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DIMENSIONAL RECURRENCE FORMULAS FOR GREEN'S FUNCTIONS OF CUBIC LATTICES

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Dimensional Recurrence Formulas for Green's Functions of Cubic Lattices.

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Abstract: I apply the theory of random walks to prove dimensional recurrence formulas for return probabilities and Green's functions of cubic lattices. I use these formulas to compute the average number of distinct sites visited by the random walker on an "almost 1-dimensional" lattice.

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1. Introduction.

Many problems in solid state physics, statistical physics and particle physics can be "latticized": then the propagation of lattice "excitations" can be described by "lattice Green's functions" or "position-space propagators" (applications to statistical physics can be found, e.g. in the classical papers by Dyson [1], while a review of solid-state physics applications is e.g. [2]). The propagation of lattice excitations is a kind of diffusion process, and it is well-known that it can be modeled by discrete random walks on the lattice: this equivalence has been used in the past to compute propagators by Montecarlo methods (see e.g. Kuti [3] and Montvay [4]).

Here I study simple random walks on cubic D-dimensional lattices and using elementary combinatorial arguments I show dimensional recurrence formulas relating the Green's function (propagator) for the D-dimensional lattice to the Green's function for the (D-1)-dimensional lattice.

In section 2 of this Letter I review some known results about the Green's functions for simple random walks on a cubic lattice: I use a formalism akin to that used in [5] and I cast the results in a combinatorial setting; in section 3 I prove the recurrence formulas. I apply the recurrence formulas to find the average number of distinct sites visited by a random walker on an "almost 1-dimensional" lattice in section 5, and section 4 contains a discussion of the results.

2. Green's functions for simple random-walks on a cubic lattice.

Take a cubic D-dimensional lattice with unit lattice spacing and let $\mathbf{r} = (x_1, \ldots, x_D)$ be a lattice vector, that is a vector that points to a lattice site (and therefore the x_i's are integer coordinates when measured in units of lattice spacings). Also, let p(j) be the probability for the random walker to step from its current site $\mathbf{r}$ to $\mathbf{r}+\mathbf{j}$, let $\mathbf{0}$ be the random walker's starting point and let $P_D(\mathbf{r},n)$ be the probability of reaching r after n steps (not necessarily for the first time). Then the $P_D(\mathbf{r},n)$'s are related to the single-step probabilities p(j) by

$$P_D(\mathbf{r},n+1) = \sum_{\mathbf{j}} p(\mathbf{j})\ P_D(\mathbf{r}-\mathbf{j},n) \tag{1}$$

($\sum_{\mathbf{j}}$ denotes the sum over all lattice points j) with the initial condition

$$P_D(\mathbf{r},0) = \delta_{\mathbf{r},\mathbf{0}}. \tag{1.1}$$

This recurrence equation can be solved using standard Fourier methods after introducing the functions

$$\lambda(\mathbf{t}) = \sum_{\mathbf{j}} p(\mathbf{j})\ \exp(i\ \mathbf{j}\cdot\mathbf{t}) \tag{2}$$

($\lambda(\mathbf{t})$ is also called the "structure function" of the random walk) and

$$L_n(\mathbf{t}) = \sum_{\mathbf{r}} P_D(\mathbf{r},n)\ \exp(i\ \mathbf{r}\cdot\mathbf{t}). \tag{3}$$

Then (1) and (1.1) become:

$$L_{n+1}(\mathbf{t}) = \lambda(\mathbf{t})\ L_n(\mathbf{t}) \tag{4}$$

$$L_0(\mathbf{t}) = 1 \tag{4.1}$$

so that

$$L_n(\mathbf{t}) = [\lambda(\mathbf{t})]^n \tag{5}$$

and

$$P_D(\mathbf{r},n) = \frac{1}{(2\pi)^D} \int_{-\pi}^{\pi} [\lambda(\mathbf{t})]^n\ \exp(-i\ \mathbf{r}\cdot\mathbf{t})\ d\mathbf{t}. \tag{6}$$

