A new finite-size scaling approach to random walks

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Abstract

We present a new finite-size scaling method for the random walks (RW) superseeding a previously widely used renormalization group approach, which is shown here to be inconsistent. The method is valid in any dimension and is based on the exact solution for the two-point correlation function and on finite size scaling. As an application, the phase diagram is derived for random walks with a surface-bulk interaction where the system has either a surface or a defect. Possible extensions to disordered systems are also discussed.

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I. INTRODUCTION

Renormalization Group (RG) has been a cornerstone in the analytical evaluation of the critical exponents of various statistical models in the past two decades [1,2,3]. Its application to self-avoiding walks (SAW) was a natural consequence of the formulation of SAW as $n \to 0$ limit of the $n$-vector model whose two-point correlation function yields, in this limit, the generating function of the random walk with the excluded volume effect [4].

An extension of this approach to the case without self-avoidance was carried out by Family and Gould (FG) [5] in the absence of disorder, and by Sahimi and Jerauld (SJ) [7] and by Gould and Kohin (GK) [8] in the disordered case, where the disorder was mimicked by a site (or bond) percolation cluster. The results in the latter cases were found to be in very good agreement with those of numerical simulations [9] of random walks on a percolating cluster on the square lattice. However unlike GK who used the kinetic rule for the random walk (more precisely they solved the model which is nicknamed myopic ant) [10], SJ used the static recipe which is now recognized to correspond to the so-called ideal chain model [11,12,13,14,15]. Recent analysis [11,12,13,14,15] with various different approaches have shown that the ideal chain does not belong to the same universality class as the kinetic walks; rather it is equivalent to the random walk in a trapping environment [14]. In view of this, we felt that a better understanding of the method in the absence of disorder was needed.

By calculating exactly the two-point correlation functions for a random walk on a quadrant of the lattice (the so-called corner rule [4]), we will show that the procedure introduced by FG needs to be revised because of the uncontrolled approximations. This is also supported by an exact analytical calculation on the one-dimensional analog. We will then proceed to show how one can obtain a consistent procedure based on the finite size scaling hypothesis [16].

The outline of this paper is as follows: In Sec.1 we first recall the derivation of the formal solution of the two-point correlation function for the random walk. This solution constitutes
the basis of the real-space renormalization group approach to this problem. The standard 
procedure is then reviewed and its fundamental problems are discussed. In Sec.II, the one-
dimensional version of this problem is analyzed exactly in detail, and the inconsistencies of 
previous renormalization approaches are exposed. In Sec.IV, we introduce our new method 
which is based entirely on the widely accepted finite size scaling approach. Then in Sec.V 
this method is applied to describe the phase diagram for a problem with different fugacities 
for the surface and bulk. The results are consistent with mean field theory where applicable. 
Finally Sec.VI contains some conclusions and perspectives on the extension of this method 
to disordered systems.

II. TWO-POINT CORRELATION FUNCTION FOR RANDOM WALKS

It is well known that the unconstrained random walk on a lattice can be solved by 
using a generating function technique pioneered by Montroll [17,18,19]. Let \( P_{x_0,x}(N) \) the 
probability for the walker to be at the position \( x \in \mathbb{Z}^d \) at the (discrete) time \( N \), given that 
it started at the site \( x_0 \) at the initial time 0. The master equation to be solved is then

\[
P_{x_0,x}(N + 1) = \frac{1}{z} \sum_{y(x)} P_{x_0,y}(N)
\]  

(2.1)

where the notation \( y(x) \) means that the sum is restricted to the nearest neighbors of \( x \). The 
number \( C_{x_0,x}(N) = z^N P_{x_0,x}(N) \) of \( N \)-step walks with end points \( x_0 \) and \( x \) then satisfies 
the analogous equation,

\[
C_{x_0,x}(N + 1) = \sum_{y(x)} C_{x_0,y}(N).
\]  

(2.2)

In order to solve the master equation, it proves convenient to introduce the generating 
function \( G_{x_0,x}(k) \),

\[
G_{x_0,x}(k) = \sum_{N=0}^{\infty} k^N C_{x_0,x}(N) \\
= \sum_{w:x_0 \rightarrow x} k^{||w||}
\]  

(2.3)
where \( w \) is a walk having \( \mathbf{x}_0 \) and \( \mathbf{x} \) as the end points, and \( |w| \) is the number of steps associated with it.

By multiplying (2.2) by \( k^{N+1} \) and summing over all \( N \), one gets, taking into account the initial condition \( C_{\mathbf{x}_0,\mathbf{x}}(0) = \delta_{\mathbf{x}_0,\mathbf{x}} \),

\[
G_{\mathbf{x}_0,\mathbf{x}}(k) = k \sum_{\mathbf{y}(x)} G_{\mathbf{x}_0,\mathbf{y}}(k) + \delta_{\mathbf{x}_0,\mathbf{x}}. \tag{2.4}
\]

It is easy to see that \( G_{\mathbf{x}_0,\mathbf{x}}(k) \) is also the two-point correlation function of a scalar free-field theory and that Eq. (2.3) can be recovered from a von Neumann expansion (see e.g. [14,19]).

Generally the procedure for a RG includes two basic steps: First one coarse grains microscopic details in real space or integrates over the fast modes in momentum space. This is followed by a rescaling of the space/momentum and of the model variables while conserving the partition function and recasting the Hamiltonian in the same functional form as before.

