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The transient solution of a local-jump heterogeneous chain of diatomic systems

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Abstract. A stochastic model for the rate of conformational change in freely-jointed chain of two regularly alternating kinds of beads joined by bonds with end effects is considered. Using explicit transformations the exact time-dependent average length of bond vectors are derived as a sum of exponentials involving roots of an underlying polynomial. These roots are calculated explicitly using the properties of tridiagonal determinants, in contrast to numerical methods where computational difficulties are encountered in finding the roots. Steady-state results are deduced.

1. Introduction

The one-step (or generation–recombination or birth-and-death) processes are a special class of Markov processes, which occur in many applications [1–5]. The master equation is an equivalent form of the Chapman–Kolmogorov equation for Markov processes, but it is easier to handle and it has a more direct physical interpretation. The master equation serves to determine the resulting evolution of the system over long time periods. Many of the concepts of stochastic theory are included in the derivation of the master equation [6–10]. It has applications in diverse physical problems such as time-dependent properties of gas-phase relaxation processes [11], chemical kinetics [12], spin relaxation processes [13] and polymer dynamics.

The translational, rotational and deformational motions of chain molecules result from repeated local segmental rearrangements distributed randomly along the chain backbone. A simple stochastic model for chain diffusion deals with a freely-jointed chain molecule consisting of finite beads joined by equal length of bonds [14]. The most elementary version deals with a freely-jointed chain, there being no correlations in the directions of neighbouring links, and the local jump process is of an especially simple and restricted kind. Models have also been treated which provide correlations between nearest-neighbour links, and it is further shown that a certain kind of kinetic bias could also be introduced without altering the nature of the results. An elegant formation has been offered by Iwata [15] who considers more general local conformational rate processes in more realistic chains. After a 'coarse-graining' operation on his basic master equation, he obtains, for sufficiently slow motions, precisely the diffusion equation of the bead-and-spring model. Thus local-jump models that appear on physical grounds are more attractive than beads and springs.

Stockmayer *et al* [16] have outlined the general nature of finite local-jump models and extended the treatment to a broader class of local processes and to chains whose elements do not all need to exhibit equiprobable tendencies to relaxation. They have

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found the exact average bond length for the basic model with the same kind of beads and discussed a freely-jointed chain of two regularly alternating kinds of beads with the structure ... ABABAB .... All bonds have the same length, but the two kinds of beads have jump rates λ and μ alternating between neighbouring bonds. Ignoring the end effects they found the approximate solution to evaluate the time-dependent average length of the bond vectors. It is shown that the slow time-dependent behaviour of a flexible chain molecule is phenomenologically invariant with respect to the fine details of its molecular structure, but that for short times or high frequencies the individual structural features lead to differences in relaxation behaviour.

The mathematical problems of equilibrium statistical mechanics are well defined, because the equations involved are simple, and thus relatively straightforward techniques can be employed. However, it is pertinent to study the time-dependent solution of systems undergoing large-scale changes with time. The purpose of this paper is to obtain the exact time-dependent average length of bond vectors for a finite local-jump model of heterogeneous chain dynamics. The differential-difference equations are converted to a system of difference equations using Laplace transforms. Then the average bond length can be expressed as a rational function by studying the associated matrix equation. Certain interesting transformations and identities of tridiagonal determinants yield the roots of the denominator polynomials of the rational functions. Irrespective of the order of the matrices involved, these roots are calculated analytically in closed form for this model; this is in contrast to the usual numerical methods where computational difficulties are encountered in finding the roots when the matrices become large. Making use of these roots, the solution is obtained by inversion. It is observed that there is a significant difference in the time-dependent solution when the number of bonds between beads are even or odd. Steady-state results are deduced. The exact transient solutions have already been found for an infinite local-jump model in terms of generalized modified Bessel functions [17].