Therefore the generating function for the return probabilities $P_D(\mathbf{r},n)$ is

$$G_D(\mathbf{r},z) = \sum_{n=0}^{\infty} P_D(\mathbf{r},n)\, z^n =$$

$$= \sum_{n=0}^{\infty} \left(\frac{1}{(2\pi)^D} \int_{-\pi}^{\pi} [\lambda(\mathbf{t})]^n \exp(-i\ \mathbf{r}\cdot\mathbf{t})\ d\mathbf{t} \right) z^n$$

$$= \frac{1}{(2\pi)^D} \int_{\pi}^{\pi} \frac{\exp(-i\ \mathbf{r}\cdot\mathbf{t})}{1 - z\ \lambda(\mathbf{t})}\, d\mathbf{t}. \qquad (7)$$

In a simple random-walk the $p(\mathbf{j})$'s are non-zero only if $\mathbf{j}$ is a unit lattice vector, i.e. one of the vectors $\pm\mathbf{e}_i$, where $\mathbf{e}_1 = (1,0,0, \ldots ,0)$, $\mathbf{e}_2 = (0,1,0, \ldots ,0)$, ... , $\mathbf{e}_D = (0,0,0, \ldots ,1)$; then the structure function becomes

$$\lambda(\mathbf{t}) = \sum_{k=1}^{D} \left[p(+\mathbf{e}_k) \exp(-it_k) + p(-\mathbf{e}_k) \exp(it_k) \right], \qquad (8)$$

where $\mathbf{t} = (t_1, \ldots ,t_D)$. Furthermore if one also assumes that there is no net drift motion, then $p(+\mathbf{e}_k) = p(-\mathbf{e}_k) \equiv p_k$ and (8) and (7) become respectively

$$\lambda(\mathbf{t}) = 2 \sum_{k=1}^{D} p_k \cos(t_k), \qquad (9)$$

and

$$G_D(\mathbf{r},z) = \frac{1}{\pi^D} \int_0^{\pi} \frac{\prod_{k=1}^{D} \cos(x_k\ t_k)\ dt_k}{1 - 2\ z \sum_{k=1}^{D} p_k \cos t_k} \qquad (10)$$

where $\mathbf{r} = (x_1, \ldots ,x_D)$ as before, and (10) is seen to be the usual expression for the scalar boson propagator in position space on a cubic D-dimensional lattice; if $p_i = \frac{1}{2D}$

for all i's, z is related to the usual "hopping parameter" K, $K=\frac{z}{2D}$, while the mass of the "hopping particle" is given by $M^2 = 2D(1-z)$ [6].

Now I turn to the problem of explicitly computing the $P_D(\mathbf{r},n)$'s. Assume the random-walker to be in $\mathbf{r} = (x_1, \ldots, x_D)$ at the n-th step; then the number $k_{\pm i}$ of steps taken in the direction $\pm\mathbf{e}_i$ must satisfy the constraint $k_{+i} - k_{-i} = x_i$. On the other hand there are $\frac{n!}{k_{+1}!\, k_{-1}! \ldots k_{+D}!\, k_{-D}!}$ such sequences of n steps with the constraint $k_{+1}+ k_{-1}+ \ldots + k_{+D}+ k_{-D}= n$, and each of them has a probability $\prod_{k=1}^{D} p_i^{k_{+i}+k_{-i}}$ of actually occurring (the p_i's are the single step probabilities defined above). Then the probability that the random-walker be in $\mathbf{r}$ at the n-th step is:

$$P_D(\mathbf{r},n) = \sum_{\sum_{i=1}^{D} k_{+i}+k_{-i}=n;\; k_{+i}-k_{-i}=x_i;\; k_{\pm i}\geq 0} n! \prod_{i=1}^{D} \frac{p_i^{k_{+i}+k_{-i}}}{k_{+i}!\, k_{-i}!} . \qquad (11)$$