In the case of the random walk, the requirement of the conservation of the partition function amounts to a mapping between the rescaled and original fugacities which can be formally expressed as:

\[
P(\{k\}', w') = \sum_{w | w'} P(\{k\}, w) \tag{2.5}
\]

where \( k' \) and \( w' \) are the fugacity and walk on the rescaled lattice, respectively, \( P \) stands for the partition function, and the sum is constrained to all \( w \) consistent with \( w' \). In the case of self-avoiding walks, this procedure leads to a well known polynomial recursion relation between \( k' \) and \( k \) whose linearization around the fixed point leads to the value of the correlation length exponent \( \nu \). On the other hand, once the self-avoidance is turned off, the polynomial recursion becomes an infinite series since there are an infinite number of walks even in the smallest possible cell. One is thus faced with the problem of finding either a way of summing over an infinite number of walks or a truncation procedure. Some time ago Family and Gould [5] devised a recipe along the latter line. Their idea was that if \( L = ba \) (\( a \) being the lattice constant) is the size of the system, then walks with number of steps \( N \) larger than \( N_{\text{MAX}} \) given by
\[ N_{\text{MAX}} \sim [< R_N^2 >]_{\text{MAX}} \sim L^2 \] (2.6)

will give a negligible contribution to the sum in Eq. (2.3).

An \( L \times L \) cell can be mapped into an \( L' \times L' \) cell by the requirement (2.5) as

\[ \chi_\hat{n}(k', \frac{1}{L'}) = \chi_\hat{n}(k, \frac{1}{L}) \] (2.7)

where we defined the quantity

\[ \chi_\hat{n}(k, \frac{1}{L}) \equiv \sum_{N=0}^{\infty} C_\hat{n}(x_0, N)k^N \] (2.8)

and \( C_\hat{n}(x_0, N) \) is the number of \( N \)-step walks in the cell starting from \( x_0 \) and exiting in the direction \( \hat{n} \) \((n = 1, 2)\). According to the assumption of FG, \( \chi \) can be approximated as

\[ \chi_\hat{n}(k, \frac{1}{L}) \approx \sum_{N=N_{\text{MIN}}}^{N_{\text{MAX}}} C_\hat{n}(x_0, N)k^N \] (2.9)

where \( N_{\text{MAX}} \) is related to the system size by Eq. (2.6) and \( N_{\text{MIN}} \) is the minimum number of steps needed to reach the closest exit of the \( L \times L \) cell.

As an example (cf. Fig.1), if we take \( L' = a \) and \( L = 2a \), then we have from Eqs. (2.7) and (2.9):

\[ k' \approx \sum_{N=N_{\text{MIN}}}^{N_{\text{MAX}}} C_\hat{n}(x_0, N)k^N = k^2 + 2k^3 + 5k^4 + 14k^5 \] (2.10)

On the other hand the total number of \( N \)-step walks having \( x_0, x \) as the end points can be calculated easily from Eq. (2.4) which gives the quantity (2.3) exactly. Therefore both sides of Eq. (2.7) can be calculated exactly without any truncation procedure. In Fig.2 we compare the right-hand side of Eq. (2.8) calculated exactly with the one calculated using the FG truncation procedure, which can clearly be recovered upon numerical Taylor expansion of the exact result up to the desired order. It is apparent that although in general the FG truncation procedure seems to reproduce rather well the trend of the fixed point \( k^* \), it fails to reproduce the singularity present in (2.8). This singularity moves closer and closer to the fixed point as the cell size increases. The physical origin of this singularity stems from the fact that, unlike other systems where criticality is reached only in the infinite volume limit,
the random walk has a criticality in any finite cell, by taking the limit \( N \to \infty \). This has a consequence, as seen in Table I, that the value of the exponent \( \nu \) overshoots the exact value \( 1/2 \) already at a very small cell size. This would also be the case with the FG truncation recipe if the size of the cell were pushed to a sufficiently large value (although the behavior of such an approximation scheme for very large cell size is not known and may be complicated, see [6]).

In the next section we will see how the same trend is found in the one-dimensional analog, where everything can be calculated analytically for any value of the system size \( L \).

III. THE ONE-DIMENSIONAL PROBLEM

In order to gain firm understanding of the problems associated with the standard renormalization approach, in this section we solve a one-dimensional version of the aforementioned corner rule renormalization method. Subsequently a semi-infinite one-dimensional model in the presence of an infinite, repulsive barrier at the origin will also be discussed.

A. Transfer matrix solution for the one-dimensional corner rule

Let us consider a one-dimensional lattice where \( x = 0, 1, 2, \ldots, L \) and the sites \( x = -1, L + 1 \) have an infinitely repulsive barrier (see Fig. 3). (The lattice constant \( a \) is set equal to 1 for simplicity.) The analog of Eq. (2.4) for the correlation function for \( x \geq 1 \) is

\[
G_{0,x}(k) = k[G_{0,x-1}(k) + G_{0,x+1}(k)]
\]

along with the boundary conditions:

\[
G_{0,0}(k) = kG_{0,1}(k) + 1
\]

and

\[
G_{0,L}(k) = kG_{0,L-1}(k)
\]
where we have assumed that all walks start from \( x = 0 \).

We can put this equation in a transfer matrix form,

\[
\Psi_x(k) = T\Psi_{x+1}(k) \quad , \quad x = 1, 2, \ldots, L - 1
\]

(3.4)

where we defined

\[
T = \begin{pmatrix}
0 & 1 \\
-1 & \frac{1}{k}
\end{pmatrix}, \quad \Psi_x = \begin{pmatrix}
G_{0,x}(k) \\
G_{0,x-1}(k)
\end{pmatrix}
\]

(3.5)

The eigenvalues of the matrix \( T \) are clearly

\[
\lambda_{\pm} = \frac{1 \pm \sqrt{1 - 4k^2}}{2k}
\]

(3.6)

which are real if \( 0 < k \leq 1/2 \) and form a complex conjugate pair if \( 1/2 < k < 1 \) (we consider \( k < 1 \) in order to make the generating functions sensible). Note that \( \lambda_+ \cdot \lambda_- = 1 \) in both cases. The right \( \{U_\alpha\} \) and left \( \{U^\alpha\} \) eigenvectors \((\alpha = \pm)\), are given by:

\[
U_\pm = \begin{pmatrix}
1 \\
\lambda_{\pm}
\end{pmatrix}, \quad U^\pm = \pm \frac{1}{\lambda_+ - \lambda_-} \begin{pmatrix}
-\lambda_+ \\
1
\end{pmatrix}
\]

(3.7)

where we normalized so that \(< U_\alpha | U_\beta > = \delta_\alpha^\beta \).