2. Model description

Consider a chain molecule consisting of two regularly alternating kinds of $N+2$ beads, joined by $N+1$ bonds. Label the beads from 0 to $N+1$ and the bonds from 0 to N. Without loss of generality, we assume that initially each bond length is a_i such that $\sum_{i=0}^{N} a_i = 1$. The direction of the bond from bead $(i-1)$ to bead i is described by the unit vector σ_{i-1}. Thus, the configuration of a chain is specified by the set of $N+1$ vectors $\sigma_0, \sigma_1, \ldots, \sigma_N$. To vary the chain conformation, beads are allowed to move one at a time. The motion of bead i consists of a jump or 'flip' whereby the vectors σ_{i-1} and σ_i are changed to new values σ'_{i-1} and σ'_i.

Let the probability density in σ-space that the chain at time t has the conformation $\{\sigma_0, \sigma_1, \ldots, \sigma_N\} \equiv \{\sigma^N\}$ be designated by $p(\sigma^N, t)$. The nature of the treatment, though differing in trivial details, is inspired by and similar to that of Glauber [18] for spin relaxation on a linear Ising lattice. In this model we shall ignore correlations between neighbouring bond vectors, so that the basic jump process for bead i depends only on the state of its two bonds with the adjacent beads. Specifically, the length of a bond at a site either changes to the length of the succeeding bond or changes to the length of the preceeding bond. Let the conditional probability per unit time that a pair of adjacent bond vectors σ_i and σ_{i+1} rotate through an angle ϕ to the new conformation σ'_i and σ'_{i+1} be denoted by $w_i(\sigma_i, \sigma_{i+1}|\sigma'_i, \sigma'_{i+1})$. The time evolution of the conformational probability density then

follows the master equation [18]:

$$\frac{\partial p(\sigma^N,t)}{\partial t} = -\sum_i \iint p(\sigma^N,t) w_i(\sigma_i,\sigma_{i+1}|\sigma_i',\sigma_{i+1}')\,\mathrm{d}\sigma_i'\,\mathrm{d}\sigma_{i+1}'$$
$$+\sum_i \iint \big(p(\sigma_0,\ldots,\sigma_i',\sigma_{i+1}',\ldots,\sigma_N,t)$$
$$\times w_i(\sigma_i',\sigma_{i+1}'|\sigma_i,\sigma_{i+1})\big)\,\mathrm{d}\sigma_i'\,\mathrm{d}\sigma_{i+1}'. \tag{1}$$

This is an expression of the fact that the rate of change of configuration of the bond vectors in time is the difference between the rates of creation and annihilation. Let $q_j(t)$ be the average length of bond j at time t. To extract simple results from the master equation it is convenient to work with the average values of the bond vectors. Our interest is in evaluating these time dependent average length values of the bond vectors, which we arrive at by multiplying the master equation (1) by $\sigma_j(t)$ and integrate over all configuration space, i.e.

$$q_j(t) \equiv \langle \sigma_j(t)\rangle = \int\cdots\int \sigma_j\, p(\sigma^N,t)\,\mathrm{d}\sigma_0\cdots\mathrm{d}\sigma_N. \tag{2}$$

Stockmayer *et al* [16] discussed a freely-jointed chain of two regularly alternating kinds of beads, with the structure ...ABABAB.... The local-jump process is described as a rotation of beads i about an axis passing through beads $i-1$ and $i+1$. These two kinds of beads have alternating jump rates λ and μ, respectively. i.e. the forward and backward jump rates for even labelled beads are respectively λ and μ, and these rates are reversed for odd labelled beads. Ignoring the end effects they have found the approximate solution to evaluate average length of bond vectors. By taking into consideration the end effects, we have found the exact time-dependent average length of bond vectors. Because of the alternating jump rates, the expressions of master equations is different for even numbered bonds and odd numbered bonds. Incorporating our assumptions in equation (1), we obtain

