $\mathbb{Z}^d$ to determine ν in dimension d. As a proof of concept we have implemented the pivot algorithm on $\mathbb{Z}^2$ and used the sample configurations to estimate $\langle R^2 \rangle^{1/2}$ at varying walk lengths N.

V. CONCLUSION

We have introduced and examined multiple models of the SAW. The benefit of studying different variants of this model becomes clear when we attempt to define an RG flow for the couplings. On a lattice, an approximate real space RG is best suited for the task, while a field theory of a SAW is easier studied with perturbative momentum shell RG methods. Although many of the results obtained are well known, it is our hope that our demonstration of the course-graining for the Edwards Hamiltonian constitutes a novel contribution. We concluded our results with a numerical simulation of a SAW, supporting some of our previous results. There is much more to be said about the SAW, it is a well-studied problem in many fields of science and engineering. It is my hope that this project provides a sufficiently technical introduction to the topic, in the context of the Renormalization Group.

[1] S. Havlin and D. Ben-Avraham, New approach to self-avoiding walks as a critical phenomenon, Journal of Physics A: Mathematical and General **15**, L321 (1982).

[2] K. G. Wilson and M. E. Fisher, Critical exponents in 3.99 dimensions, Physical Review Letters **28**, 240 (1972).

[3] K. F. Freed, Polymers and random walks renormalization group description and comparison with experiment, Journal of Rcsearch of the National Bureau of Stancards **90** (1985).

[4] P.-G. de Gennes, Exponents for the excluded volume problem as derived by the wilson method, Physics Letters A **38**, 339 (1972).

[5] D. Dhar, Self-avoiding random walks: Some exactly soluble cases, Journal of Mathematical Physics **19**, 5 (1978).

[6] M. Kardar, *Statistical physics of fields* (Cambridge University Press, 2007).

[7] R. J. Creswick, H. A. Farach, C. P. Poole, and C. Poole, *Introduction to renormalization group methods in physics* (Wiley-Interscience, 1992).

[8] P.-G. De Gennes and P.-G. Gennes, *Scaling concepts in polymer physics* (Cornell university press, 1979).

[9] P. Grassberger, R. Hegger, and L. Schafer, Self-avoiding walks in four dimensions: logarithmic corrections, Journal of Physics A: Mathematical and General **27**, 7265 (1994).

[10] J. Cardy, *Scaling and renormalization in statistical physics*, Vol. 5 (Cambridge university press, 1996).

[11] S. F. Edwards, The statistical mechanics of polymers with excluded volume, Proceedings of the Physical Society (1958-1967) **85**, 613 (1965).

[12] J. McGreevy, The renormalization group (2018).

[13] S. Caracciolo, G. Parisi, and A. Pelissetto, Random walks with short-range interaction and mean-field behavior, Journal of Statistical Physics **77**, 519 (1994).

[14] N. Clisby, Accurate estimate of the critical exponent ν for self-avoiding walks via a fast implementation of the pivot algorithm, Physical review letters **104**, 055702 (2010).