Then expanding \( \Psi_L(k) \) in terms of the right eigenvectors and using the boundary condition (3.3) we get the coefficients of \( U_\pm \),

\[
c^\pm_{L+1} = \pm \frac{G_{0,L}}{\lambda_+ - \lambda_-}.
\]

(3.8)

Expressing \( \Psi_1(k) \) by iteration of Eq. (3.4) and using (3.8), we get

\[
G_{0,1} = \frac{G_{0,L}}{\lambda_+ - \lambda_-}(\lambda_+^L - \lambda_-^L),
\]

(3.9)

\[
G_{0,0} = \frac{G_{0,L}}{\lambda_+ - \lambda_-}(\lambda_+^{L+1} - \lambda_-^{L+1}),
\]

(3.10)

which determine \( G_{0,L} \) if we further impose the other boundary condition (3.2). Thus we find,

\[
G_{0,L}(k) = \frac{\lambda_+ - \lambda_-}{\lambda_+^{L+1} - \lambda_-^{L+1} - k(\lambda_+^L - \lambda_-^L)}
\]

(3.11)
for the system size $L = 1, 2, ...$

Note that, although this solution is valid for arbitrarily large $L$, the boundary condition (3.3) makes the system finite. This distinction will become more clear in the next subsection.

Once $G_{0,L}(k)$ has been obtained, the one-dimensional analog of Eq. (2.8), namely

$$\chi_1(k, 1/L) \equiv G_{0,x}(k)_{x=L},$$

gives the recursion relation corresponding to (2.7):

$$\chi_1(k', 1/L') = \chi_1(k, 1/L)$$

The fixed point $k^*(L, L')$ is obtained by setting $k = k' = k^*$ in (3.12). Using (3.11) and (3.12) for renormalization from a cell of size $L + 1$ to that of size $L$, we get an implicit solution for the fixed point $k^*(L + 1, L)$,

$$k^*_L \equiv k^*(L + 1, L) = \frac{\lambda^*_L + 2 - \lambda^*_L + 2 - (\lambda^*_L + 1 - \lambda^*_L + 1)}{\lambda^*_L + 1 - \lambda^*_L + 1 - (\lambda^*_L - \lambda^*_L)}$$

where $\lambda^*_L$ is $\lambda_\pm$ evaluated at $k = k^*_L$.

We expect $k^*_L$ to approach $1/2$ as $L \to \infty$ because the critical fugacity $k_c$ for the infinite, one-dimensional problem is exactly $1/2$. Given this limit, we now look for the $L$ dependence of $k^*_L$ for large but finite $L$. For this purpose, we need to distinguish the following two cases due to the square root in the expression (3.3) for $\lambda$:

(a) Case $0 < k^*_L \leq 1/2$.

If this were the case, the eigenvalues $\lambda^*_\pm(k)$ would be real. By introducing an auxiliary variable $\alpha$ by $\tanh \alpha = \sqrt{1 - 4k^2_L}$ and expressing (3.13) in terms of hyperbolic functions, we get

$$1/2 = \frac{(1 + \tanh \alpha)^L + 2 - (1 - \tanh \alpha)^L + 2 - [(1 + \tanh \alpha)^L + 1 - (1 - \tanh \alpha)^L + 1] \cosh \alpha}{(1 + \tanh \alpha)^L + 1 - (1 - \tanh \alpha)^L + 1 - [(1 + \tanh \alpha)^L - (1 - \tanh \alpha)^L] \cosh \alpha}.$$  

(3.14)

We see that the right hand side of (3.14) tends to $1$ as $\alpha \to 0$ (i.e., $k^*_L \to (1/2)^-$). This shows that $k^*_L$ cannot be in this range at least for large $L$.

(b) Case $1/2 < k^*_L < 1$. 

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Here the eigenvalues $\lambda_\pm$ form a complex conjugate pair. Again it is convenient to introduce a new variable $\theta$ by $\tan \theta = \sqrt{4k^2 - 1}$. Using $\theta$, (3.11) can be expressed as

$$G_{0,L}(k) = \frac{\sin \theta}{\sin[(L + 1)\theta] - k \sin[L\theta]} \quad (3.15)$$

and the fixed point equation (3.13) as

$$\tan(L\theta_L^*) = \left[\left(\frac{k}{L}\right)^2 - 1\right]^2 \left(\frac{k}{L}\right)^2 + k \left(1 - \cos \theta\right) \bigg| _{k=k_L^*, \theta=\theta_L^*}, \quad (3.16)$$

where $\theta_L^*$ is the value of $\theta$ at $k = k_L^*$. Now in the limit $k^* \rightarrow (\frac{1}{2})^+$ we can use a small $\theta^*$ expansion. Since the right-hand side of (3.16) diverges as $\theta^* \rightarrow 0$, small values of $\theta^*$ are achieved only in the large $L$ limit (as expected). Thus, the aforesaid limit is equivalent to the limit $L \rightarrow \infty$.