$$q_0'(t) = -\lambda q_0(t) + \lambda q_1(t) \tag{3}$$

$$q_j'(t) = \left\{ \begin{array}{ll} \lambda q_{j-1}(t) - (\lambda+\mu) q_j(t) + \mu q_{j+1}(t) & j \text{ odd} \\ \mu q_{j-1}(t) - (\lambda+\mu) q_j(t) + \lambda q_{j+1}(t) & j \text{ even} \end{array} \right\} \qquad j = 1,2,\ldots,N-1 \tag{4}$$

$$q_N'(t) = \left\{ \begin{array}{ll} \lambda q_{N-1}(t) - \lambda q_N(t) & N \text{ odd} \\ \mu q_{N-1}(t) - \mu q_N(t) & N \text{ even} \end{array} \right. \tag{5}$$

with

$$q_i(0) = a_i \qquad \forall\, i.$$

By setting the derivatives to zero on the left-hand sides of equations (3), (4) and (5), we find that after a very long time the average values of the bond lengths are equal to $1/(N+1)$. We observe that these equilibrium measures are independent of the jump rates and the position of the bond vectors. The transient solutions differ considerably depending on whether N is odd or even. In sections 3 and 4 we derive the time-dependent average length of bond vectors for N odd or even. First we consider the case when there are an even number of bonds, i.e. N is odd. We observe that Laplace transforms are very helpful in changing the differential-difference equations to difference equations, which are easily amenable to analysis.

3. Even number of bonds

Let $\psi_n(s)$ be the Laplace transform of $q_n(t)$. Then from equations (3), (4) and (5) we have

$$\begin{aligned}
&(s+\lambda)\psi_0(s) - \lambda\psi_1(s) = a_0 \\
&-\lambda\psi_{n-1}(s) + (s+\lambda+\mu)\psi_n(s) - \mu\psi_{n+1}(s) = a_n \qquad n = 1, 3, \ldots, N-2 \\
&-\mu\psi_{n-1}(s) + (s+\lambda+\mu)\psi_n(s) - \lambda\psi_{n+1}(s) = a_n \qquad n = 2, 4, \ldots, N-1 \\
&-\lambda\psi_{N-1}(s) + (s+\lambda)\psi_N(s) = a_N.
\end{aligned} \tag{6}$$

This system of equations can be written as

$$A\Psi = [a_0 \ a_1 \ \ldots \ a_N]' \tag{7}$$

where

$$A = \begin{pmatrix}
s+\lambda & -\lambda & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
-\lambda & s+\lambda+\mu & -\mu & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & -\mu & s+\lambda+\mu & -\lambda & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & -\mu & s+\lambda+\mu & -\lambda \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\lambda & s+\lambda
\end{pmatrix}_{N+1}$$

and $\Psi = [\psi_0(s), \ \psi_1(s), \ \ldots \ , \psi_N(s)]'$. Let $D_r(s)$ be the determinant formed by the $r \times r$ square matrix at the top left-hand corner of the matrix A. We define this subdeterminant recursively as follows:

$$\begin{aligned}
&D_0(s) = 1 \\
&D_1(s) = s+\lambda \\
&D_r(s) = \left\{ \begin{array}{ll} (s+\lambda+\mu)D_{r-1}(s) - \lambda^2 D_{r-2}(s) & r \text{ even} \\ (s+\lambda+\mu)D_{r-1}(s) - \mu^2 D_{r-2}(s) & r \text{ odd} \end{array} \right\} \qquad r = 2, 3, \ldots, N.
\end{aligned} \tag{8}$$

Now we obtain the transient solution for the case when N is odd.

