Analytic expression for the mean time to absorption for a random walker on the Sierpinski gasket. II. The eigenvalue spectrum

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We continue the study of a particle (atom, molecule) undergoing an unbiased random walk on the Sierpinski gasket, and obtain for the gasket and tower the eigenvalue spectrum of the associated stochastic master equation. Analytic expressions for recurrence relations among the eigenvalues are derived. The recurrence relations obtained are compared with those determined for two Euclidean lattices, the closed chain with an absorbing site and a finite chain with an absorbing site at one end. We check and confirm the internal consistency between the smallest eigenvalue and the mean walklength in each of the cases studied. Attention is drawn to the relevance of the results obtained to a problem of electron transfer in proteins.

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I. INTRODUCTION

The original motivation for this study and earlier ones [1,2] followed from an expository article by Hahn [3] on "Geometry and Intuition." There, Hahn first reviewed the geometry of ordinary points, end points and branch points. In that order, "a point on a curve is called an end point if there are arbitrarily small neighborhoods surrounding it, each of whose boundaries has only a single point in common with the curve. A point on the curve that is not an end point is called an ordinary point if it has arbitrarily small neighborhoods each of whose boundaries has exactly two points in common with the curve. A point on a curve is called a branch point if the boundary of any of its arbitrarily small neighborhoods has more than two points in common with the curve. Intuition seems to indicate that it is impossible for a curve to be made up of nothing but end points or branch points. As far as end points are concern, this intuitive conviction has been confirmed by logical analysis, but as regards branch points it has been refuted. The Polish mathematician W. Sierpinski proved in 1915 that there are curves all of whose points are branch points."

Hahn then reviewed Sierpinski's construction of what today is called the gasket, viz., inscribing equilateral triangles within equilateral triangles and "erasing" the interior of the inscribed triangle. "The points of the original equilateral triangle that survive the infinitely numerous erasures can be shown to form a curve all of whose points, with the exceptions of the vertex points of the original triangle, are branch points." In fact, by coalescing the three vertices into a single point, all of the points of the resulting curve are branch points. Hahn's message was that "in geometrical questions, even very simple and elementary ones, intuition is a wholly unreliable guide."

Consider first a curve defined by a discrete set of ordinary points and two end points. Ergodic flows on the consequent $d=1$ dimensional lattice can be studied using the theory of finite Markov processes [4]. Specifically, for an unbiased "random walk" problem on a closed chain (no end points) having a single absorbing site, Montroll [5] in 1969 obtained an analytic solution for the mean walklength $\langle n\rangle$, viz.,

$$\langle n\rangle = N(N+1)/6. \tag{1}$$

If, on the other hand, one places the absorbing site at one of the end points, and imposes zero-flux boundary conditions at the other, one obtains a slightly different analytic expression for the mean walk length

$$\langle n\rangle = N(2N-1)/3 \tag{2}$$

or, if the absorbing site is at an ordinary point and zero flux conditions are imposed at both end points [6],

$$\langle n\rangle = N(N+1)/3. \tag{3}$$

Now, consider a curve, all of whose points are branch points (except for the vertices, one of which is an absorbing site), i.e., the Sierpinski gasket. For an unbiased random walk on a finite nth generation Sierpinski gasket embedded in Euclidean dimension $d=2$, an exact formula was derived [1] for the mean walk length $T^{(n)}$. Then, in [2] an exact formula for $T^{(n)}$ for the Sierpinski tower embedded in Euclidean dimension $d=3$ was obtained. Also presented in [2] was the exact result for the generalization to the case of an nth generation tower embedded in an arbitrary number of Euclidean dimensions d, viz.

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$$T^{(n)} = \frac{d[(d+1)^n(d+3)^{n+1} + (d+2)(d+3)^n - (d+1)^n]}{(d+2)[(d+1)^{n+1} + d - 1]}. \tag{4}$$

The program followed to obtain these results took advantage of the self-similarity of the gasket, introduced time scaling on the gasket, and mobilized a decimation procedure.

Recalling that the mean walk length $\langle n \rangle$ is the first moment of an underlying probability distribution function, the question posed in this study is whether one can obtain analytic results for the full distribution function. While the general problem is challenging, a particular case yields to exact analysis, and this is the subject of the present contribution. In particular, we consider the transient behavior of a random walker on a chain with a set of ordinary points bracketed by end points, versus a chain with multiple branch points (the Sierpinski gasket). Proceeding from the stochastic master equation, we obtain numerically exact results for the eigenvalue spectrum, and explore whether these eigenvalues satisfy a recurrence relation.

To study the dynamics, we proceed from the probability distribution function $\rho_n(t)$ describing system's evolution. If i denotes the initial state of the system, and $\rho_n(t)$ is the probability of being in a specific, intermediate state n at time t, then the stochastic master equation is

$$\frac{d\rho_n(t)}{dt} = -\sum_m^N G_{nm}\rho_m(t). \tag{5}$$

solved subject to the initial condition

$$\rho_n(t=0) = \delta_{n,i}. \tag{6}$$

In Eq. (5), G_{nm} is the transition rate of the probability to the state n from the state m. The **G** matrix is linked to the $N \times N$ Markov transition probability matrix **P** with elements p_{nm} defined via the relation

$$G_{nm} = \delta_{n,m} - p_{nm}. \tag{7}$$

Here, p_{nm} is the probability that the random walker, conditional on being in state m at time t will be in the state n in the next step, until the terminal state is reached. The transition probability is equal to one divided by the coordination number of the starting site.

