

## Random Walks and Chemical Graph Theory

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Simple random walks probabilistically grown step by step on a graph are distinguished from walk enumerations and associated equipose random walks. Substructure characteristics and graph invariants correspondingly defined for the two types of random walks are then also distinct, though there often are analogous relations. It is noted that the connectivity index as well as some resistance-distance-related invariants make natural appearances among the invariants defined from the simple random walks.

### 1. INTRODUCTION

Simple random walks with each step taken independently and randomly naturally are anticipated as a basis for novel chemical graph theory. These are distinct from the frequently studied enumerations of walks, and analogues to invariants defined in terms of walk enumerations may be anticipated. Further one might wonder whether the simple random walks are related to other already known invariants, say involving resistance distances<sup>1,2</sup> or connectivity index<sup>3</sup> and related descriptors.<sup>4,5</sup>

Here we describe theory for the simple random walks and some related invariants, and we identify some relations to earlier indices. But, first some relevant graph-theoretical definitions<sup>6–8</sup> are presented.

A *walk* in a (molecular) graph  $G$  is an alternating sequence of vertices and edges of  $G$ , such that each edge  $e$  begins and ends with the vertices immediately preceding and following  $e$  in the sequence. The *length* of a walk is the number of edges in it. Repetition of vertices and edges is allowed in a walk. A *self-returning walk* is a walk starting and ending at the same vertex. Walks have been extensively applied by Rucker and Rucker<sup>9–14</sup> and others<sup>15–24</sup> as measures of the complexity of graphs and molecules, particularly for use as molecular descriptors in structure–property modeling.<sup>25–30</sup>

A *random walk* in a (molecular) graph is naturally designated by a probability measure, of which there are at least two natural intrinsic ones. First is the probability measure that entails starting walks from each vertex with equal probability, and subsequent steps are such that each neighboring vertex is stepped to with equal probability, so that the probability of stepping from vertex  $i$  to vertex  $j$  is  $1/d_i$ , where  $d_i$  is the *degree* (or valency) of vertex  $i$ . The walks of the consequently generated distribution are referred

to<sup>31</sup> as *simple random walks*. Second is the probability measure that takes each possible walk of a given length as equally probable. These probability measures are generally quite different, though if a graph is regular (i.e., having all vertices of the same degree), then these two probability measures are equivalent. We call the walks generated by this second probability measure *equipose random walks*. The simple random walks have rather infrequently been used in chemical graph theory, whereas the equipose random walks have rather frequently been used.<sup>9–24</sup> Often either equipose or simple random walks have been called just *random*, likely without recognition of the alternative type—or perhaps with confusion of the two possibilities. Rather broadly the simple random walks have been studied in mathematics and physics, as modeling different sorts of diffusion processes. See, e.g., Doyle and Snell's charming book<sup>31</sup> *Random Walks and Electrical Networks* or Montroll and Schlesinger's also charming review<sup>32</sup> *On the Wonderful World of Random Walks*. Very often in the rather extensive literature relating to diffusion the walks are taken on translationally symmetric vertex-regular lattice graphs, for which case the problems of random and equipose walks end up coinciding, but occasionally allowance is made for the more general circumstance, e.g. ref 33. In polymer chemistry (as in Flory's classic text<sup>34</sup>) the equipose random walks have been viewed as simple descriptions of ensembles of polymer chains, though more properly the walks should be self-avoiding. In mathematics another case where random walks appear is in Polya's fundamental result<sup>35</sup> that for (simple) random walks on a translationally symmetric  $d$ -dimensional lattice the probability of never returning to the starting point is  $>0$  if and only if  $d > 2$ . And another area in which simple random walks occur is in the analysis of functions (e.g., *landscape functions*<sup>36,37</sup>) on the vertices of a (often large) graph. In computer science, in particular in the analysis of algorithms, random walks have been an important tool whose debut can be traced back to the seminal paper of Aleliunas et al.<sup>38</sup> and has found its way into textbooks such as that of Motwani and Raghavan.<sup>39</sup> Perhaps the most comprehensive mathematical reference to random walks is the monograph of

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Aldous and Fill,<sup>40</sup> which has been in the making, and available on line, for about a decade.

Granted the distinction between simple and equipoise random walks, it is natural to address analogies between their treatment and corresponding walk-based graph invariants and also to look into relations to already introduced invariants.