Theorem 1. When N is odd, then for $j = 0, 1, \ldots, N$,

$$\begin{aligned}
q_j(t) = \frac{1}{N+1} + \sum_{k=1}^{N} \Bigg\{ &\sum_{i=0}^{j} a_i (\lambda\mu)^{(j-i)/2} C_{ij} \frac{D_i(s_k) D_{N-j}(s_k) \mathrm{e}^{s_k t}}{b_k} \\
&+ \sum_{i=j+1}^{N} a_i (\lambda\mu)^{(i-j)/2} C_{ij}^{-1} \frac{D_j(s_k) D_{N-i}(s_k) \mathrm{e}^{s_k t}}{b_k} \Bigg\}
\end{aligned} \tag{9}$$

where

$$s_1 = -2\lambda$$

$$s_k = \left\{ \begin{array}{ll} -(\lambda+\mu) - \sqrt{(\lambda+\mu)^2 - 4\lambda\mu \sin^2(k\pi/(N+1))} & 2 \leqslant k \leqslant \frac{1}{2}(N+1) \\ -(\lambda+\mu) + \sqrt{(\lambda+\mu)^2 - 4\lambda\mu \sin^2(k\pi/(N+1))} & \frac{1}{2}(N+3) \leqslant k \leqslant N \end{array} \right. \tag{10}$$

$$C_{ij} = \left\{ \begin{array}{ll} \sqrt{\lambda/\mu} & i \text{ even, } j \text{ odd} \\ \sqrt{\mu/\lambda} & i \text{ odd, } j \text{ even} \\ 1 & \text{otherwise} \end{array} \right. \tag{11}$$

and

$$b_k = s_k \prod_{\substack{r=1 \\ r\neq k}}^{N} (s_k - s_r) \qquad 1 \leqslant k \leqslant N. \tag{12}$$

Proof. To analyse Ψ in (7), roots of $|A| = 0$ are to be computed. Certain interesting transformations and idendities of tridiagonal determinants (see the appendix) are used to achieve this. Using identity A1

$$|A| = s \begin{vmatrix} s+2\lambda & -\lambda\mu & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & s+2\mu & -\lambda\mu & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & s+2\lambda & -\lambda\mu & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & s+2\mu & -\lambda\mu \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & s+2\lambda \end{vmatrix}_N .$$

By identity A4

$$|A| = \frac{s}{\phi} \begin{vmatrix} \theta\phi - \lambda\mu & -\lambda\mu & \cdot & \cdot & \cdot & \cdot & \cdot \\ -\lambda\mu & \theta\phi - 2\lambda\mu & -\lambda\mu & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\lambda\mu & \theta\phi - 2\lambda\mu & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -\lambda\mu & \theta\phi - 2\lambda\mu & -\lambda\mu \\ \cdot & \cdot & \cdot & \cdot & \cdot & -\lambda\mu & \theta\phi - \lambda\mu \end{vmatrix}_{(N+1)/2}$$

where $\theta = s + 2\lambda$ and $\phi = s + 2\mu$. Again applying identity A1

$$|A| = s\theta \begin{vmatrix} \theta\phi - 2\lambda\mu & -\lambda\mu & \cdot & \cdot & \cdot & \cdot & \cdot \\ -\lambda\mu & \theta\phi - 2\lambda\mu & -\lambda\mu & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\lambda\mu & \theta\phi - 2\lambda\mu & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -\lambda\mu & \theta\phi - 2\lambda\mu & -\lambda\mu \\ \cdot & \cdot & \cdot & \cdot & \cdot & -\lambda\mu & \theta\phi - 2\lambda\mu \end{vmatrix}_{(N-1)/2} .$$

Using identity A5

$$|A| = s\theta \prod_{k=1}^{(N-1)/2} \left(\theta\phi - 2\lambda\mu - 2\lambda\mu \cos\left(\frac{2k\pi}{N+1} \right) \right).$$