The plan of this paper is the following. In Sec. II we consider first the Sierpinski gasket and determine exact expressions for the recurrence relations satisfied by the eigenvalues of the gasket and tower. The analytic approach taken was inspired by a seminal paper published in 1983 by Domany, Alexander, Bensimon, and Kadanoff [7] on "Solutions to the Schroedinger equation on some fractal lattices." We sketch their procedure, and highlight the particular stage in their program where we specialize to the classical, gasket problem.

We note that the method and results obtained by Domany *et al.* [7] in 1983 were subsequently discovered independently and/or mobilized in obtaining important results on several related problems. Although not intended to be inclusive, we draw attention to the work of Cosenza and Kapral [8] on the exact spectrum of the dual Sierpinski gasket.

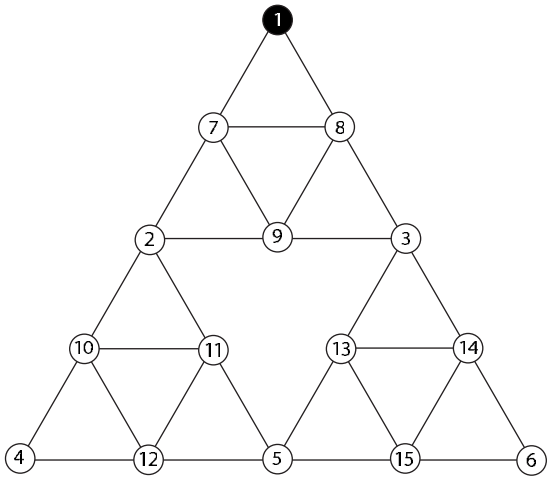

FIG. 1. Sierpinski Gasket of orders $n=2$ and $n=3$.

These authors obtained important results on the stability and bifurcations of spatially synchronized, periodic states on the Sierpinski gasket. Also relevant is the work of Agliari, Blumen and Muelken [9] on the coherent propagation of quantum walks, where the formal relationship between the Schrödinger equation and the classical master equation was exploited to study the problem of electronic energy transfer through the photosynthetic antenna system. Methods introduced in [7,8], and in a recent study by Agliari [10], could have been tailored to the problem at hand; that we have not done so is because our intent here was to stay as close as possible to the formal methods introduced in [7].

To place the results obtained in Sec. II in a slightly more general context, we take up in Secs. III and IV the problem of the closed chain and the finite chain, and obtain analytic expressions for the spectrum of eigenvalues for each. In the concluding Sec. V we review the results obtained and comment on their relevance to a specific experimental problem under active investigation today: electron transfer in the protein, azurin.

II. SIERPINSKI GASKET

To illustrate the approach taken in this study we proceed by showing how the spectrum of the transition matrix of a Sierpinski gasket SG_n of order n is related to that of the previous one. Consider for example the case $n=2$. SG_2 has six vertices, numbered 1 to 6, and we will assume throughout that the sink is at vertex 1 (see Fig. 1). The transition matrix P_2 for the sites other than the sink is thus

$$P_2 = \begin{bmatrix} 1 & -1/4 & -1/4 & -1/4 & 0 \\ -1/4 & 1 & 0 & -1/4 & -1/4 \\ -1/2 & 0 & 1 & -1/2 & 0 \\ -1/4 & -1/4 & -1/4 & 1 & -1/4 \\ 0 & -1/2 & 0 & -1/2 & 1 \end{bmatrix}. \tag{8}$$

The gasket SG_3 can now be obtained by adding vertices 7 to 15 as shown in Fig. 1. Let α be the set of the original vertices, and β the set of the added vertices.

Writing the eigenvalue problem for the transition matrix P_3 in block form

$$\begin{bmatrix} P_{\alpha,\alpha} & P_{\alpha,\beta} \\ P_{\beta,\alpha} & P_{\beta,\beta} \end{bmatrix} \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} = \lambda_3 \begin{bmatrix} u_\alpha \\ u_\beta \end{bmatrix} \tag{9}$$

leads to

$$P_{\alpha,\alpha}u_\alpha + P_{\alpha,\beta}u_\beta = \lambda_3 u_\alpha, \tag{10}$$

$$P_{\beta,\alpha}u_\alpha + P_{\beta,\beta}u_\beta = \lambda_3 u_\beta, \tag{11}$$

and finally gives

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_3 - P_{\beta\beta})^{-1}P_{\beta\alpha}]u_\alpha = \lambda_3 u_\alpha. \tag{12}$$

As there are no transitions between sites belonging to the α sublattice, $P_{\alpha\alpha}$ reduces to the identity matrix, and furthermore the 9×9 matrix $P_{\beta\beta}$ is block diagonal, each block being the same 3×3 matrix corresponding to transitions within the inserted triangles. One finds

$$P_3 = P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_3 - P_{\beta\beta})^{-1}P_{\beta\alpha} = \begin{bmatrix} p & q & q & q & 0 \\ q & p & 0 & q & q \\ 2q & 0 & p & 2q & 0 \\ q & q & q & p & q \\ 0 & 2q & 0 & 2q & p \end{bmatrix}, \tag{13}$$

where

$$p = \frac{8\lambda_3^2 - 12\lambda_3 + 3}{8\lambda_3^2 - 14\lambda_3 + 5}, \quad q = \frac{1}{4}\frac{2\lambda_3 - 3}{8\lambda_3^2 - 14\lambda_3 + 5}. \tag{14}$$