## 2. SIMPLE RANDOM AND EQUIPOISE WALKS

**Random Walks.** Walks can be generated<sup>16,25</sup> from powers of the vertex-adjacency matrix  $A$ . And this may be viewed as an identification of the distribution for equipoise random walks. Rather similarly, the distribution for simple random walks can be generated by powers of a Markov matrix  $M$  with elements which are probabilities for associated individual steps:

$$(M)_{ij} \equiv \begin{cases} 1/d_j & i \sim j \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

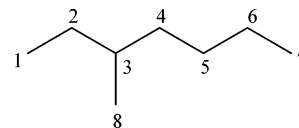
Then  $(M^l)_{ij}$  is the probability for an  $l$ -step random walk beginning at vertex  $j$  to end at vertex  $i$ .

One feature that equipoise walks have is that one is able to work with integer arithmetic. And perhaps it should be pointed out that one can similarly deal with simple random walks and their associated characteristics. The probabilities being summed (as in the powers of  $M$ ) are of course generally noninteger rationals, but for chemical graphs these rationals typically have denominators with a rather small least common multiple. For instance, if attention is limited to graphs characteristic of conjugated networks, then every single-step probability when multiplied by 6 becomes an integer, so that if the computations are done with  $6M$  in place of  $M$  all the arithmetic is integer arithmetic, though at the end (of computing results for  $l$ -step walks) one needs to understand that the result is to be divided by  $6^l$ . And in dealing with general alkane graphs (with degrees up to 4) one would use  $12M$  and ultimately divide by  $(12)^l$ .

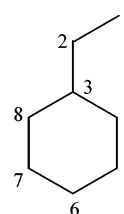
Another point of interest concerns a probabilistic local-growth view for equipoise random walks. That is, one may view *weighted simple random walks* to be such that there is the following: first, a *local* probabilistic growth with a probability for any step along an edge from site  $i$  being  $1/d_i$ ; second, a *weight* for such a step being  $d_i$ ; and third, a weight for a walk as a whole being the product of its step weights. Then it is seen that the consequent probabilistic expectation values for walk weights give results for the *equipoise* walks.

**Vertex Characteristics and Graph Invariants.** Associated to the equipoise case there is<sup>9</sup> a vertex characteristic termed the atomic length- $l$  walk-count  $(awc)_l(i)$  representing the number of all possible walks of length  $l$  which start at a specified vertex (atom)  $i$  and end somewhere. For simple random walks one might be tempted to define an analogue invariant giving the sum of the probabilities for length- $l$  walks starting from vertex  $i$  to end at some vertex—but this value is  $=1$  (so long as  $i$  is not an isolated vertex). However  $(awc)_l(i)$  is also the number of walks ending at  $i$  having started anyplace, and so we introduce a *random-walk count*  $(rwc)_l$  at vertex  $i$  as

$$(rwc)_l(i) = \sum_{j=1}^N (M^l)_{ij} \quad (2)$$



**Figure 1.** Labeled tree representing 3-methylheptane.



**Figure 2.** Labeled graph representing vinylbenzene.

which can interpreted as  $N$  times the probability  $(rwc)_l(i)/N$  that one ends after  $l$  steps at vertex  $i$  having started randomly at any vertex. Another vertex characteristic is based on self-returning  $l$ -step random walks

$$(srrw)_l(i) = (M^l)_{ii} \quad (3)$$

which of course is the probability for a simple random walk starting at vertex  $i$  to return to  $i$  after  $l$  steps. These vertex characteristics in fact have already arisen in ref 41 in the context of general *sum rules* for *resistance distances*,<sup>1</sup> though  $(srrw)_l(i)$  was there denoted  $w_l(i)$ .

Parallel to what has been done with walk counts<sup>16</sup> one can invoke vertex codes now for simple random walks. Thence a self-returning random-walk code for vertex  $i$  is a sequence  $(srrw)_l(i)$  with  $l$ th member  $(srrw)_l(i)$ . One point raised by Randić<sup>16</sup> is that some inequivalent vertices (i.e., vertices not in the same orbit of the automorphism group of  $G$ ) may turn out to have the same equipoise self-returning-walk codes. One example of this is 3-methylheptane (see Figure 1) where carbons 3 and 5 turn out to have the same equipoise code.

However, our present simple-random-walk analogue code neatly distinguishes these two vertices, even at the comparatively low member of  $l = 2$ , for which  $(srrw)_2(3) = 2/3$  while  $(srrw)_2(5) = 1/2$ . Moreover, there are other cases such as this such as the carbon atoms 4 and 7 of vinylbenzene (see Figure 2), for which we obtain  $(srrw)_2(4) = 1/2$  while  $(srrw)_2(7) = 2/3$ .

Thence the present code offers the possibility of being more faithfully distinguishing than the earlier self-returning equipoise walk code.