The constraint $k_{+i}+k_{-i}=x_i$ can be used to eliminate k_{-i}, and if one lets $k_i \equiv k_{+i}$, then:

$$P_D(\mathbf{r},n) = \sum_{2\sum_{i=1}^{D} k_i=n+\sum_{i=1}^{D} x_i;\; k_i\geq \max(0,x_i)} n! \prod_{i=1}^{D} \frac{p_i^{2k_i-x_i}}{k_i!\, (k_i-x_i)!} . \qquad (12)$$

Notice that the constraint $2\sum_{i=1}^{D} k_i= n + \sum_{i=1}^{D} x_i$ forces $n+\sum_{i=1}^{D} x_i$ to be even, therefore n and $\sum_{i=1}^{D} x_i$ must have the same parity: if this is not the case then $P_D(\mathbf{r},n)=0$. In the specially important case $\mathbf{r} = \mathbf{0}$, n must be even and (12) becomes

$$P_D(\mathbf{0},2n) = \sum_{\sum_{i=1}^{D} k_i = n} (2n)! \prod_{i=1}^{D} \frac{p_i^{2k_i}}{(k_i!)^2} . \tag{13}$$

If the single step probabilities p_i are all equal and the number of random walkers is conserved (i.e. $\sum_{i=1}^{D} p_i = \frac{1}{2}$) then $p_i = \frac{1}{2D}$, and (13) reduces to

$$P_D(\mathbf{0},2n) = (2D)^{-2n} \sum_{\sum_{i=1}^{D} k_i = n} \frac{(2n)!}{\prod_{i=1}^{D} (k_i!)^2} . \tag{14}$$

If D=1 or D=2, the sum (14) can be easily evaluated to yield

$$P_1(0,2n) = \frac{1}{2^{2n}} \binom{2n}{n}, \tag{15}$$

$$P_2(\mathbf{0},2n) = \frac{1}{4^{2n}} \binom{2n}{n}^2, \tag{16}$$

and if D=1 it is also easy to find the nonzero probabilities for even (r=2x) and odd (r=2x-1) lattice points:

$$P_1(2x,2n) = \frac{1}{2^{2n}} \binom{2n}{n+x}, \tag{17}$$

$$P_1(2x-1,2n+1) = \frac{1}{2^{2n+1}} \binom{2n+1}{n+x} . \tag{18}$$

If D>2 and/or the p_i's are not all equal, the P's have more complicated expressions, but there is a simple gaussian approximation (see, e.g. [5]), which is valid when $np_i >> x_i$:

$$P_D(\mathbf{r},n) \approx \frac{2}{(4\pi n)^{D/2}} \left[\prod_{i=1}^{D} p_i \right]^{-1/2} \exp\left\{ -\frac{1}{2n} \sum_{i=1}^{D} \frac{x_i^2}{2p_i} \right\}, \tag{19}$$

where it is understood that $\mathbf{r}$ and n have the same parity, and that $P_D(\mathbf{r},n) = 0$ if $\sum_{i=1}^{D} x_i > n$.

I remark here that for the 1-dimensional simple random walk there is an exact expression for the Green function in closed form [7]:

$$G_1(k,z) = \frac{1}{\sqrt{1-z^2}}\left[\frac{1}{z} - \sqrt{\frac{1-z^2}{z^2}}\right]^{|k|} . \qquad (20)$$

3. The dimensional recurrence formulas.

The single step probabilities are often chosen to be $p_i = \frac{1}{2D}$: the resulting random-walk is "isotropic". Now let $p_i = p$ for $i=1,...,D-1$ and $p_D = \alpha p$, then:

$$p_i = \frac{1}{2(D-1+\alpha)} \quad \text{for } i=1,...,D-1, \text{ and} \quad p_D = \frac{\alpha}{2(D-1+\alpha)} , \qquad (21)$$

(I assume the normalization condition $\sum_{i=1}^{D} p_i = \frac{1}{2}$ which means that the number of randow walkers is conserved) and when α changes from 1 to 0, it interpolates continuously between the D-dimensional and the (D-1)-dimensional case.