After considerable simplifications, we get

$$\begin{aligned} |A| &= s(s+2\lambda) \prod_{k=1}^{(N-1)/2} \left(s^2 + 2s(\lambda+\mu) + 4\lambda\mu \sin^2\left(\frac{k\pi}{N+1} \right) \right) \\ &= s \prod_{k=1}^{N} (s - s_k) \end{aligned} \tag{13}$$

where the s_k are given by (10). The root $s = 0$ gives the equilibrium solutions. Solving the linear system of equation (7), for $j = 0, 1, \ldots, N$ we obtain

$$\begin{aligned} \psi_j(s) = \frac{1}{|A|} \times \Bigg\{ & \sum_{i=0}^{j} a_i (\lambda\mu)^{(j-i)/2} C_{ij} D_i(s) D_{N-j}(s) \\ & + \sum_{i=j+1}^{N} a_i (\lambda\mu)^{(i-j)/2} C_{ij}^{-1} D_j(s) D_{N-i}(s) \Bigg\} \end{aligned} \tag{14}$$

where C_{ij} and $D_n(s)$ are given by (11) and (8), respectively. Expanding (14) in partial fractions,

$$\psi_j(s) = \frac{q_j}{s} + \sum_{k=1}^{N} \frac{A_{jk}}{(s - s_k)} \qquad j = 0, 1, \ldots, N \tag{15}$$

where the q_j, $j = 0, 1, \ldots, N$, are the equilibrium solutions and the A_{jk} are constants yet to be determined. On inverting (15) we obtain

$$q_j(t) = q_j + \sum_{k=1}^{N} A_{jk} \mathrm{e}^{s_k t} \qquad j = 0, 1, \ldots, N. \tag{16}$$

In order to obtain q_j and A_{jk} we set $s = 0$, $s = s_k$ $(1 \leqslant k \leqslant N)$ and

$$D_n(0) = \left\{ \begin{array}{ll} (\lambda\mu)^{n/2} & n \text{ even} \\ \lambda(\lambda\mu)^{(n-1)/2} & \text{otherwise} \end{array} \right\} \qquad n = 1, 2, \ldots, N \tag{17}$$

in (14) and after considerable algebra, we get

$$q_j = \frac{1}{N+1} \qquad 0 \leqslant j \leqslant N \tag{18}$$

and

$$A_{jk} = \frac{1}{b_k} \left\{ \sum_{i=0}^{j} a_i (\lambda\mu)^{(j-i)/2} C_{ij} \frac{D_i(s_k) D_{N-j}(s_k)}{b_k} + \sum_{i=j+1}^{N} a_i (\lambda\mu)^{(i-j)/2} C_{ij}^{-1} \frac{D_j(s_k) D_{N-i}(s_k)}{b_k} \right\}$$

$$j = 0, 1, \ldots, N \tag{19}$$

where the b_k are given by (12). Hence the theorem follows by substituting equations (18) and (19) in (16). □

Next we obtain the transient solution for the case when there are odd number of bonds, i.e. for N even.

4. Odd number of bonds

Taking the Laplace transform of equations (3), (4) and (5), we obtain

$$\begin{aligned}
&(s + \lambda)\psi_0(s) - \lambda\psi_0(s) = a_0 \\
&-\lambda\psi_{n-1}(s) + (s + \lambda + \mu)\psi_n(s) - \mu\psi_{n+1}(s) = a_n \qquad n = 1, 3, \ldots, N-1 \\
&-\mu\psi_{n-1}(s) + (s + \lambda + \mu)\psi_n(s) - \lambda\psi_{n+1}(s) = a_n \qquad n = 2, 4, \ldots, N-2 \\
&-\mu\psi_{N-1}(s) + (s + \mu)\psi_N(s) = a_N.
\end{aligned} \tag{20}$$

Observe the subtle change between the set of equations (20) and (6). Equations (20) can be written as

$$B\Psi = [a_0 \; a_1 \ldots a_N]' \tag{21}$$

where

$$B = \begin{pmatrix}
s+\lambda & -\lambda & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
-\lambda & s+\lambda+\mu & -\mu & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & -\mu & s+\lambda+\mu & -\lambda & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & -\lambda & s+\lambda+\mu & -\mu \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -\mu & s+\mu
\end{pmatrix}_{N+1}.$$