A $1/L$ expansion of (3.16) and use of the relation $\tan^{-1} x = \pi/2 - \tan^{-1} 1/x$ yields, after some algebra,

$$\theta^* = \frac{\pi}{2L} - \frac{5\pi}{4L^2} + \frac{25\pi}{8L^3} + O\left(\frac{1}{L^4}\right). \quad (3.17)$$

This translates, in terms of the fixed point value, to

$$k_L^* = \frac{1}{2} + \left(\frac{\pi}{4}\right)^2 \frac{1}{L^2} + O\left(\frac{1}{L^3}\right). \quad (3.18)$$

The critical value $k_c$ is obtained exactly from $k_L^*$ in the $L \rightarrow \infty$ limit as expected. However the exponent $\nu$ does not have the correct limiting value (which is $1/2$) as we show now.

Linearizing the recursion relation (3.12) around the fixed point, we get the eigenvalue

$$\Lambda = \frac{\partial k'}{\partial k} \bigg| _{k=k^*(L,L')} = \frac{\partial G_{0,L}(k)/\partial k}{\partial G_{0,L'}(k')/\partial k'} \bigg| _{L' \leq L-1},$$

$$= \frac{\partial G_{0,L}(\theta)^{-1}/\partial \theta}{\partial G_{0,L'}(\theta')^{-1}/\partial \theta'} \bigg| _{\theta=\theta^*(L,L')} \quad (3.19)$$

Using the expression (3.13) and the large $L$ expansions (3.17) and (3.18) for renormalization from a cell of size $L + 1$ to one of size $L$, we get after some straightforward but lengthy algebra,
\[ \frac{\partial G_{0,L}(\theta)^{-1}}{\partial \theta}|_{\theta=\theta^*_L} = -(\frac{2}{\pi^2})L^2[1+(5-\frac{\pi^2}{8})\frac{1}{L} + O(\frac{1}{L^2})] \].

(3.20)

This serves as the denominator in (3.19), while the numerator must be calculated by substituting \( L + 1 \) for \( L \) in Eq. (3.15), differentiating as in (3.19), and then substituting the expansions (3.17) and (3.18). Thus we finally obtain

\[ \Lambda_L = 1 + (2 + \frac{\pi^2}{4})\frac{1}{L} + O(\frac{1}{L^2}) \]  

(3.21)

and

\[ \nu = \lim_{L \to \infty} \frac{\ln[(L + 1)/L]}{\ln \Lambda_L} = \frac{1}{2 + \pi^2/4} = 0.2238... \]  

(3.22)

This exactly calculated exponent \( \nu \) therefore badly overshoots the correct value \( \nu = 1/2 \) in the same fashion as in the numerical evaluation of the previous section. Up to this point, however, it could still be a consequence of the finite size \( L \) imposed by the boundary condition (3.3). In the next subsection we will remove one of the boundaries and work with a semi-infinite one-dimensional system.

**B. Generating function solution for the semi-infinite system**

Let us again consider a one-dimensional lattice where \( x = 0, 1, 2, ... \) and the site \( x = -1 \) has an infinitely repulsive barrier (see Fig. 3), but there is no longer a barrier at the other end. For this calculation we will exploit a different method, namely the Laplace-Fourier method (see, e.g. second reference in [9]).

The master equation for the bulk is:

\[ P_{0,x}(N+1) = \frac{1}{2}[P_{0,x-1}(N) + P_{0,x+1}(N)] \]  

(3.23)

for \( x = 1, 2, ... \) and the boundary condition at the surface \( x = 0 \) is:

\[ P_{0,0}(N+1) = \frac{1}{2}P_{0,1}(N) \]  

(3.24)

We introduce the Fourier transform for the semi-infinite line by
\[ \hat{P}(q, N) = \sum_{x=0}^{\infty} e^{-i qx} P_{0,x}(N) \quad \longleftrightarrow \quad P_{0,x}(N) = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} e^{i qx} \hat{P}(q, N) . \]  

(3.25)

Multiplying (3.23) by \( e^{-i qx} \) and summing from \( x = 1 \) to \( \infty \), and using the boundary condition (3.24), we get

\[ \hat{P}(q, N + 1) = \hat{P}(q, N) \cos q - \frac{1}{2} e^{i q} P_{0,0}(N) . \]  

(3.26)

We now Laplace transform in \( N \) by defining the generating function,

\[ \tilde{G}(q, \lambda) = \sum_{N=0}^{\infty} \lambda^N \hat{P}(q, N) = \sum_{x=0}^{\infty} e^{-i qx} G_{0,x}(\lambda) \]  

(3.27)

where \( G_{0,x}(\lambda) \) is the generating function for the probability \( P_{0,x}(N) \). Then from equation (3.26) and the initial condition \( P_{0,x}(0) = \delta_{0,x} \) we get

\[ \tilde{G}(q, \lambda) = 1 - \frac{1}{2} \lambda e^{i q} G_{0,0}(\lambda) \frac{1 - \lambda \cos q}{1 - \lambda \cos q} . \]  

(3.28)

This allows the determination of \( G_{0,0}(\lambda) \). Integrating (3.28) over the first Brillouin zone, we get

\[ G_{0,0}(\lambda) = \frac{I_0(\lambda)}{1 + \frac{1}{2} \lambda I_1(\lambda)} \]  

(3.29)

where we have defined the integrals

\[ I_x(\lambda) = \int_{-\pi}^{+\pi} \frac{dq}{2\pi} \frac{e^{i qx}}{1 - \lambda \cos q} \]  

(3.30)

for \( x = 0, 1, 2, ... \). This integral can be easily computed as a contour integral

\[ I_x(\lambda) = \frac{i}{\pi} \oint_{|z|=1} dz \frac{z^x}{\lambda(z - z_+)(z - z_-)} \]  

(3.31)

where

\[ z_{\pm} = \frac{1 \pm \sqrt{1 - \lambda^2}}{\lambda} . \]  