Now denote with $P_D(\mathbf{r},n;\alpha)$ the return probability computed from (12) with single step probabilities given by (21) (and therefore $P_D(\mathbf{r},n;1) = P_D(\mathbf{r},n)$, and $P_D(\mathbf{r},n;0) = P_{D-1}(\mathbf{r},n)$), and let $\mathbf{r} = \mathbf{0}$, $k \equiv k_D$, then

$$P_D(\mathbf{0},2n;\alpha) = \sum_{\sum_{i=1}^{D} k_i = n} \frac{(2n)!}{\prod_{i=1}^{D} (k_i!)^2} \frac{\alpha^{2k_D}}{\left[2(D-1+\alpha)\right]^{2n}} ; \qquad (22)$$

this can be rearranged to give

$$\left[2(D-1+\alpha)\right]^{2n} P_D(\mathbf{0},2n;\alpha) = \sum_{k=0}^{n} \frac{\alpha^{2k}}{(k!)^2} \sum_{\sum_{i=1}^{D-1} k_i = n-k} \frac{(2n)!}{\prod_{i=1}^{D-1} (k_i!)^2} =$$

$$= \sum_{k=0}^{n} \frac{\alpha^{2k}}{(k!)^2} \frac{(2n)!}{(2n-2k)!} [2(D-1)]^{2n-2k} P_{D-1}(\mathbf{0},2n-2k) \quad . \tag{23}$$

In particular, if $\alpha=1$,

$$[2D]^{2n} P_D(\mathbf{0},2n) = \sum_{k=0}^{n} \frac{(2n)!}{(2n-2k)!\,(k!)^2} [2(D-1)]^{2n-2k} P_{D-1}(\mathbf{0},2n-2k). \tag{24}$$

Denote with $G_D(\mathbf{r},z;\alpha)$ the Green's function for the lattice defined by the single-step probabilities (21) (so that $G_D(\mathbf{r},z;1) = G_D(\mathbf{r},z)$, and $G_D(\mathbf{r},z;0) = G_{D-1}(\mathbf{r},z)$): if one multiplies (23) times z^{2n} and sums over n one obtains

$G_D(\mathbf{0},2(D-1+\alpha)z;\alpha) =$

$$= \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{\alpha^{2k}}{(k!)^2} \frac{(2n)!}{(2n-2k)!} [2(D-1)]^{2n-2k} P_{D-1}(\mathbf{0},2n-2k) \; z^{2n} =$$

$$= \sum_{k=0}^{\infty} \frac{\alpha^{2k}}{(k!)^2} \sum_{n=k}^{\infty} \frac{(2n)!}{(2n-2k)!} [2(D-1)]^{2n-2k} P_{D-1}(\mathbf{0},2n-2k) \; z^{2n} \tag{25}$$

Since

$$\frac{(2n)!}{(2n-2k)!} z^{2n} = z^{2k} \frac{d^{2k}}{dz^{2k}} (z^{2n}) \tag{26}$$

(25) becomes:

$G_D(\mathbf{0},2(D-1+\alpha)z;\alpha) =$

$$=\sum_{k=0}^{\infty} \frac{\alpha^{2k}}{(k!)^2} z^{2k} \frac{d^{2k}}{dz^{2k}}\left[z^{2k} \sum_{n=k}^{\infty} [2(D-1)]^{2n-2k} P_{D-1}(\mathbf{0},2n-2k)\, z^{2n-2k}\right] =$$

$$=\sum_{k=0}^{\infty} \frac{(\alpha z)^{2k}}{(k!)^2} \frac{d^{2k}}{dz^{2k}}\left[z^{2k}\, G_{D-1}(\mathbf{0},2(D-1)z)\right] , \qquad (27)$$

and, once again, if $\alpha=1$,

$$G_D(\mathbf{0},2Dz) = \sum_{k=0}^{\infty} \frac{z^{2k}}{(k!)^2} \frac{d^{2k}}{dz^{2k}}\left[z^{2k}\, G_{D-1}(\mathbf{0},2(D-1)z)\right] , \qquad (28)$$