To obtain graph invariants a particular vertex characteristic may be summed over all vertices. Thus one obtains invariants  $(rwc)_l$  and  $(srrw)_l$ .

## 3. RANDOM-WALK MATRICES

**Eigen-Resolution.** The  $(rwc)_l(i)$  or  $(srrw)_l(i)$  can be computed by means of eigenvalues of the matrix  $M$ . However, it should be noted that the matrix is generally nonsymmetric, when the graph is not regular. But in the general case the eigenvalues are related to those of a symmetric matrix, since  $M$  can be expressed as

$$M = AD^{-1} \quad (4)$$

where  $A$  is the vertex-adjacency matrix,  $D$  is the diagonal

matrix with elements  $(D)_{ii} = d_i$  the degree of site  $i$ , and  $D^{-1}$  is its inverse (presuming that  $G$  has no isolated vertices). Now, we introduce the following matrix

$$H \equiv D^{-1/2} M D^{1/2} \quad (5)$$

where  $D^{1/2}$  is the diagonal matrix with elements  $(D^{1/2})_{ii} = d_i^{1/2}$  and  $D^{-1/2}$  is its inverse  $(D^{-1/2})^{-1}$ . Matrices  $H$  and  $M$  are related by a similarity transformation, so that  $H$  has the same eigenvalues as  $M$  and eigenvectors  $\vec{c}'$  which are simply related to those  $\vec{c}$  of  $M$ . In particular, if  $H\vec{c}' = \lambda\vec{c}'$  and we define  $\vec{c} \equiv D^{1/2}\vec{c}'$ , then

$$M\vec{c} = M D^{1/2}\vec{c}' = D^{1/2}(D^{-1/2} M D^{1/2})\vec{c}' = \lambda D^{1/2}\vec{c}' \quad (6)$$

so that  $M\vec{c} = \lambda\vec{c}$ . And conversely if  $M\vec{c} = \lambda\vec{c}$  and we define  $\vec{c}' \equiv D^{-1/2}\vec{c}$ , then  $\vec{c}' = \lambda\vec{c}'$ . That is,  $M$  and  $H$  have eigenvectors with common eigenvalues such as to be interrelated

$$\vec{c} \stackrel{D^{-1/2}}{D^{1/2}} \vec{c}' \quad (7)$$

Next since

$$H = D^{-1/2} A D^{-1/2} \quad (8)$$

one sees that  $H$  is symmetric, whence one can use more standard symmetric-matrix diagonalization routines to obtain the  $\vec{c}$  and associated eigenvalues  $\lambda$ . Then

$$(rwc)_i(i) = \sum_{\lambda} c_{\lambda i} d_{\lambda i}^{-1/2} \lambda^l \sum_{j=1}^N c_{\lambda j} d_{\lambda j}^{-1/2} \quad (9)$$

where the  $c_{\lambda i}$  are components of the normalized eigenvector  $\vec{c}_{\lambda}$  for eigenvalue  $\lambda$ . Again the analogous expressions for equipose walks are already found in the work of Rucker and Rucker<sup>9-14</sup> and see ref 42. For  $(srrw)_i(i)$  a similar expression applies with the  $j$ -sum eliminated and  $j$  set =  $i$ .

Eigen-expansions for random walks (either simple or equipose) are typically especially convenient in asymptotic analysis, e.g., as in refs 33, 43, and 44.

**Laplacian Relations.** The random-walk-based matrices are related to fundamental *Laplacian* matrices. First  $I - H$  (where  $I$  is the identity matrix) is what is sometimes called the *normalized Laplacian* matrix (or even just the Laplacian matrix<sup>45</sup>). But also there is the *combinatorial Laplacian matrix*  $L$  (or oft times termed just the Laplacian matrix<sup>46,47</sup>) which is given as

$$L = D - A = D^{1/2} (I - H) D^{1/2} \quad (10)$$

Thus, the  $H$  matrix can (by way of  $L$ ) also lead<sup>1,49,50</sup> for acyclic structures to the Wiener index  $W$ , it turning out that<sup>51</sup>  $W = \sum_{\lambda \neq 0} 1/\lambda$  with the  $\lambda$  eigenvalues of  $L$ . This index  $\sum_{\lambda \neq 0} 1/\lambda$  extended to cycle-containing structures has been termed<sup>51</sup> the *quasi-Wiener* or *Kirchhof* index and is also obtained via a generalized inverse of  $L$ .