It will be noticed that this matrix is very similar to P_2. In fact it is simply

$$P_3 = (p + 4q)I_5 - 4qP_2, \tag{15}$$

where I_5 is the 5×5 identity matrix. Consequently the spectrum $\{\lambda_3\}$ of the transition matrix P_3 is related to that of P_2 by

$$\lambda_3 = \frac{8\lambda_3^2 - 10\lambda_3 - (2\lambda_3 - 3)\lambda_2}{8\lambda_3^2 - 14\lambda_3 + 5}. \tag{16}$$

Multiplying the left-hand side of this equation by the denominator of the right-hand side leads to

$$\lambda_3(8\lambda_3^2 - 14\lambda_3 + 5) = 8\lambda_3^2 - 10\lambda_3 - (2\lambda_3 - 3)\lambda_2. \tag{17}$$

Expanding the left-hand side now gives

$$8\lambda_3^3 - 14\lambda_3^2 + 5\lambda_3 = 8\lambda_3^2 - 10\lambda_3 - (2\lambda_3 - 3)\lambda_2, \tag{18}$$

and transposing terms from the left-to the right-hand side we obtain

$$8\lambda_3^3 - 14\lambda_3^2 + 5\lambda_3 - 8\lambda_3^2 + 10\lambda_3 + (2\lambda_3 - 3)\lambda_2 = 0, \tag{19}$$

or, on collecting terms of same power,

$$8\lambda_3^3 - 22\lambda_3^2 + 15\lambda_3 + (2\lambda_3 - 3)\lambda_2 = 0. \tag{20}$$

We now notice that

$$8\lambda_3^3 - 22\lambda_3^2 + 15\lambda_3 = (2\lambda_3 - 3)(4\lambda_3^2 - 5\lambda_3), \tag{21}$$

so the equation for λ_3 reads

$$(2\lambda_3 - 3)(4\lambda_3^2 - 5\lambda_3 + \lambda_2) = 0. \tag{22}$$

So that part of the spectrum of P_3 which is related to the one of P_2 is provided by the roots of

$$4\lambda_3^2 - 5\lambda_3 + \lambda_2 = 0, \tag{23}$$

which are given by,

$$\lambda_3 = \frac{5 \pm \sqrt{25 - 16\lambda_2}}{8}. \tag{24}$$

Thus from the five values for λ_2, namely $\{3/4, 3/2, 3/2, (5 \pm \sqrt{17})/8\}$ one finds ten values for λ_3, respectively,

$$\frac{5 \pm \sqrt{13}}{8}, \frac{3}{4}, \frac{1}{2}, \frac{3}{4}, \frac{1}{2}, \frac{5 \pm \sqrt{15 \pm 2\sqrt{17}}}{8}, \tag{25}$$

but the values of 1/2 are spurious since they correspond to a noninvertible matrix $\lambda_3 - P_{\beta,\beta}$. The remaining six eigenvalues are to be found among those singular values for which the analysis breaks down, namely 3/2 ($q=0$) and 5/4 (p and q not defined).

It now remains to show that in general one always has the recurrence

$$4\lambda_{n+1}^2 - 5\lambda_{n+1} + \lambda_n = 0 \rightarrow \lambda_{n+1} = \frac{5 \pm \sqrt{25 - 16\lambda_n}}{8}. \tag{26}$$

For all values of n, the Sierpinski gasket of order $n+1$ can be obtained by inserting three further vertices on the edges of each "cell" of SG_n. Focusing on one such cell and calling $\alpha=\{1,2,3\}$ the vertices of SG_n and $\beta=\{9,8,7\} \equiv \{1',2',3'\}$ the additional set (see Fig. 1), it is clear that the contribution to the transition matrix P_{n+1} can be written in block form, with

$$(P_{\alpha,\alpha})_{i,j} = \delta_{i,j}, \tag{27}$$

$$(P_{\alpha,\beta})_{i,j} = (P_{\beta,\alpha})_{j,i} = -\frac{1}{4}(1 - \delta_{i,j}), \tag{28}$$

$$(P_{\beta,\beta})_{i,j} = \delta_{i,j} - \frac{1}{4}(1 - \delta_{i,j}). \tag{29}$$

Therefore

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_n - P_{\beta\beta})^{-1}P_{\beta\alpha}]_{i,j} = \sum_{k,l=1}^{3} (P_{\alpha\beta})_{i,k}(\lambda_n - P_{\beta\beta})^{-1}_{k,l}(P_{\beta\alpha})_{l,i}, \tag{30}$$

and since

$$(\lambda_n - P_{\beta\beta})^{-1} = \begin{bmatrix} \lambda_n - 1 & 1/4 & 1/4 \\ 1/4 & \lambda_n - 1 & 1/4 \\ 1/4 & 1/4 & \lambda_n - 1 \end{bmatrix}^{-1}, \tag{31}$$

it follows that

$$(\lambda_n - P_{\beta\beta})^{-1}_{k,l} = \begin{cases} -\dfrac{1}{4(\lambda_n - 1/2)(\lambda_n - 5/4)} & \text{if } k \neq l \\ \dfrac{\lambda_n - 3/4}{(\lambda_n - 1/2)(\lambda_n - 5/4)} & \text{if } k = l \end{cases}. \tag{32}$$