If $\mathbf{r} \neq \mathbf{0}$ one obtains, by similar manipulations, the following results:

a. if $\mathbf{r}$ is even (i.e. $\sum_{i=1}^{D} x_i = 2L$) then

$\left[2(D-1+\alpha)\right]^{2n} P_D(\mathbf{r},2n;\alpha) =$

$$= \sum_{k=x}^{n-L+x} \frac{\alpha^{2k-x}}{k!(k-x)!} \frac{(2n)!}{(2n-2k+x)!} [2(D-1)]^{2n-2k+x} P_{D-1}(\mathbf{r}',2n-2k+x); \qquad (29)$$

and

b. if $\mathbf{r}$ is odd (i.e. $\sum_{i=1}^{D} x_i = 2L-1$) then

$\left[2(D-1+\alpha)\right]^{2n+1} P_D(\mathbf{r},2n+1;\alpha) =$

$$= \sum_{k=x}^{n-L+x+1} \frac{\alpha^{2k-x}}{k!(k-x)!} \frac{(2n+1)!}{(2n+1-2k+x)!} [2(D-1)]^{2n+1-2k+x} P_{D-1}(\mathbf{r}',2n+1-2k+x), \qquad (30)$$

where $\mathbf{r} = (x_1, \ldots ,x_D)$ is a D-dimensional lattice vector as before, $\mathbf{r}' = (x_1, \ldots ,x_{D-1})$ is a (D-1)-dimensional lattice vector, and $x \equiv |x_D|$. The Green's functions are related by the formula

$$G_D(\mathbf{r},2(D-1+\alpha)z;\alpha) = \sum_{k=x}^{\infty} \frac{(\alpha z)^{2k-x}}{k!(k-x)!} \frac{d^{2k-x}}{dz^{2k-x}} \left[z^{2k-x}\, G_{D-1}(\mathbf{r}',2(D-1)z) \right], \quad (31)$$

which generalizes (27) and, if $\alpha=1$,

$$G_D(\mathbf{r},2Dz) = \sum_{k=x}^{\infty} \frac{z^{2k-x}}{k!(k-x)!} \frac{d^{2k-x}}{dz^{2k-x}} \left[z^{2k-x}\, G_{D-1}(\mathbf{r}',2(D-1)z) \right], \quad (32)$$

which generalizes (28).

4. An application to the average number of distinct sites visited by a random walker.

The average number of distinct lattice sites visited by a random walker is an important statistics, relevant to trapping problems (see e.g. [5] and [8]): if S_n denotes the number of distict sites visited after n steps on a lattice without traps, and if c denotes the concentration of traps, then it is easy to see that the probability that the random walker survives trapping after n steps is (with the assumptions that traps are perfect absorbers and that the origin may also be a trap):

$$f_n = \langle (1-c)^{S_n} \rangle, \quad (33)$$

where the average is over all walks of n steps on the lattice without traps, and over all trap configurations. The calculation of these survival probabilities is a difficult mathematical problem which has attracted the attention of many researchers [8,9]; however it has been argued [8] that for very small concentrations the Rosenstock approximation

$$f_n \approx (1-c)^{\langle S_n \rangle} \quad (34)$$

is a sufficiently good approximation of (33), and therefore one may turn to the $\langle S_n \rangle$'s to estimate the survival probabilities.