(3.32)

It is worth mentioning that these poles are the same as the eigenvalues \( \lambda_{\pm} \) derived in the previous subsection, since the relation between the two fugacities is \( \lambda = 2k \). Again the
case $0 < \lambda < 1$ and $1 < \lambda < \infty$ have to be distinguished. In the first case the poles $z_{\pm}$ lie on the real axis and $z_-$ is always interior to the unit circle, while $z_+$ is always exterior. In the second case the poles $z_{\pm}$ are complex conjugate and lie on the unit circle symmetrically with respect to the real axis. The result for the integral is

$$I_x(\lambda) = \begin{cases} I_0(\lambda)z_-^x & \text{if } 0 < \lambda < 1 \\ \frac{1}{\lambda} \frac{z_+^x - z_-^x}{z_+ - z_-} & \text{if } 1 < \lambda < \infty \end{cases}$$

(3.33)

where

$$I_0(\lambda) = \begin{cases} 1/\sqrt{1-\lambda^2} & \text{if } 0 < \lambda < 1 \\ 0 & \text{if } 1 < \lambda < \infty \end{cases}$$

(3.34)

We now proceed to compute the $G_{0,x}(\lambda)$ in the two cases. From Eq. (3.28) and (3.29), we find by inverse transforming in $q$,

$$G_{0,x}(\lambda) = \frac{I_x(\lambda)}{1 + \frac{1}{2} \lambda z_- I_0(\lambda)}$$

(3.35)

in the case $0 < \lambda < 1$, and

$$G_{0,x}(\lambda) = I_x(\lambda)$$

(3.36)

for the case $1 < \lambda < \infty$.

Consider first the case of $1 < \lambda < \infty$. In this case, we introduce an angle $\theta$ by

$$z_{\pm} = e^{\pm i\theta}, \quad \tan \theta = \sqrt{\lambda^2 - 1}$$

(3.37)

Then, from (3.33) and (3.36), we get

$$G_{0,L}(\lambda)^{-1} = -\frac{\sin \theta}{\cos \theta \sin L\theta}$$

(3.38)

For large $L$, this expression changes sign rapidly as $\theta$ (or $\lambda$) varies, and thus unacceptable as the correlation function on physical grounds.

Therefore, we now consider the case $0 < \lambda < 1$. If we define, as before, an angle $\alpha$ from

$$z_{\pm} = e^{\pm \alpha}, \quad \tanh \alpha = \sqrt{1 - \lambda^2}$$

(3.39)
we find

\[ G_{0,L}(\lambda)^{-1} = e^{\alpha L} \left[ \tanh \alpha + \frac{e^{-\alpha}}{2 \cosh \alpha} \right]. \tag{3.40} \]

We note that this is an exact result independent of any renormalization procedure. Now since the only singularity of \( G_{0,L}(\lambda) \) is at \( \lambda = 1 \) (or \( \alpha = 0 \)) where \( \frac{\partial G_{0,L}}{\partial \lambda} \) diverges, we must interpret \( \lambda = 1 \) to be the critical point \( \lambda_c \). Thus, it is also consistent with the mean field theory for semi-infinite systems where the transverse correlation at criticality behaves as the separation \( L \) goes to \( \infty \) as \( L^{-(d-1)} \) for \( d \) dimensions.

Now, applying the idea of cell renormalization discussed before to this result, we turn to the equation for the fixed point,

\[ G_{0,L'}(\lambda^*) = G_{0,L}(\lambda^*) \tag{3.41} \]

where \( L' \leq L - 1 \) and \( L = 1, 2, \ldots \). This gives the fixed point at \( \alpha^* = 0 \) or \( \lambda^* = 1 \) exactly independent of \( L \) or \( L' \), which is consistent with \( \lambda_c = 1 \). Turning to the critical exponent, we calculate the *eigenvalue*

\[ \Lambda = \left. \frac{\partial \lambda'}{\partial \lambda} \right|_{\lambda^*} = \left. \frac{\partial G_{0,L}(\lambda)}{\partial \lambda} \right|_{\lambda^*} \left. \frac{\partial G_{0,L'}(\lambda')}{\partial \lambda'} \right|_{\lambda^*} \tag{3.42} \]

by linearizing the recursion relation around the fixed point \( \lambda^* = 1 \). Note that, since \( G_{0,L}(\lambda) \) is singular at \( \lambda = 1 \), what we are attempting to do is to linearize around a singular fixed point. After some manipulation we find

\[ \Lambda(L, L') = \frac{L + 1}{L' + 1}, \tag{3.43} \]

which is clearly wrong, since it would yield \( \nu = 1 + 0(1/L)! \)

Even though the renormalization approach based on Eq. (2.7) with (3.40) results in a nonsensical exponent value, the result for the two-point correlation function \( G_{0,L}(\lambda) \) itself is correct. Indeed it is easy to check that it reproduces the exact results for the critical exponents \( \nu \) and \( \gamma_1 \) (a surface exponent [16]) if they are calculated directly from it. More specifically one finds in the grand-canonical ensemble,
\[ \chi_1(\lambda) = \sum_{L=0}^{\infty} G_{0,L}(\lambda) \lambda^{-1} (1 - \lambda)^{-1/2} \]  

(3.44)

which is the exact result for the surface exponent \( \gamma_1 = 1/2 \) (see next section) and

\[ \xi^2(\lambda) = \sum_{L=0}^{\infty} \frac{L^2 G_{0,L}(\lambda)}{\sum_{L=0}^{\infty} G_{0,L}(\lambda)} \lambda^{-1} (1 - \lambda)^{-1} \]  

(3.45)

which again gives the exact result \( \nu = 1/2 \). The latter result can also be read off directly from (3.40) by noting that \( \alpha \sim \sqrt{1 - \lambda} \) near \( \lambda^* = 1 \).

