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An invariance property of the repton model

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Abstract

It is required on physical grounds that the eigenvalues of the transition-rate matrix of the Rubinstein–Duke repton model for all values of the spatial wave number q be invariant to the choice of marker repton. This is not immediately obvious from the structure of the transition-rate matrix itself, but we show that these matrices for different choices of marker are related by similarity transformation and therefore have the same eigenvalues.

1. Introduction

Rubinstein introduced a lattice model with which to describe the dynamics of a polymer chain in a medium with a high density of obstructions [1]. The model incorporates and is an expression of de Gennes' reptation mechanism, according to which the motion of the chain results from the diffusion of stored length along the chain's own contour [2]. Rubinstein's picture was then adapted by Duke as a model of the electrophoresis of charged polymers (DNA) in a gel [3]. The model is the object of much current interest [4–8].

In its projected version [1], the model is as pictured in Fig. 1 [3]. It is a chain of N elements ("reptons") connected by $N-1$ bonds. Each element of the chain is permanently confined to its own track running in the x direction, where x is a coordinate that takes only the discrete values $\ldots, -2, -1, 0, 1, 2, \ldots$. The x coordinates of adjacent reptons may differ by only 0 or ± 1, and this is assured by the move rules. Arrows attached to the reptons show the moves they are allowed to make, each such move increasing ($\uparrow$) or decreasing ($\downarrow$) the x coordinate of that repton by 1. The rule is that an interior repton (repton l, $2 \leqslant l \leqslant N-1$) is not allowed to move (so carries no arrow) unless it is the end one of a sequence ("cluster") of two or more consecutive reptons all at the same x; and then it may move only in the direction

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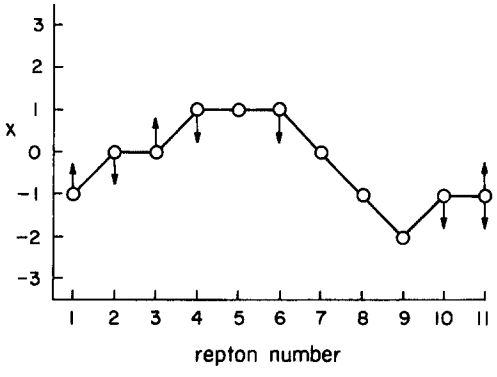

Fig. 1. Typical configuration of a chain of $N = 11$ reptons. Arrows on the reptons indicate allowed moves. The chain drifts and diffuses in the x direction.

of that one of its two neighbors which does not belong to the cluster; i.e., which lies one unit ahead of or behind it in the x direction. An end repton ($l = 1$ or N) that is the end member of a cluster (repton 11 in the example in the figure) is allowed to move either up ($\uparrow$) or down ($\downarrow$) by one unit, while an end repton that is not the end member of a cluster (repton 1 in the figure) may move, but only in the direction to which its neighbor lies ($\uparrow$, in the example in the figure).

With each arrow there is associated a transition rate (transition probability per unit time) proportional to a parameter B if the arrow is $\uparrow$ and B^{-1} if it is $\downarrow$. Here $\ln B$ is proportional to an external field E that acts on each repton as a force in the x-direction: $B = \exp(E/2)$, say, so $B = B^{-1} = 1$ when there is no field. (For simplicity we take B and E dimensionless but the dimensions are easily restored [9].)

A chain of N reptons has 3^{N-1} possible internal configurations, these being the 3^{N-1} distinct sequences of bond variables $j_1, \ldots, j_{N-1}$ where $j_l \equiv x_{l+1} - x_l = 0$ or ± 1. Let $y = 1, \ldots, 3^{N-1}$ index these chain configurations; i.e., these 3^{N-1} different sequences of bond variables. Choose any repton of the chain to be the "marker"; i.e., the one whose x coordinate locates the chain as a whole in the x direction. By specifying simultaneously the coordinate x of the marker repton and the internal configuration y of the chain we fix the coordinate x_l of every repton l and so the exact location of the chain and each of its elements.