Further yet random walks arise in designating the elements of the resistance distance matrix

$$\Omega_{ij} = 1/(d_i P_{j \rightarrow i}) \quad (11)$$

where  $P_{j \rightarrow i}$  is the probability that a random walk starting from site  $i$  will arrive at  $j$  before returning to  $i$ . This was first

noted by Nash-Williams,<sup>52</sup> but also see, e.g., ref 31. That this  $\Omega_{ij}$  is a (intrinsic) distance function (or metric) on graphs is established in ref 1. Computation of the  $\Omega_{ij}$  is discussed in ref 53. In chemical graph theory this random-walk interpretation of resistance distances has been particularly used by Palacios<sup>54,55</sup> but also by some others.<sup>41,56,57</sup>

In fact, the triple interaction of chemistry, random walks, and electric networks provides new insights and sometimes elegant proofs of facts related to one of these three areas with tools borrowed from another area. Here is an example (see ref 58 for a different approach) for which we need to extend the transition probabilities defined in (12) to a more general situation where the edge  $ij$  may have associated with it a conductance  $C_{ij}$  (or equivalently, a resistance  $r_{ij} = 1/C_{ij}$ ) not necessarily equal to 1; in this general case we define the probability for a random walk to go from vertex  $i$  to a neighbor vertex  $j$  in one step as

$$P_{ij} = C_{ij}/C(i) \quad (12)$$

where  $C(i) = \sum_j C_{ij}$ . In this general case we also need to rewrite eq 11 as

$$P_{j \rightarrow i} = 1/C(i) \Omega_{ij} \quad (13)$$

It should be noted that the effective resistance  $\Omega_{ij}$  has been defined in (11) and (13) in probabilistic terms, but it can be computed by using Ohm's laws in the "electric network". In this context we can prove the following fact: multiplying by the same factor  $r$  the resistance of every "resistor" (i.e., edge) in an "electric network" (i.e., graph) implies that the effective resistance  $\Omega_{ij}$  between any two sites  $i$  and  $j$  of the network is multiplied by the same factor  $r$ . Indeed, we notice that the left-hand side of (13) is purely probabilistic and the right-hand side is purely electric. Think of the transformed network where all resistors have been multiplied by  $r$  and use a hat superscript for the corresponding variables for the transformed network. Then

$$\hat{p}_{vw} = \hat{C}_{vw}/\hat{C}(v) = (1/r)C_{vw}/(1/r)C(v) = p_{vw} \quad (14)$$

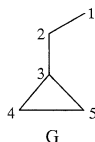
In other words, the probabilistic structure of the transformed network is the same as that of the original network, and thus the left-hand side of (13) is the same for the original and the transformed networks. The right-hand side of (2) for the transformed network is  $1/\hat{\Omega}_{ij}(1/r)C(i)$ , and therefore we must have  $\hat{\Omega}_{ij} = r\Omega_{ij}$ , as claimed.

A further sequence of symmetric simple-random-walk matrices has been defined<sup>41</sup> with the  $l$ th such walk matrix having elements  $w_l(i,j) \equiv (M^l)_{ij} d_j$ , and used in relation to resistance distances. This or  $H^l$  or the nonsymmetric  $M^l$  may be viewed as the random-walk analogue of Dobrynin's<sup>20</sup> path layer matrix for equipose random walks, and in turn this may be used to generate invariants much after the fashion that Dobrynin<sup>20</sup> and Diudea<sup>21</sup> have done for equipose walks.

One such equipose-based matrix  $P$  was introduced by Randić.<sup>22</sup> It has 0 on it diagonal, and otherwise its  $(i,j)$ th element is  $(A^l)_{ij}/(awc)_l(j)$  where  $l$  depending on  $i$  and  $j$  is the shortest-path distance  $d(i,j)$  between  $i$  and  $j$ . That is,  $P_{ij}$  (for  $i \neq j$ ) is the probability for an equipose random walk of *minimal* length  $d(i,j)$  from vertex  $j$  to end at vertex  $i$ . (In fact Randić defined his matrix as the transpose of the present  $P$ , though here we follow the traditional convention in

**Table 1.** Numerical Example

(i) Labeled molecular graph  $G$  representing the carbon skeleton of ethylcyclopropane



(ii) The vertex-adjacency matrix  $A$  and the diagonal matrix  $D$  of  $G$

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad D = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{bmatrix}$$

(iii) The simple-random-walk Markov matrix  $M$  of  $G$

$$M = \begin{bmatrix} 0 & 1/2 & 0 & 0 & 0 \\ 1 & 0 & 1/3 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 1/2 \\ 0 & 0 & 1/3 & 0 & 1/2 \\ 0 & 0 & 1/3 & 1/2 & 0 \end{bmatrix}$$