So what is wrong with applying Eq. (2.7) to our \( G_{0,L}(\lambda) \)? In the present calculation, \( L \) is not the size of the system (which is infinite), but it refers only to a site of the semi-infinite, one-dimensional lattice. Therefore, the ideas of cell renormalization has no basis of application in this case. In fact, for general dimension \( d \), the transverse correlation at criticality should behave as

\[ G_{0,L}(\lambda)|_{\lambda=\lambda_c} \sim \frac{1}{L^{d-2+\eta}} \]  

(3.46)

for \( L \) large. Since \( \eta = 1 \) for random walks, such behaviour cannot be consistent with Eq. (2.7) for any \( d \) other than 1. (We just saw that it does not work even for \( d = 1 \).)

If we assume instead

\[ G_{0,L'}(\lambda') = \left( \frac{L'}{L} \right)^a G_{0,L}(\lambda) \]  

(3.47)

for an unknown exponent \( a \), then this would lead to

\[ \lambda^* = 1 - O\left( \frac{1}{L} \right) , \]  

(3.48)

\[ \nu = \frac{1}{a + 1} + O\left( \frac{1}{L} \right) , \]  

(3.49)

for renormalization from \( L + 1 \) to \( L \). The choice of \( a = 1 \) then leads to the correct limiting values as \( L \to \infty \). (This is also true for any ratio \( L/L' \) as shown in the Appendix.) The extra factor \( (L/L)^a \) could be considered to correspond to the rescaling step of the renormalization transformation. However, this choice of \( a \) is not in agreement with the intuitive guess of \(-d + 2 - \eta \) for \( d = 1 \). Rather, it would correspond to \(-d + 2 - \eta \) where \( \eta = 0 \) is the bulk
exponent. Thus it is not straightforward to repair this approach in a satisfactory way, even where exact correlation functions are available, not to mention that in most cases we do not have such luxury.

**IV. FINITE SIZE SCALING AND SURFACE CRITICAL BEHAVIOUR**

We learned from the previous calculations that, in the usual form, the cell renormalization procedure cannot be consistent. That is, it is not assured that, as the size of the cell increases, the results for the critical exponents improve and become exact in the limit of an infinite cell. If an improvement is attempted by using exact correlation functions, an inconsistency is again found stemming from the basic recursion relation (2.7) itself. On the other hand one might still hope that, as the cell size grows, the approximate renormalization procedure of FG’s truncation recipe could give better and better results. Unfortunately, however, this also appears not to be the case. Therefore, we need an alternative procedure which is both consistent in principle and workable in practice.

The clue of where to start comes from the result (3.18) where we calculated how the fixed point was becoming exact in the $L \to \infty$ limit. This is indeed compatible with the finite size scaling hypothesis (see e.g [16] and references therein),

$$k_c(L) = k_c(\infty) + A \left(\frac{1}{L}\right)^{1/\nu} \tag{4.1}$$

where $k_c(\infty) = 1/2$ is the exact critical fugacity in the infinite lattice limit and $\nu = 1/2$ in this case. The idea, therefore, is that one can estimate $k_c(L)$ by looking at the divergences of the (bulk) susceptibility defined as

$$\chi_B(k) = \frac{1}{|\Lambda|} \sum_{\mathbf{x}_0 \in \Lambda} \sum_{N=0}^{\infty} C(\mathbf{x}_0, N; \Lambda) k^N$$

$$= \frac{1}{|\Lambda|} \sum_{\mathbf{x}_0 \in \Lambda} \sum_{\mathbf{x} \in \Lambda} G_{\mathbf{x}_0, \mathbf{x}}(k) \tag{4.2}$$

where $C(\mathbf{x}_0, N; \Lambda)$ is the number of $N$-step walks starting from a point $\mathbf{x}_0$ and entirely contained in the volume $\Lambda$ and $G_{\mathbf{x}_0, \mathbf{x}}(k)$ is its generating function. The subscript $B$ refers
to bulk in the sense that the endpoints $x_0$ and $x$ can be anywhere in volume $\Lambda$. Then, either by fixing the exact value of $\nu = 1/2$ one can calculate $k_c(\infty)$ or by fixing the exact value of $k_c(\infty)$ one can calculate the value of the exponent $\nu$.

The results for the square lattice are shown in Fig.4 and Fig.5, and they are consistent with the expected values. Indeed a best fit for both cases gives $k_c(\infty) = 0.25 \pm 0.01$ and $1/\nu = 1.94 \pm 0.02$ and in the case of $\nu$ improves if we include more and more terms corresponding to larger cell sizes.

The presence of the surface also changes the entropic critical exponents as it is well known [10]. Indeed if the system is sufficiently large to make the distinction between surface and bulk sensible, one can decompose the total free energy $F_L$ as:

$$F_L(\Delta k, h, h_1, \frac{1}{L}) \approx L^d f_B(\Delta k, h, \frac{1}{L}) + L^{d-1} f_S(\Delta k, h, h_1, \frac{1}{L})$$ (4.3)

where $h$ and $h_1$ are the external fields associated with the bulk and the surface respectively and $\Delta k = k - k_c$. By differentiating twice with respect to the proper external field and by using the finite size scaling ansatz, one gets the well known general results

$$\tilde{\chi}_B(L) \approx L^{\gamma/\nu}$$  
$$\tilde{\chi}_1(L) \approx L^{\gamma_1/\nu}$$  
$$\tilde{\chi}_{1,1}(L) \approx L^{\gamma_{1,1}/\nu},$$ (4.4)

at the critical values $\Delta k = 0, h = h' = 0$. Here we have defined the local susceptibilities:

$$\chi_1(k) = \frac{1}{|\partial\Lambda|} \sum_{x_0 \in \partial\Lambda} \sum_{x \in \Lambda} G_{x_0,x}(k)$$
$$\chi_{1,1}(k) = \frac{1}{|\partial\Lambda|} \sum_{x_0 \in \partial\Lambda} \sum_{x \in \partial\Lambda} G_{x_0,x}(k)$$ (4.5)

where we mean by $\partial\Lambda$ the boundaries of the volume $\Lambda$.