The probability $p_{x,y}(t)$ that at time t the chain is at the position and in the internal configuration represented by x, y is given by [9]

$$p_{x,y}(t) = \sum_n \int_{-\pi}^{\pi} c_n(q) f_y^{(n)}(q) \, e^{iqx + \lambda_n(q)t} \, dq \tag{1.1}$$

with

$$c_n(q) = (2\pi)^{-1} \sum_x \sum_y e^{-iqx} g_y^{(n)}(q) \, p_{x,y}(0), \tag{1.2}$$

where $f_y^{(n)}(q)$, $g_y^{(n)}(q)$, and $\lambda_n(q)$ are, respectively, the y components of the nth right and left eigenvectors $\boldsymbol{f}^{(n)}(q)$ and $\boldsymbol{g}^{(n)}(q)$, and the nth eigenvalue, of a $3^{N-1} \times 3^{N-1}$ transition-rate matrix $\boldsymbol{\Lambda}(q)$ to be defined presently; and where the eigenvectors are normalized by

$$\boldsymbol{g}^{(n)}(q) \cdot \boldsymbol{f}^{(n)}(q) = 1 \,. \tag{1.3}$$

The rows and columns of $\boldsymbol{\Lambda}(q)$ are labeled by the configuration index y. If the chain is in configuration y and one of the reptons then moves in the direction of an arrow that is attached to it in that configuration, the chain then finds itself in a new configuration, y'. The off-diagonal element $\Lambda_{y'y}(q)$ of $\boldsymbol{\Lambda}(q)$ is 0 if the two configurations y and y' are not connected by an allowed transition (an allowed move by any repton); B if the transition $y \to y'$ results from an allowed move $\uparrow$ by a repton other than the marker repton and $B\mathrm{e}^{-\mathrm{i}q}$ if from a move $\uparrow$ by the marker; and B^{-1} if the transition $y \to y'$ results from an allowed move $\downarrow$ by a repton other than the marker and $B^{-1}\mathrm{e}^{\mathrm{i}q}$ if from a move $\downarrow$ by the marker. The diagonal element Λ_{yy} is independent of q (and of the choice of marker) and is given by

$$\Lambda_{yy} = -\sum_{y'(\neq y)} \Lambda_{y'y}(0) \,. \tag{1.4}$$

The evolution in time of the locations and configurations of the chains in an ensemble of such chains is determined by the eigenvalues and eigenvectors of $\boldsymbol{\Lambda}(q)$ via Eqs. (1.1)–(1.3). One of the eigenvalues – call it $\lambda_0(q)$ – is 0 at $q = 0$. Then in particular the drift velocity (terminal velocity) and diffusion coefficient of the chains are expressible in terms of the values at $q = 0$ of the first and second derivatives, $\mathrm{d}\lambda_0/\mathrm{d}q$ and $\mathrm{d}^2\lambda_0/\mathrm{d}q^2$, of $\lambda_0(q)$ [9].

The left-hand side of (1.1) is independent of the choice of marker repton because, as remarked above, specifying x and y simultaneously is equivalent to specifying the location x_l of every repton l in the chain. [The x and y in (1.2) are dummy variables, which are summed over.] It must therefore be that the right-hand side of (1.1) is also independent of the choice of marker. This invariance is not immediately obvious from the structure of the right-hand side of (1.1), nor from the structure of the transition-rate matrix $\boldsymbol{\Lambda}(q)$, whose elements $\Lambda_{y'y}$, as seen above, depend on the choice of marker: that choice determines how many and which of the off-diagonal elements are $B\mathrm{e}^{-\mathrm{i}q}$ and $B^{-1}\mathrm{e}^{\mathrm{i}q}$. The invariance of the right-hand side of (1.1) for all t requires, in particular, that the eigenvalues $\lambda_n(q)$ be independent of the choice of marker even though the matrix $\boldsymbol{\Lambda}(q)$ of which they are the eigenvalues is not.

The necessity of that invariance on physical grounds was recognized earlier, and was explicitly verified for short chains (small N), but was not derived in general [9]. Here we demonstrate the invariance of the $\lambda_n(q)$ to the choice of marker by showing that the matrices $\boldsymbol{\Lambda}(q)$ and $\bar{\boldsymbol{\Lambda}}(q)$ for any two different choices are related by a similarity transformation. The structure of the argument for general N will be clear from the special case $N = 3$, which we present in the next section. The argument for general N is in Section 3.