Montroll and Weiss [10] showed that the generating function of the $<S_n>$'s is related to the Green's function:

$$S_D(z) = \sum_{n=0}^{\infty} <S_n> z^n = \frac{1}{(1-z)^2 \, G_D(\mathbf{0},z)}, \qquad (35)$$

then, using (20):

$$S_1(z) = \frac{1}{1-z}\sqrt{\frac{1+z}{1-z}} = 1+ 2z + \frac{5}{2}z^2 + 3z^3 + \frac{27}{8}z^4 + \frac{15}{4}z^5 + \ldots =$$

$$= 1 + 2z + 2.5 z^2 + 3 z^3 + 3.375 z^4 + 3.75 z^5 + \ldots \qquad (36)$$

Now, if one takes a simple random walk on a 2-dimensional lattice with single step probabilities

$$p_x = \frac{1}{2(1+\alpha)}, \quad \text{and} \quad p_y = \frac{\alpha}{2(1+\alpha)}, \qquad (37)$$

one can use (27) to find an approximation for the Green function:

$$G_2(0,z;\alpha) = \frac{1}{\sqrt{1-z^2}} - \frac{z^2}{(1-z^2)^{3/2}}\alpha + \frac{z^2(8+z^2)}{4\,(1-z^2)^{5/2}}\alpha^2 - \frac{z^2(12+12z^2+z^4)}{4\,(1-z^2)^{7/2}}\alpha^3 + \ldots \qquad (38)$$

and then, from (35), after some tedious algebra, one obtains the generating function of the $<S_n>$'s for an anisotropic 2-dimensional walk:

$$S_2(z;\alpha) = \frac{1}{1-z}\sqrt{\frac{1+z}{1-z}} + \frac{z^2}{(1-z)^2\sqrt{1-z^2}}\alpha + \frac{z^2(3z^2-8)}{4\,(1-z)^2\,(1-z^2)^{3/2}}\alpha^2 + \ldots \qquad (39)$$

I have expanded $S_2(z;\alpha)$, and the results of the expansion are compared in the figure with data from a Montecarlo program for 2-dimensional simple random-walks with $\alpha = 0.05$. The figure can be better understood recalling a Tauberian theorem ([11] and [5]) which relates the large n behaviour of the $<S_n>$'s to the divergence near z=1:

(39) shows that higher correction terms have an increasingly divergent behaviour near z=1, so that higher order corrections become more and more important for large n's.