(iv) The  $H$  matrix of  $G$

$$H = \begin{bmatrix} 0 & 1/\sqrt{2} & 0 & 0 & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{6} & 0 & 0 \\ 0 & 1/\sqrt{6} & 0 & 1/\sqrt{6} & 1/\sqrt{6} \\ 0 & 0 & 1/\sqrt{6} & 0 & 1/\sqrt{4} \\ 0 & 0 & 1/\sqrt{6} & 1/\sqrt{4} & 0 \end{bmatrix}$$

(v) The connectivity index of  $G$

$$\chi = \frac{1}{2} \sum_{i \neq j} (H)_{ij} \cong 2.432$$

(vi) The (normalized Laplacian) matrix  $I - H$  of  $G$

$$I - H = \begin{bmatrix} 1 & -1/\sqrt{2} & 0 & 0 & 0 \\ -1/\sqrt{2} & 1 & -1/\sqrt{6} & 0 & 0 \\ 0 & -1/\sqrt{6} & 1 & -1/\sqrt{6} & -1/\sqrt{6} \\ 0 & 0 & -1/\sqrt{6} & 1 & -1/\sqrt{4} \\ 0 & 0 & -1/\sqrt{6} & -1/\sqrt{4} & 1 \end{bmatrix}$$

(vii) The (combinatorial) Laplacian matrix  $L$  of  $G$

$$L = D^{1/2}(I - H)D^{1/2} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{bmatrix}$$

(viii) The quasi-Wiener number or the Kirchhoff index of  $G$

$$W^* = K = N \sum_{\lambda \neq 0} 1/\lambda = 15$$

dealing with Markov processes.) The simple random-walk analogue  $Q$  then has off-diagonal elements which are probabilities  $(M^{d(i,j)})_{ij}$  for a simple random walk of (minimum) length  $d(i,j)$  from vertex  $j$  to end at vertex  $i$ . Clearly this formulation provides a convenient and efficient way to compute  $Q$ : simply raise  $M$  to successive powers, with the first time that that an element of a power  $M^l$  becomes nonzero identifying the value of the corresponding element of  $Q$ .

#### 4. RANDOM WALKS AND THE CONNECTIVITY INDEX

**Relation to the Connectivity Index.** The connectivity index was introduced by Randić in 1975<sup>3</sup> to distinguish degrees of *branching* and designed so as to correlate to

selected molecular properties. Soon thereafter rather diverse applications in structure–property–activity modeling were made,<sup>26,27</sup> and now is the most used molecular descriptor in the topological-index modeling of molecular properties.<sup>28–30</sup> The connectivity index is defined as

$$\chi = \sum_{i \sim j}^G (d_i d_j)^{-1/2} \quad (15)$$

where the sum is over adjacent pairs of sites (i.e., over edges). Then also the connectivity index  $\chi$  is given as the half-sum of the off-diagonal elements of  $H$ :

$$\chi = \frac{1}{2} \sum_{i \neq j} H_{ij} \quad (16)$$

Evidently the connectivity index is thence interpreted as a sum over *symmetrized* neighbor-hopping probabilities. Another relation of  $\chi$  to resistance distances is given in ref 41.

Further  $\chi$  may be represented in terms of the so-called normalized Laplacian matrix  $I - H \equiv L_{\text{norm}}$

$$\chi = -\frac{1}{2} \sum_{i \neq j} (L_{\text{norm}})_{ij} \quad (17)$$

so that it is also a representative sum of the elements of this important operator. For comparison it may be noted that the half-sum of the off-diagonal elements of the combinatorial Laplacian  $L$  is the number  $e(G)$  of edges of  $G$ , while the sum of the elements of the related  $D^{1/2}HD^{-1/2} = M$  is the number  $N$  of sites of  $G$ , so that the sum of (14) might naturally also be anticipated to be a comparably important invariant.

This then constitutes our effort to uncover underlying physico-mathematical fundamentals on which  $\chi$  is based, so as to indicate its great success in modeling physical, chemical, and biological properties of molecules. A numerical example is elaborated in Table 1.

#### 5. CONCLUSION

It is seen that simple random walks and equipoise random walks are quite distinct. There are analogous relations, which lead to a variety of analogous graph-theoretic quantities (vertex characteristics, vertex codes, edge characteristics, and graph invariants), as here indicated. Further the simple random walks are seen to be intimately related to several earlier graph invariants, including those related to resistance distances, and significantly also to the connectivity index. Yet further uses far outside of chemical graph theory are noted, with the idea that such should prove more widely useful. As such it is suggested that simple-random-walk-based quantities should prove of further use, not yet fully recognized in chemical graph theory.

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