2. $N=3$

There are $3^{N-1} = 9$ possible configurations y of the chain, which we number $y = 1, \ldots, 9$ and show in Fig. 2 [9]. Two essentially different choices of marker repton are possible: either of the two end ones (they are equivalent by symmetry) or the middle one. Let $\Lambda(q)$ be the transition-rate matrix when the left-end repton is chosen as marker and let $\bar{\Lambda}(q)$ be that matrix when the middle repton is the marker. From the prescription given earlier for constructing these matrices, and with the allowed repton moves as indicated by the arrows in Fig. 2, we have

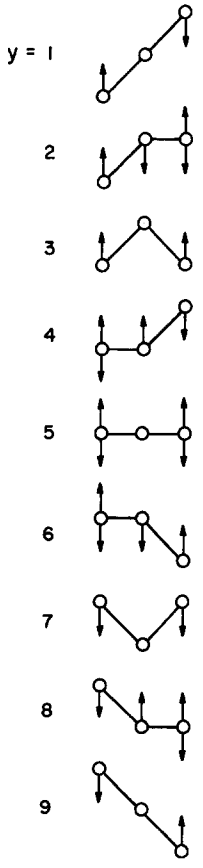

Fig. 2. The nine possible configurations, labeled $y = 1, \ldots, 9$, of a chain of three reptons. Arrows show allowed moves, as in Fig. 1.

$\Lambda(q) =$

$y =$	1	2	3	4	5	6	7	8	9
1	$-(B+B^{-1})$	B	0	$B^{-1}e^{iq}$	0	0	0	0	0
2	B^{-1}	$-2(B+B^{-1})$	B	B	$B^{-1}e^{iq}$	0	0	0	0
3	0	B^{-1}	$-2B$	0	0	$B^{-1}e^{iq}$	0	0	0
4	Be^{-iq}	B^{-1}	0	$-2(B+B^{-1})$	B	0	$B^{-1}e^{iq}$	0	0
5	0	Be^{-iq}	0	B^{-1}	$-2(B+B^{-1})$	B	0	$B^{-1}e^{iq}$	0
6	0	0	Be^{-iq}	0	B^{-1}	$-2(B+B^{-1})$	0	B	$B^{-1}e^{iq}$
7	0	0	0	Be^{-iq}	0	0	$-2B^{-1}$	B	0
8	0	0	0	0	Be^{-iq}	B^{-1}	B^{-1}	$-2(B+B^{-1})$	B
9	0	0	0	0	0	Be^{-iq}	0	B^{-1}	$-(B+B^{-1})$

(2.1)

and

$\bar{\Lambda}(q) =$

$y =$	1	2	3	4	5	6	7	8	9
1	$-(B+B^{-1})$	B	0	B^{-1}	0	0	0	0	0
2	B^{-1}	$-2(B+B^{-1})$	B	Be^{-iq}	B^{-1}	0	0	0	0
3	0	B^{-1}	$-2B$	0	0	B^{-1}	0	0	0
4	B	$B^{-1}e^{iq}$	0	$-2(B+B^{-1})$	B	0	B^{-1}	0	0
5	0	B	0	B^{-1}	$-2(B+B^{-1})$	B	0	B^{-1}	0
6	0	0	B	0	B^{-1}	$-2(B+B^{-1})$	0	Be^{-iq}	B^{-1}
7	0	0	0	B	0	0	$-2B^{-1}$	B	0
8	0	0	0	0	B	$B^{-1}e^{iq}$	B^{-1}	$-2(B+B^{-1})$	B
9	0	0	0	0	0	B	0	B^{-1}	$-(B+B^{-1})$

(2.2)