Thus, our new method forgoes the usual corner rule renormalization per se, and instead, calculates various quantities associated with a finite cell and interprets them in terms of surface finite size scaling. From Fig.6 one can see that this method very accurately reproduces the values predicted by the mean field theory [10,20], namely $\gamma/\nu = 2, \gamma_1/\nu = 1, \gamma_{1,1}/\nu = -1$. 

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V. PHASE DIAGRAM FOR SURFACE-BULK RANDOM WALKS

As an application of the method just described, we now present the finite size scaling solution of the problem of the interplay between the bulk Λ (with fugacity $k$) and the surface $\partial\Lambda$ (with fugacity $k_1$) (see Fig.7), based on the exact calculation of the finite cell susceptibilities.

Physically the possibility of changing the strength of the surface fugacity with respect to the strength of the bulk fugacity allows the surface to make up for the missing bonds. Clearly one expects that if $k_1$ is sufficiently strong almost all walks lie on the surface, and then the critical point and the universality class should both change: when all the ”interactions” in the bulk are zero, the walks are not allowed to stay in the bulk and we have the adsorbed phase. Since $k_1 = 1/2$ and $k = 1/4$ are the exact critical values corresponding to an infinite surface (a line in this case) and an infinite bulk, one then expects a qualitative phase diagram as shown in Fig.8.

For this calculation we eliminated the corner and imposed a periodic boundary condition into the vertical direction $\hat{2}$, while the horizontal direction $\hat{1}$ is of size $L$ and has free edges. The result is shown in Fig.9. It appears that there is a tricritical point (called special point) which is the intersection of three different lines (corresponding to three different second order phase transitions). Below the special point there is the ordinary transition, where the bulk and the surface undergo a transition at the same critical point. Above the special point there is a line of surface transitions, which take place if $k_1$ is bigger then the special point ordinate, where the surface goes into an ordered state (where the susceptibility is singular) while the bulk is still disordered, as well as another line called the extraordinary line where the bulk also becomes ordered.

Our estimate of the special point $SP$ is at $k = 0.25 \pm 0.01$, and $k_1 = 0.35 \pm 0.01$, corresponding to a ratio $k_1/k = 1.40 \pm 0.06$. This is in reasonably good agreement with a simple mean-field argument which would predict the ratio of $4/3$. The errors were estimated graphically.
The qualitative features contained in this phase diagram also appear in the case of the self-avoiding walks [21] and in percolation [22].

Quite similar features are found in the case of a defect (which is a $d-1$-dimensional surface inserted into a $d$-dimensional bulk). The phase diagram obtained looks very similar to the one for the surface. The special point $SP$ is found when $k_1/k = 1$ again consistent with mean field arguments.

VI. CONCLUSIONS

In this paper we have given a detailed analysis of the difficulties associated with the usual cell renormalization approach to the random walk problem and presented an alternative method to calculate critical properties which does not suffer from similar difficulties. This new approach is shown to give results which improve as the size of the cell increases, unlike the previous approaches which are shown here not to have this essential feature, relying on an uncontrolled approximation. Our approach is based only on the finite size scaling hypothesis. Using this approach we have computed the full phase diagram of the effect of the surface fugacity having a different value from the bulk fugacity, and calculated the exponents $\gamma_1$ and $\gamma_{1,1}$ as well $\nu$. All the results are consistent with simple mean field arguments as expected. Analogous results are obtained for the case of a defect.

The real challenge now is to use this method for the situations where no simple mean field results are useful and the exponents are unknown. A timely example of such a case is the one where the substrate on which the random walks are constrained is disordered or otherwise self-similar. Although this problem is potentially important as it has essential features of transport through disordered media, an important materials problem, the results of previous investigations [8,4] are not reliable. This extension is not expected to be straightforward, however, since various numerical approaches [12,13,14,15] all agree on the result that the susceptibility singularity for an ideal chain or trapped ant (which can also be thought as the limit of the self-avoiding walk in absence of self-avoidance) is not a simple power law in the
presence of strongly correlated disorder, but rather an *essential singularity*. Further work will then be needed in order to implement this extension.

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APPENDIX: EXACT DECIMATION FOR AN ARBITRARY SCALE FACTOR

We will show in this Appendix that, unlike in the corner rule renormalization, an exact decimation procedure (which gives exact scaling relations) always gives the exact critical point and the exact critical exponent irrespective of the choice of the scaling ratio $l \equiv L/L'$. Without loss of generality, we will do this for decimation from $L$ to $a = 1$ ($a$ being the lattice constant), with the rescaling ratio of $L$.

It is not hard to convince oneself that a decimation of the $L$ sites next to the origin gives rise to the recursion,

$$k'_L = \frac{k^L}{1 - 2k^2A_L(k)} \prod_{p=1}^L A_p(k), \quad (k \equiv k_1) \tag{A1}$$

and

$$G_{0,x'=x/L} (k') = (1 - 2k^2A_L(k))G_{0,x} (k) \tag{A2}$$

where $A_L(k)$ is such that

$$A_{L+1} = \frac{1}{1 - k^2A_L} \tag{A3}.$$ 

In the previous expressions $k_L$ refers to the fugacity $k$ when the lattice constant is $L$. We can show by induction that $k^*_L = \frac{1}{2}$ ($\forall L \in \mathbb{N}$). Indeed if we assume $k^*_L = k^*_1 = \frac{1}{2} \equiv k^*$, then we would have from Eq. (A1),

$$k^*_{L+1} = k^*_L D_L(k^*) \tag{A4}$$

where

$$D_L(k^*) = [kA_{L+1}(k) \frac{1 - 2k^2A_L(k)}{1 - 2k^2A_{L+1}(k)}]_{k=k^*} \tag{A5}.$$ 

Thus the claim is equivalent to showing that $D_L(k^*) = 1$, which is easy to derive using Eq. (A3).