Consequently

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_n - P_{\beta\beta})^{-1}P_{\beta\alpha}]_{i,j} = \begin{cases} \dfrac{1}{16}\dfrac{\lambda_n - 3/2}{(\lambda_n - 1/2)(\lambda_n - 5/4)} & \text{if } i \neq j \\ 1 + \dfrac{1}{8}\dfrac{\lambda_n - 1}{(\lambda_n - 1/2)(\lambda_n - 5/4)} & \text{if } i = j \end{cases}. \tag{33}$$

However when the full transition matrix P is evaluated for the complete gasket, it must be borne in mind that each α vertex belongs to two cells, with two exceptions: the lower left vertex (for example, vertex 4 in Fig. 1, and given the generic label A in what follows), and the lower right vertex (e.g., vertex 6 in Fig. 1, and given the generic label B). In other words the above expressions are correct for the nondiagonal terms (different values for i and j determine one cell), but for the diagonal terms one obtains

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_n - P_{\beta\beta})^{-1}P_{\beta\alpha}]_{i,i} = 1 + \frac{1}{4}\frac{\lambda_n - 1}{(\lambda_n - 1/2)(\lambda_n - 5/4)}. \tag{34}$$

Consequently it is again possible to relate the spectra $\{\lambda_{n+1}\}$ and $\{\lambda_n\}$ with a scaling and transition which are exactly those found in the case $n=2$, provided it can be shown that this transformation is also valid for the vertices A and B. An unexpected result occurs at this step of the analysis, where a special feature of sites A and B emerges, a feature different from the role of these sites in [7]. In [7] sites A and B are fixed by the boundary conditions, but in the present case they belong to the set of variables. Note that A belongs to only one triangle [see Fig. 1]. For vertex A, the $P_{\beta,\beta}$ matrix is unchanged, but

$$P_{A,1} = P_{A,3} = -1/2, \quad P_{1,A} = P_{3,A} = -1/4 \tag{35}$$

and

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_n - P_{\beta\beta})^{-1}P_{\beta\alpha}]_{A,A} \tag{36}$$

$$= 1 + \sum_{k=1,3}\sum_{l=1,3}(P_{\alpha\beta})_{A,k}[(\lambda_n - P_{\beta\beta})^{-1}]_{k,l}(P_{\beta\alpha})_{l,A} \tag{37}$$

$$= 1 + \frac{1}{8}\left[-2\frac{1}{4(\lambda_n - 1/2)(\lambda_n - 5/4)} + 2\frac{\lambda_n - 3/4}{(\lambda_n - 1/2)(\lambda_n - 5/4)}\right] \tag{38}$$

$$= 1 + \frac{1}{4}\frac{\lambda_n - 1}{(\lambda_n - 1/2)(\lambda_n - 5/4)}. \tag{39}$$

As to the nondiagonal elements they are equal to

TABLE I. Eigenvalues for the $d_f = \ln 3/\ln 2$ Sierpinski gasket of N sites.

N	λ
3	1/2, 3/2
6	3/4, 3/2 {2}, $5/8 \pm (1/8)\sqrt{17}$
15	3/4 {2}, 5/4, 3/2 {5}, $5/8 \pm (1/8)\sqrt{13}$, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{17}}$
42	3/4 {5}, 5/4 {4}, 3/2 {14}, $5/8 \pm (1/8)\sqrt{5}$, $5/8 \pm (1/8)\sqrt{13}$,{2}, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{13}}$, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{15 \pm 2\sqrt{17}}}$
123	3/4 {14}, 5/4 {13}, 3/2 {41}, $5/8 \pm (1/8)\sqrt{5}${4}, $5/8 \pm (1/8)\sqrt{13}${5}, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{5}}$, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{13}}$ {2}, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{15 \pm 2\sqrt{13}}}$, $5/8 \pm (1/8)\sqrt{15 \pm 2\sqrt{15 \pm 2\sqrt{15 \pm 2\sqrt{17}}}}$

$$[P_{\alpha\alpha} + P_{\alpha\beta}(\lambda_n - P_{\beta\beta})^{-1}P_{\beta\alpha}]_{A,1} \tag{40}$$

$$= 1 + \sum_{k=1,3}\sum_{l=1,3}(P_{\alpha\beta})_{A,k}[(\lambda_n - P_{\beta\beta})^{-1}]_{k,l}(P_{\beta\alpha})_{l,A} \tag{41}$$

$$= \frac{1}{8}\left[-3\frac{1}{4(\lambda_n - 1/2)(\lambda_n - 5/4)} + \frac{\lambda_n - 3/4}{(\lambda_n - 1/2)(\lambda_n - 5/4)}\right] \tag{42}$$

$$= \frac{1}{8}\frac{\lambda_n - 3/2}{(\lambda_n - 1/2)(\lambda_n - 5/4)}, \tag{43}$$

and it will be noticed that both the scaling and the translation are the *same* for these corner vertices A and B as for all the sites of the gasket. Armed with the recurrence relation for the eigenvalues of the Sierpinski gasket given in Eq. (26), one can reproduce the values displayed in Table I for the first five generations of the Sierpinski gasket, obtained via exact numerical solution of Eq. (5) subject to Eq. (6).

Turning to the Sierpinski tower, numerically exact values for the eigenvalues were obtained for the first three generations of the tower. In following the above program, everything goes through as for the gasket, *including* the factors for the sites in the corner of the base. The recurrence relation for the eigenvalues in the Sierpinski tower reads

$$\lambda_{n+1} = \frac{3 \pm \sqrt{9 - 6\lambda_n}}{6}. \tag{44}$$

The first generation, $N=4$ tower has as eigenvalues 1/3 and 4/3 {2} (where the braces {} indicate the degeneracy of the eigenvalue), and these give for the $N=10$ tower, respectively,

TABLE II. Eigenvalues for the $d_f = \ln 4/\ln 2$ Sierpinski tower of N sites.