Let $\Delta_r(s)$ be the determinant formed by the $r \times r$ square matrix at the bottom right-hand corner of the matrix B. We define this subdeterminant recursively as follows:

$$\Delta_0(s) = 1$$

$$\Delta_1(s) = s + \mu$$

$$\Delta_r(s) = \left\{ \begin{array}{ll} (s+\lambda+\mu)\Delta_{r-1}(s) - \mu^2\Delta_{r-2}(s) & r \text{ even} \\ (s+\lambda+\mu)\Delta_{r-1}(s) - \lambda^2\Delta_{r-2}(s) & r \text{ odd} \end{array} \right\} \qquad r = 2, 3, \ldots, N. \tag{22}$$

Now we find the transient solution for the case when N is even.

Theorem 2. When N is even, the transient solution for $j = 0, 1, \ldots, N$ are given by

$$q_j(t) = \frac{1}{N+1} + \sum_{k=1}^{N} \left\{ \sum_{i=0}^{j} a_i C_{ij} \frac{D_i(x_k)\Delta_{N-j}(x_k)\mathrm{e}^{x_k t}}{V_k} + \sum_{i=j+1}^{N} a_i C_{ij}^{-1} \frac{D_j(x_k)\Delta_{N-i}(x_k)\mathrm{e}^{x_k t}}{V_k} \right\} \tag{23}$$

where

$$x_k = \left\{ \begin{array}{ll} -(\lambda+\mu) - \sqrt{(\lambda+\mu)^2 - 4\lambda\mu\sin^2(k\pi/(N+1))} & 1 \leqslant k \leqslant \frac{1}{2}N \\ -(\lambda+\mu) + \sqrt{(\lambda+\mu)^2 - 4\lambda\mu\sin^2(k\pi/(N+1))} & \frac{1}{2}N < k \leqslant N \end{array} \right. \tag{24}$$

and

$$V_k = x_k \prod_{\substack{r=1 \\ r\neq k}}^{N} (x_k - x_r) \qquad 1 \leqslant k \leqslant N. \tag{25}$$

Proof. To analyse Ψ in (21), roots of $|B| = 0$ are to be computed. Using identities A1, A2, A3 and A5, we obtain

$$\begin{aligned} |B| &= s \prod_{k=1}^{N/2} \left(s^2 + 2s(\lambda+\mu) + 4\lambda\mu\sin^2\left(\frac{k\pi}{N+1}\right)\right) \\ &= s\prod_{k=1}^{N}(s - x_k) \end{aligned} \tag{26}$$

where the x_k are given by (24). Now, solving the linear system of equation (21), for $j = 0, 1, \ldots, N$ we obtain

$$\begin{aligned} \psi_j(s) = \frac{1}{|B|} \times \Bigg\{ &\sum_{i=0}^{j} a_i(\lambda\mu)^{(j-i)/2} C_{ij} D_i(s)\Delta_{N-j}(s) \\ &+ \sum_{i=j+1}^{N} a_i(\lambda\mu)^{(i-j)/2} C_{ij}^{-1} D_j(s)\Delta_{N-i}(s) \Bigg\} \end{aligned} \tag{27}$$

where C_{ij} and $D_n(s)$ are given by equations (11) and (8), respectively. Hence the theorem follows, by using

$$\Delta_n(0) = \left\{ \begin{array}{ll} (\lambda\mu)^{n/2} & n \text{ even} \\ \mu(\lambda\mu)^{(n-1)/2} & \text{otherwise} \end{array} \right\} \qquad n = 1, 2, \ldots, N$$

and the arguments used in theorem 1. □

Remark. The transient solution of average length of bonds are symmetric when $\lambda = \mu$, $q_n(t) = q_{N-n}(t)$ for all n and corresponding change in initial bond length of the chain.