Next we will show, again by induction, that $\nu = \frac{1}{2}$ independent of $L$. From
\[ k'_{L+1} = k'_{L} D_{L}(k) \quad . \] (A6)

Upon differentiation with respect to \( k \), we have from Eq. (A6),

\[
\frac{\partial k'_{L+1}}{\partial k} = \frac{\partial k'_{L}}{\partial k} D_{L}(k) + k'_{L} \frac{\partial D_{L}(k)}{\partial k}
\] (A7)

Since by hypothesis,

\[
\frac{\partial k'_{L}}{\partial k} \bigg|_{k^*} = \lambda_{MAX}(L) \big[D_{L}(k)\big]_{k = k^*} + k'_{L} \big[\frac{\partial D_{L}(k)}{\partial k}\big]_{k = k^*}
\] (A8)

after some manipulations we get, at the fixed point \( k^* = \frac{1}{2} \),

\[
D_{L}(k^*) = 1, \quad \frac{\partial D_{L}(k)}{\partial k} \bigg|_{k^*} = 2(2L + 1)
\] (A9)

Therefore, substituting in (A7), we get

\[
\frac{\partial k'_{L+1}}{\partial k} \bigg|_{k^*} = (L + 1)^2 = \lambda_{MAX}(L + 1)
\] (A10)

which is what we wanted to prove.
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FIGURES

FIG. 1. Corner rule for the case of the smallest cell $2a \times 2a$. By symmetry the number of walks starting from the origin 0 and exiting in the direction $\hat{1}$ or $\hat{2}$ are equal.

FIG. 2. Comparison between the exact and approximate $G_{L}^{1}(k) \equiv \chi_{2}(k,1/L)$ in the cases $L = 1, 2, 3$. The three solid lines correspond to the exact evaluations, while the two dotted lines are the approximate results as discussed in text. The intersections of the the solid lines correspond to the exact fixed points $k^{*} = 0.3157, 0.2950$, while the intersections of the dotted lines correspond to the Family-Gould fixed points $k_{FG}^{*} = 0.3470, 0.3108$ for a scaling from $L = 2, 3$ to $L' = 1, 2$ respectively.

FIG. 3. One-dimensional case. In (a) the sites $x = -1$ and $x = L + 1$ have an infinitely repulsive barrier, corresponding to the corner rule in $d = 1$. The second case (b) is a semi-infinite one-dimensional lattice with an infinitely repulsive barrier only at $x = -1$.

FIG. 4. Finite-size scaling result for the critical value $k_{c}(\infty)$, which corresponds to the true critical point for the square lattice. A best fit over all points gives $k_{c}(\infty) = 0.25 \pm 0.01$, while the exact value is $k_{c} = 1/4$.

FIG. 5. Finite-size scaling result for the exponent $\nu$. A best fit over all points gives $1/\nu = 1.94 \pm 0.02$, while the exact value is $1/\nu = 2$.

FIG. 6. Evaluation of the bulk and surface susceptibilities in the finite-size scaling approach. The estimates for $\chi_{B}$ ($\bigcirc$), $\chi_{1}$ ($\triangle$) and $\chi_{1,1}$ (+) are obtained from the slopes of the lines shown in the log-log plots. The exact values according to the mean field calculation are $\gamma/\nu = 2$, $\gamma_{1}/\nu = 1$ and $\gamma_{1,1}/\nu = -1$.

FIG. 7. Example of a surface-bulk problem where the surface fugacity $k_{1}$ and the bulk fugacity $k$ are shown.
FIG. 8. A sketch of the expected phase diagram. The lines shown correspond to the ordinary transition (O), the surface transition (S) and the extraordinary transition (E). Also shown is the tricritical point called the special transition (SP).

FIG. 9. Computed phase diagram for the surface-bulk problem of Fig. 7. The points shown have been calculated for different system sizes, $L = 4$ (○), $L = 10$ (△), and $L = 20$ (◇). The dotted and dashed lines correspond to slopes $k_1/k = 1, 2$ respectively. The special point is estimated to be at $k = 0.25 \pm 0.01$, $k_1 = 0.35 \pm 0.01$. 
TABLE I. Behaviour of $\nu$ as functions of the cell size $b = L/a$ where $a$ is the lattice constant. The first two columns refer to the present work, while the second two refer to the results using the approximate recipe of Family and Gould ref [5].

| Scaling length $b/b'$ | $k^*$  | $\nu$  | $k^*_FG$ | $\nu_{FG}$ |
|-----------------------|--------|--------|----------|------------|
| 2/1                   | 0.3156 | 0.5438 | 0.3470   | 0.5853     |
| 3/1                   | 0.2950 | 0.5132 | 0.3108   | 0.5571     |
| 3/2                   | 0.2770 | 0.4441 | 0.2920   | 0.5129     |
| 4/1                   | 0.2825 | 0.4937 | 0.2926   | 0.5412     |
| 4/3                   | 0.2711 | 0.4485 | 0.2743   | 0.4868     |
| 5/1                   | 0.2745 | 0.4792 | 0.2838   | 0.5398     |
| 5/4                   | 0.2640 | 0.4351 | 0.2693   | 0.5148     |