N	λ
4	1/3, 4/3 {2}
10	2/3 {2}, 4/3 {5}, $1/2 \pm \sqrt{7/6}$
34	2/3 {5}, 1 {3}, 4/3 {17}, $1/2 \pm \sqrt{5/6}$ {2}, $1/2 \pm \sqrt{6 \pm \sqrt{7}/6}$

$$1/2 \pm \frac{\sqrt{7}}{6}, \quad \frac{2}{3} \quad \text{and} \frac{1}{3} \tag{45}$$

but the last value must be rejected as it would involve a singularity in the recurrence. Then for the $N=34$ tower, the first pair gives

$$\frac{1}{2} \pm \frac{\sqrt{6 \pm \sqrt{7}}}{6} \tag{46}$$

and 2/3 gives

TABLE III. Eigenvalues for a linear chain of N sites subject to periodic boundary conditions.

N	λ
3	1/2, 3/2
4	$1, 1 \pm \sqrt{2}$
5	$3/4 \pm (1/4)\sqrt{5}$, $5/4 \pm (1/4)\sqrt{5}$
6	$1, 1/2, 3/2, 1 \pm \sqrt{3}$
7	$(1/12)(28+i84\sqrt{3})^{1/3}+(7/3)(28+i84\sqrt{3})^{-1/3}+5/6$, $-(1/24)(28+i84\sqrt{3})^{1/3}-(7/6)(28+i84\sqrt{3})^{-1/3}+5/6$ $\pm(1/4)i\sqrt{3}[(1/6)(28+i84\sqrt{3})^{1/3}-(14/3)(28+i84\sqrt{3})^{-1/3}]$, $(1/12)(-28+i84\sqrt{3})^{1/3}+(7/3)(-28+i84\sqrt{3})^{-1/3}+7/6$, $-(1/24)(-28+i84\sqrt{3})^{1/3}-(7/6)(-28+i84\sqrt{3})^{-1/3}+7/6$ $\pm(1/4)i\sqrt{3}[(1/6)(-28+i84\sqrt{3})^{1/3}-(14/3)(-28+i84\sqrt{3})^{-1/3}]$
8	$1, 1 \pm \sqrt{2}, 1 \pm (1/2)\sqrt{2+\sqrt{2}}, 1 \pm (1/2)\sqrt{2-\sqrt{2}}$
9	1/2, 3/2, $(1/4)(-4+i4\sqrt{3})^{1/3}+(-4+i4\sqrt{3})^{-1/3}+1$, $-(1/8)(-4+i4\sqrt{3})^{1/3}-(1/2)(-4+i4\sqrt{3})^{-1/3}+1$ $\pm(1/4)i\sqrt{3}[(1/2)(-4+i4\sqrt{3})^{1/3}-2(-4+i4\sqrt{3})^{-1/3}]$, $(1/4)(4+i4\sqrt{3})^{1/3}+(4+i4\sqrt{3})^{-1/3}+1$, $-(1/8)(4+i4\sqrt{3})^{1/3}-(1/2)(4+i4\sqrt{3})^{-1/3}+1$ $\pm(1/4)i\sqrt{3}[(1/2)(4+i4\sqrt{3})^{1/3}-2(4+i4\sqrt{3})^{-1/3}]$
10	$1, 3/4 \pm (1/4)\sqrt{5}, 5/4 \pm (1/4)\sqrt{5}$, $1 \pm (1/4)\sqrt{10+2\sqrt{5}}, 1 \pm (1/4)\sqrt{10-2\sqrt{5}}$
11	Table IV
12	$1, 1/2, 3/2, 1 \pm (1/2)\sqrt{2}, 1 \pm (1/2)\sqrt{3}$, $1 \pm (1/4)\sqrt{6} \pm (1/4)\sqrt{2}$
13	Table IV

$$\frac{1}{2} \pm \frac{\sqrt{5}}{6} \tag{47}$$

and so on as shown in Table II.

III. CLOSED CHAIN

Consider a linear chain of N sites, with a single deep trap and subject to periodic boundary conditions. Reported in Table III is the set $\{\lambda_i\}$ determined via numerical solution of the stochastic master equation, Eq. (5), for lattices up to $N=13$ sites. As is evident, there appears to be a repetition of (certain) eigenvalues for small lattices that reappear for larger ones, suggesting the possible existence of an underlying recurrence relation.

The results presented in Table III are given in integer format, except for the values for $N=11$ and $N=13$. In these two cases, polynomial representations for the eigenvalues are obtained (see Table IV) which then can be used to determine the eigenvalues in decimal format. Specifically, one solves for the roots of the equation

$$P_N(w) = 0. \tag{48}$$

In general, the analytic procedure for obtaining the eigenvalues of the stochastic master equation (by diagonalizing the fundamental matrix of the theory of Markov processes) proceeds first through such polynomial representations. In some (though certainly not all) cases, representation of the

TABLE IV. Polynomial representations of the data in Table III.