5. Conclusion

Time-dependent analysis of master equations plays a vital role in several physical problems. The exact transient solution for the conformational change in a freely jointed chain with different jump rates between alternating kinds of beads is outlined, for the first time. The above solution involves roots, namely the s_k and x_k, which are found analytically in closed form irrespective of the order of the matrices involved. This is in contrast to numerical methods, where computational difficulties are encountered in calculating some values of the parameters, because the diagonal elements of the underlying matrix become large, making the roots large and thus causing overflow while running the program. We observe that there is a significant change in the transient solution when N is odd or even. Also we observe that the steady-state measures are independent of jump rates and the position of the bond vectors.

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Appendix

Here we give some identities of tridiagonal determinants [19] which are useful in finding the time-dependent solution of the model under consideration.

Identity A1.

$$\begin{vmatrix} A+a_0 & a_0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ b_1 & A+a_1+b_1 & a_1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & b_2 & A+a_2+b_2 & a_2 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & b_{n-1} & A+a_{n-1}+b_{n-1} & a_{n-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b_n & A+b_n \end{vmatrix}_{n+1}$$

$$= A \times \begin{vmatrix} g_0 & b_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_1 & g_1 & b_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & a_2 & g_2 & b_3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_{n-2} & g_{n-2} & b_{n-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{n-1} & g_{n-1} \end{vmatrix}_n$$

where $g_j = A + a_j + b_{j+1}$, $j = 0, 1, \ldots, n-1$.

Identity A2.

$$\begin{vmatrix} \theta_1 & d_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & \phi & d_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \theta_2 & d_3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \theta_m & d_{2m-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \phi \end{vmatrix}_{2m}$$

$$= \begin{vmatrix} \gamma_1 & d_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ d_2 & \gamma_2 & d_3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & d_4 & \gamma_3 & d_5 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & d_{2m-4} & \gamma_{m-1} & d_{2m-3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & d_{2m-2} & \gamma_m \end{vmatrix}_m$$

where $\gamma_j = d_{2j-2} + \theta_j\phi + d_{2j-1},\ j = 1, 2, \ldots, m$ with $d_0 = 0$.

Identity A3.

$$\begin{vmatrix} y_0 & a_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_2 & y_1 & a_3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & a_4 & y_2 & a_5 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & a_{n-4} & y_{(n-4)/2} & a_{n-3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & a_{n-2} & y_{(n-2)/2} \end{vmatrix}_{n/2}$$

$$= \begin{vmatrix} x & a_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & x & a_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & x & a_3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & x & a_{n-1} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & x \end{vmatrix}_n$$

where $y_j = x^2 + a_{2j} + a_{2j+1},\ j = 0, 1, \ldots, (n-2)/2$ with $a_0 = 0$.

Identity A4.

$$\begin{vmatrix} \theta_1 & d_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ -1 & \phi & d_2 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -1 & \theta_2 & d_3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \phi & d_{2m-2} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & -1 & \theta_m \end{vmatrix}_{2m-1}$$

$$= \frac{1}{\phi} \begin{vmatrix} \gamma_1 & d_1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ d_2 & \gamma_2 & d_3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & d_4 & \gamma_3 & d_5 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & d_{2m-4} & \gamma_{m-1} & d_{2m-3} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & d_{2m-2} & \gamma_m \end{vmatrix}_m$$

where $\gamma_j = d_{2j-2} + \theta_j\phi + d_{2j-1},\ j = 1, 2, \ldots, m$ with $d_0 = 0$ and $d_{2m-1} = 0$.

Identity A5.

$$\begin{vmatrix} A & a & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ b & A & a & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & b & A & a & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & b & A & a \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & b & A \end{vmatrix}_N = \prod_{j=1}^{N} \left(A - 2\sqrt{ab} \cos\left(\frac{j\pi}{N+1} \right) \right).$$

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