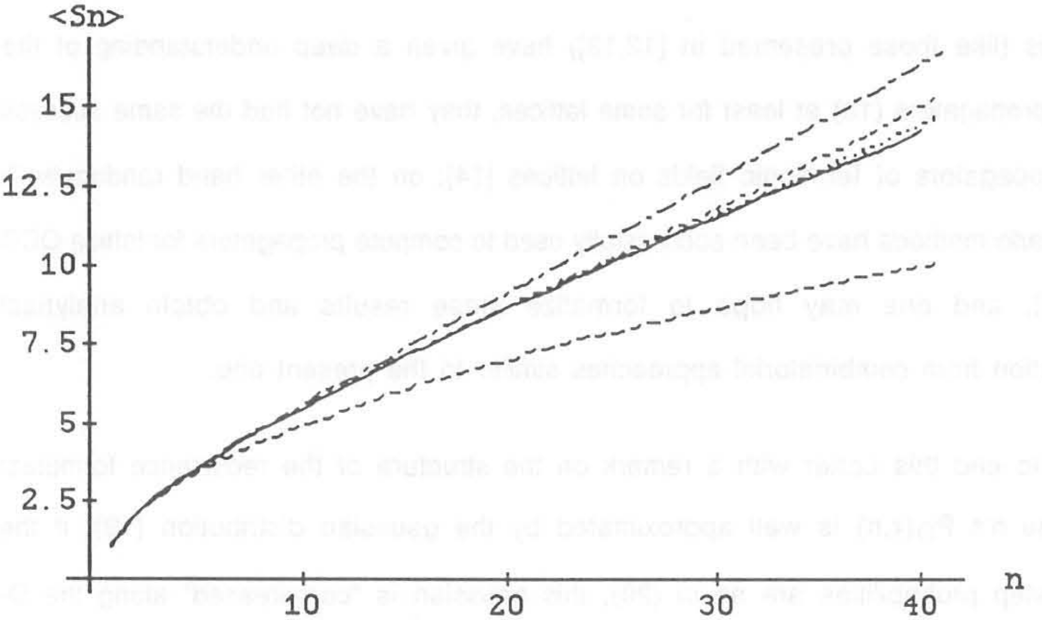

Figure: The average number of distinct sites visited by simple random-walks on 2-dimensional anisotropic lattices (with α=0.05, see text) vs. the step number n. The data points have been joined with straight segments for greater clarity: the solid curve joins the data points obtained from a Montecarlo simulation (10^5 random-walks have been generated), the dashed curve below the Montecarlo data shows $\langle S_n \rangle$ for the 1-dimensional simple random-walk, while the upper curves are obtained from (39), retaining terms respectively up to first order in α (dashed-dotted curve), to second order (short dashes) and to third order (dots).

5. Conclusions.

I have shown recurrence formulas for the probabilities $P_D(r,n)$ and the lattice Green's functions $G_D(r,z)$: the concept of dimensional recurrence for cubic lattices is a natural one, and in the past other authors have proven similar formulas which display recurrence in integral forms (see e.g. [7] and [12]). However, I think that the present approach has two merits: the first is that it yields useful approximations for anisotropic lattices (as shown in section 4). The other is that it points to a rather direct way of obtaining the Green's functions from microscopic bases. While integral methods (like those presented in [12,13]) have given a deep understanding of the boson propagators (10) at least for some lattices, they have not had the same success with propagators of fermionic fields on lattices [14]; on the other hand random-walk Montecarlo methods have been successfully used to compute propagators for lattice QCD [3,4,14], and one may hope to formalize these results and obtain analytical information from combinatorial approaches similar to the present one.

I wish to end this Letter with a remark on the structure of the recurrence formulas: for large n's $P_D(\mathbf{r},n)$ is well approximated by the gaussian distribution (19): if the single-step probabilities are as in (20), this gaussian is "compressed" along the D-th axis and has a disk-like shape. Consider now the assignment $p_i = \alpha' p$ for i=1,...,D-1 and $p_D = p$, then:

$$p_i = \frac{\alpha'}{2(1+(D-1)\alpha')} \quad \text{for } i=1,\dots,D-1, \text{ and} \quad p_D = \frac{1}{2(1+(D-1)\alpha')}, \qquad (40)$$

and one can find recurrence formulas just as before. However it is not necessary to work them out explicitly, because the substitution $\alpha' \to \frac{1}{\alpha}$ changes (32) into (20), and therefore the recurrence formula for Green's functions becomes:

$$G'_D(\mathbf{r},2(1+(D-1)\alpha')z;\alpha') = G_D(\mathbf{r},2(D-1+\alpha)z;\alpha) =$$

$$= \sum_{k=x}^{\infty} \frac{(\alpha z)^{2k-x}}{k!(k-x)!} \frac{d^{2k-x}}{dz^{2k-x}} \left[z^{2k-x} G_{D-1}(\mathbf{r}',2(D-1)z) \right]$$

$$= \sum_{k=x}^{\infty} \frac{(z/\alpha')^{2k-x}}{k!(k-x)!} \frac{d^{2k-x}}{dz^{2k-x}} \left[z^{2k-x} G_{D-1}(\mathbf{r}',2(D-1)z) \right], \qquad (41)$$

where G'_D is the Green's function defined by (32) and G_D is defined as in (30). Now $\alpha'=1$ gives $G_D(\mathbf{r},2Dz)$, while $G'_D(\mathbf{r},2(1+(D-1)\alpha')z;\alpha') = G_1(x,2z)$ if $\alpha'=0$. The gaussian (19) is now "elongated" along the D-th axis and if $\alpha' \to 0$ it represents an "almost" one-dimensional diffusion process. The latter limit is important in some lattice formulations of gauge theories where space is "latticized" while time is "continuous" [14].

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