$P_3 = 4w^2 - 8w + 3$

$P_4 = 8w^3 - 24w^2 + 20w - 4$

$P_5 = 16w^4 - 64w^3 + 84w^2 - 40w + 5$

$P_6 = 32w^5 - 160w^4 + 288w^3 - 224w^2 + 70w - 6$

$P_7 = 64w^6 - 384w^5 + 880w^4 - 960w^3 + 504w^2 - 112w + 7$

$P_8 = 128w^7 - 896w^6 + 2496w^5 - 3520w^4 + 2640w^3 - 1008w^2 + 168w - 8$

$$P_9 = 256w^8 - 2048w^7 + 6720w^6 - 11648w^5 + 11440w^4 - 6336w^3 + 1848w^2 - 240w + 9$$

$$P_{10} = 512w^9 - 4608w^8 + 17408w^7 - 35840w^6 + 43680w^5 - 32032w^4 + 13728w^3 - 3168w^2 + 330w - 10$$

$$P_{11} = 1024w^{10} - 10240w^9 + 43776w^8 - 104448w^7 + 152320w^6 - 139776w^5 + 80080w^4 - 27456w^3 + 5148w^2 - 440w + 11$$

$$P_{12} = 2048w^{11} - 22528w^{10} + 107520w^9 - 291840w^8 + 496128w^7 - 548352w^5 - 183040w^4 + 51480w^3 - 8008w^2 + 572w - 12$$

$$P_{13} = 4096w^{12} - 49152w^{11} + 259072w^{10} - 788480w^9 + 1532160w^8 - 1984512w^7 + 1736448w^6 - 1018368w^5 + 388960w^4 - 91520w^3 + 12012w^2 - 728w + 13$$

eigenvalues in integer format can be obtained, as displayed in Table III.

The key to uncovering recurrence relations for this Euclidean lattice trapping problem resides in the polynomial representations given in Table IV. These results can be used to construct a general expression for the polynomial $P_{N+1}(w)$, valid for arbitrary N,

$$P_{N+1}(w) = 2^N w^N - \frac{2^{N-1}(2N)w^{N-1}}{1!} + \frac{2^{N-2}(2N-1)(2N-2)w^{N-1}}{2!} - \frac{2^{N-3}(2N-2)(2N-3)(2N-4)w^{N-3}}{3!} + \frac{2^{N-4}(2N-3)(2N-4)(2N-5)(2N-6)w^{N-4}}{4!} - /+ \ldots . \tag{49}$$

As will now be shown explicitly, this expression can be recast into the following exact, closed form

$$P_{N+1}(w) = \left(\frac{1}{w(2-w)}\right)^{1/2} \sin\left[(2N+2)\arccos\left(\frac{w}{2}\right)^{1/2}\right]. \tag{50}$$

With periodic boundary conditions (site $N+1$ identified with site 1), the absorbing site can always be labeled 1, so the $N \times N$ transition matrix reads

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & \ldots & \ldots & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} & \ldots & \ldots & 0 \\ 0 & \frac{1}{2} & -1 & \frac{1}{2} & \ldots & 0 \\ \vdots & \vdots & \ddots & \ldots & \ldots & \vdots \\ \vdots & \vdots & \ddots & \ldots & \ldots & \vdots \\ 0 & 0 & \ldots & \frac{1}{2} & -1 & \frac{1}{2} \\ 0 & 0 & \ldots & 0 & \frac{1}{2} & -1 \end{pmatrix}, \tag{51}$$

and after removing a factor λ (corresponding to the stationary state), the $(N-1)\times(N-1)$ characteristic determinant will be

$$\Delta_{N-1}(-\lambda) = \begin{vmatrix} -1+\lambda & \frac{1}{2} & \ldots & \ldots & 0 \\ \frac{1}{2} & -1+\lambda & \frac{1}{2} & \ldots & 0 \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ 0 & \ldots & \frac{1}{2} & -1+\lambda & \frac{1}{2} \\ 0 & \ldots & 0 & \frac{1}{2} & -1+\lambda \end{vmatrix}. \tag{52}$$

Notice that if one inserts $\lambda = 1+\cos\theta$ into the last determinant, one has

$$\Delta_{N-1} = \frac{1}{2^{N-1}} \begin{vmatrix} 2\cos\theta & 1 & \ldots & \ldots & 0 \\ 1 & 2\cos\theta & 1 & \ldots & 0 \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ 0 & \ldots & 1 & 2\cos\theta & 1 \\ 0 & \ldots & 0 & 1 & 2\cos\theta \end{vmatrix}. \tag{53}$$

This tridiagonal Toeplitz determinant is equal to the Chebyshev polynomial (see Ref. [11])

$$U_{N-1}(\cos\theta) = \frac{\sin N\theta}{\sin\theta}. \tag{54}$$

The previous, closed form expression for $P(w)$ follows by writing the determinant, Eq. (52), as

$$P_N(w) = 2^{N-1} \begin{vmatrix} -1+w & \frac{1}{2} & \ldots & \ldots & 0 \\ \frac{1}{2} & -1+w & \frac{1}{2} & \ldots & 0 \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ \vdots & \ddots & \ldots & \ldots & \vdots \\ 0 & \ldots & \frac{1}{2} & -1+w & \frac{1}{2} \\ 0 & \ldots & 0 & \frac{1}{2} & -1+w \end{vmatrix}, \tag{55}$$

and setting

$$w = 2\cos^2 t \tag{56}$$

so that

TABLE V. Eigenvalues for a linear chain of N sites subject to finite boundary conditions.

N	λ
3	$3/4 \pm (1/4)\sqrt{5}$
4	$(1/12)(28+\mathrm{i}84\sqrt{3})^{1/3}+(7/3)(28+\mathrm{i}84\sqrt{3})^{-1/3}+5/6$, $(1/24)(28+\mathrm{i}84\sqrt{3})^{1/3}-(7/6)(28+\mathrm{i}84\sqrt{3})^{-1/3}+5/6$, $\pm(1/4)\mathrm{i}\sqrt{3}[(1/6)(28+\mathrm{i}84\sqrt{3})^{1/3}-(14/3)(28+\mathrm{i}84\sqrt{3})^{-1/3}]$
5	$1/2$, $(1/4)(-4+\mathrm{i}4\sqrt{3})^{1/3}+(-4+\mathrm{i}4\sqrt{3})^{-1/3}+1$, $(-1/8)(-4+\mathrm{i}4\sqrt{3})^{1/3}-(1/2)(-4+\mathrm{i}4\sqrt{3})^{-1/3}+1$, $\pm(1/4)\mathrm{i}\sqrt{3}[(1/2)(-4+\mathrm{i}4\sqrt{3})^{1/3}-2(-4+\mathrm{i}4\sqrt{3})^{-1/3}]$
>5	See Table VI

$$P_N = \begin{vmatrix} 2\cos 2t & 1 & \cdots & \cdots & 0 \\ 1 & 2\cos 2t & 1 & \cdots & 0 \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \ddots & \cdots & \cdots & \vdots \\ 0 & \cdots & 1 & 2\cos 2t & 1 \\ 0 & \cdots & 0 & 1 & 2\cos 2t \end{vmatrix}. \tag{57}$$

Then,

$$P_N = \frac{\sin 2Nt}{\sin 2t} = \frac{\sin\left[2N \arccos\left(\frac{w}{2}\right)^{1/2}\right]}{2\left[\frac{w}{2}\left(1-\frac{w}{2}\right)\right]^{1/2}} \tag{58}$$

which is just Eq. (50).

Consequently the spectrum of the transition matrix for N sites with periodic boundary conditions is given by

$$\lambda_N(k) = 1 + \cos\frac{k\pi}{N} \quad (k = 1,2, \ldots N-1) \tag{59}$$

and the smallest of these is

$$\lambda_0 = 1 - \cos\frac{\pi}{N}. \tag{60}$$

IV. FINITE CHAIN WITH ABSORBING SITE AT ONE END

The program described in the preceding section can be mobilized for a walker on a $d=1$ Euclidean lattice of N sites, with a confining boundary at one end of the chain and a deep trap at the other. Though eigenvalues $\{\lambda_i\}$ can be determined in integer format for a few lattices [Table V], the precursor, polynomial representations can be obtained for arbitrary N; see Table VI. A series representation of these results, valid for any N, can be generated,

TABLE VI. Polynomial representations of the data in Table V.

$F_3 = 4w^2 - 6w + 1$

$F_4 = 8w^3 - 20w^2 + 12w - 1$

$F_5 = 16w^4 - 56w^3 + 60w^2 - 20w + 1$

$F_6 = 32w^5 - 144w^4 + 224w^3 - 140w^2 + 30w - 1$

$F_7 = 64w^6 - 352w^5 + 720w^4 - 672w^3 + 280w^2 - 42w + 1$

$F_8 = 128w^7 - 832w^6 + 2112w^5 - 2640w^4 + 1680w^3 - 504w^2 + 56w - 1$

$F_9 = 256w^8 - 1920w^7 + 5824w^6 - 9152w^5 + 7920w^4 - 3696w^3 + 840w^2 - 72w + 1$

$F_{10} = 512w^9 - 4352w^8 + 15360w^7 - 29120w^6 + 32032w^5 - 20592w^4 + 7392w^3 - 1320w^2 + 90w - 1$

$F_{11} = 1024w^{10} - 9728w^9 + 39168w^8 - 87040w^7 + 116480w^6 - 96096w^5 + 48048w^4 - 13728w^3 + 1980w^2 - 110w + 1$

$F_{12} = 2048w^{11} - 21504w^{10} + 97280w^9 - 248064w^8 + 391680w^7 - 396032w^6 + 256256w^5 - 102960w^4 + 24024w^3 - 2860w^2 + 132w - 1$

$F_{13} = 4096w^{12} - 47104w^{11} + 236544w^{10} - 680960w^9 + 1240320w^8 - 1488384w^7 + 1188096w^6 - 622336w^5 + 205920w^4 - 40040w^3 + 4004w^2 - 156w + 1$

$$F_{N+1}(w) = 2^N w^N - \frac{2^{N-1}(2N-1)w^{N-1}}{1!} + \frac{2^{N-2}(2N-2)(2N-3)w^{N-2}}{2!} - \frac{2^{N-3}(2N-3)(2N-4)(2N-5)W^{N-3}}{3!} + \frac{2^{N-4}(2N-4)(2N-5)(2N-6)(2N-7)w^{N-4}}{4!} - /+ \ldots \tag{61}$$

and an exact, closed-form result can be written down, viz.

$$F_{N+1}(w) = \left(\frac{2}{2-w}\right)^{1/2} \sin\left[(2N+1)\arccos\left(\frac{w}{2}\right)^{1/2}\right]. \tag{62}$$

In this case, with absorption at site 1, the transition matrix becomes

$$\begin{pmatrix} 0 & \frac{1}{2} & 0 & \cdots & \cdots & 0 \\ 0 & -1 & \frac{1}{2} & \cdots & \cdots & 0 \\ 0 & \frac{1}{2} & -1 & \frac{1}{2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \cdots & \vdots \\ \vdots & \vdots & \ddots & \cdots & \cdots & \vdots \\ 0 & 0 & \cdots & \frac{1}{2} & -1 & \frac{1}{2} \\ 0 & 0 & \cdots & 0 & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \tag{63}$$

and the characteristic determinants Δ'_{N-1} are related to the previous determinants Δ by (expand with respect to the last row)

$$\begin{aligned} \Delta'_{N-1} &= \left(-\frac{1}{2}+\lambda\right)\Delta_{N-2} - \frac{1}{4}\Delta_{N-3} \quad (N=2,3,\ldots) \\ &= \frac{1}{2^{N-2}\sin\theta}\left[\left(\frac{1}{2}+\cos\theta\right)\sin(N-1)\theta - \frac{1}{2}\sin(N-2)\theta\right] \\ &= \frac{1}{2^{N-1}}\frac{\sin\left(N-\frac{1}{2}\right)\theta}{\sin\frac{\theta}{2}}. \end{aligned}$$

The spectrum corresponds thus to the values

$$\theta_k = \frac{k\pi}{N-\frac{1}{2}} \quad (k=1,2,\ldots,N-1), \tag{64}$$

and the smallest value of $\lambda_k = 1+\cos\theta_k$ occurs for $k=N-1$,

$$\lambda_N = 1+\cos\frac{(N-1)\pi}{N-\frac{1}{2}} = 1-\cos\frac{\pi}{2N-1}. \tag{65}$$

V. DISCUSSION AND CONCLUSIONS

In this study we have focused on the transient behavior of a diffusing particle undergoing an unbiased random walk on a lattice, all of whose points are branch points (with the exception of three vertices) versus a lattice with a set of ordinary points bracketed by end points. Analytic expressions were obtained for the eigenvalues as a function of system size N. Exact recurrence relations satisfied by the smallest eigenvalue were derived.

To contextualize the results obtained, we take advantage of the inverse relation between the first moment of the probability distribution function $\rho(t)$, i.e., the mean walk length $\langle n\rangle$, and the smallest eigenvalue λ_0 of the underlying stochastic master equation, Eq. (5), a relationship which becomes exact ($\lambda_0 = 1/\langle n\rangle$) in the limit of large system size [4]. Phrasing the results obtained in terms of the system's dimensionality, previous studies [12–14] documented that for a given system size N, the mean walklength before trapping on the Sierpinski gasket, a two-dimensional uncountable set with zero measure and Hausdorff dimension

$$d_f = \frac{\log 3}{\log 2} = 1.584\,963 \tag{66}$$

(also the fractal dimension of the T fractal; see [10]), was distinctly larger than the value calculated for the triangular lattice, a regular lattice of Euclidean dimension $d=2$. Further, the walk length on the gasket was smaller than values calculated for a $d=1$ regular lattice, Eq. (1) and Eqs. (2) and (3). Subsequently, it was demonstrated [15] that the $\langle n\rangle$ for trapping on a triangular lattice of Euclidean dimension $d=2$ was smaller than the value of $\langle n\rangle$ calculated for the Sierpinski tower, which has a Hausdorff dimension

$$d_f = \frac{\log 4}{\log 2} = 2. \tag{67}$$

In light of the relationship between $\langle n\rangle$ and the smallest eigenvalue λ_0, we can check whether the expressions obtained for λ_0 in Secs. II–IV are consistent with earlier results on $\langle n\rangle$. First, from the equations for the smallest eigenvalue for the closed chain and the finite chain with an absorbing site at one end, the eigenvalue λ_0 for a finite chain of N sites is always smaller than that for a closed chain having the same number N of sites; this is consistent with Eq. (1) and Eqs. (2) and (3) for the mean walk length, where $\langle n\rangle$ for the periodic chain is always smaller than for the finite chain.

Second, for a given N, values of λ_0 for the Sierpinski gasket (see Table I) are always smaller than the values calculated using either Eqs. (60) and (65). Again, consistency with results reported earlier (see earlier paragraph) on the mean walk length $\langle n\rangle$ for these cases is found.

Finally, in his 1969 paper, Montroll proved analytically that for a given N, the higher the Euclidean dimensionality, the smaller the mean walk length. Our results on the Sierpinski gasket and tower, show that for a given N, the higher the Hausdorff dimension of a fractal, the smaller the mean walk length and the larger the smallest eigenvalue.

One motivation for considering the trapping problem on a finite chain with an absorbing site at one end derives from a problem in protein chemistry under active investigation today. Electron transfer has been studied theoretically and experimentally over the last three decades [16–19]. In experimental studies on proteins such as azurin [18,19], an electron moves along the backbone of the polypeptide chain until being "trapped" at a localized reaction center. For distances greater than 20 Å, electron transfer (ET) between a donor (D) and acceptor (A) has been shown to proceed via a tunneling mechanism. Aspects of this problem can be treated as a random walk on a finite chain with an absorbing site at one end assuming there is a single ($d=1$) pathway between donor and acceptor [20]. If, as is likely in the general case, multiple pathways may be available, a lattice of higher dimension would need to be considered. Rather than going to the next

higher Euclidean dimension, it seems sensible to consider a lattice with the Hausdorff dimensionality of the Sierpinski gasket or the T fractal [10]. The results presented in this study allow the dynamics of the electron transfer event to be explored in this more general setting and this application will be taken up in subsequent work.

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