These are of the form

$$\Lambda(q) = \begin{bmatrix} \boldsymbol{L}_{11} & \boldsymbol{L}_{12} & \boldsymbol{O} \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22} & \boldsymbol{L}_{23} \\ \boldsymbol{O} & \boldsymbol{L}_{32} & \boldsymbol{L}_{33} \end{bmatrix}, \tag{2.3}$$

$$\bar{\Lambda}(q) = \begin{bmatrix} \boldsymbol{L}_{11} & \bar{\boldsymbol{L}}_{12} & \boldsymbol{O} \\ \bar{\boldsymbol{L}}_{21} & \boldsymbol{L}_{22} & \bar{\boldsymbol{L}}_{23} \\ \boldsymbol{O} & \bar{\boldsymbol{L}}_{32} & \boldsymbol{L}_{33} \end{bmatrix}, \tag{2.4}$$

where $\boldsymbol{O}$ and the various $\boldsymbol{L}_{mn}$ and $\bar{\boldsymbol{L}}_{mn}$ are the 3×3 blocks (sub-matrices) outlined in (2.1) and (2.2). The diagonal blocks $\boldsymbol{L}_{11}$, etc. are the same in $\boldsymbol{\Lambda}$ and $\bar{\boldsymbol{\Lambda}}$. The farthest off-diagonal blocks called $\boldsymbol{O}$ are the same in both and consist entirely of zeros. The blocks $\bar{\boldsymbol{L}}_{12}$ and $\bar{\boldsymbol{L}}_{23}$ in $\bar{\boldsymbol{\Lambda}}$ are the scalar multiples e^{-iq} of $\boldsymbol{L}_{12}$ and $\boldsymbol{L}_{23}$, respectively, in $\boldsymbol{\Lambda}$, while $\bar{\boldsymbol{L}}_{21}$ and $\bar{\boldsymbol{L}}_{32}$ in $\bar{\boldsymbol{\Lambda}}$ are the scalar multiples e^{iq} of $\boldsymbol{L}_{21}$ and $\boldsymbol{L}_{32}$ in $\boldsymbol{\Lambda}$. This is the pattern we shall later find for general N.

From the foregoing observations it follows that $\boldsymbol{\Lambda}(q)$ and $\bar{\boldsymbol{\Lambda}}(q)$ in this $N = 3$ case are related by the similarity transformation

$$\boldsymbol{S} \cdot \boldsymbol{\Lambda} = \bar{\boldsymbol{\Lambda}} \cdot \boldsymbol{S}, \tag{2.5}$$

where $\boldsymbol{S}(q)$ is a diagonal matrix with elements $S_{1,1}, \ldots, S_{9,9}$ given by

$$e^{-iq}, e^{-iq}, e^{-iq}, 1, 1, 1, e^{iq}, e^{iq}, e^{iq}. \tag{2.6}$$

Then because of (2.5) the matrices $\boldsymbol{\Lambda}(q)$ and $\bar{\boldsymbol{\Lambda}}(q)$ have the same eigenvalues $\lambda_n(q)$.

3. General N

Here it will be shown that if $\boldsymbol{\Lambda}(q)$ is the transition-rate matrix with repton l chosen as marker, for any $l = 1,2, \ldots, N-1$, and if $\bar{\boldsymbol{\Lambda}}(q)$ is the corresponding matrix with repton $l+1$ as marker, then $\boldsymbol{\Lambda}$ and $\bar{\boldsymbol{\Lambda}}$ are related by a similarity transformation, as in (2.5). It then follows that the corresponding matrices for *any* two choices of marker are so related, and from that, in turn, it follows again that any two such transition-rate matrices have the same eigenvalues.

Let reptons l and $l+1$ be the two alternative choices of marker. Having chosen the value of l, make a list of the 3^{N-1} distinct configurations y of the chain, as is done for $N = 3$ in Fig. 2. We are free to order these as we wish since the eigenvalues of $\boldsymbol{\Lambda}$ and $\bar{\boldsymbol{\Lambda}}$ do not depend on this order. Choose the first 3^{N-2} entries in the list ($y = 1, \ldots, 3^{N-2}$) to be those for which the bond variable j_l has the value $+1$, the next 3^{N-2} entries those for which $j_l = 0$, and the remaining 3^{N-2} entries those for which $j_l = -1$ (as in the $N = 3$ case with the choice $l = 1$, as seen in Fig. 2). The order within each set is arbitrary but, once having been chosen, is fixed.

Next, construct the matrices $\boldsymbol{\Lambda}$ and $\bar{\boldsymbol{\Lambda}}$ according to their definition in Section 1: the first of these with repton l as marker and the second with $l+1$ as marker. Each comprises nine $3^{N-2} \times 3^{N-2}$ blocks corresponding to the division of the configurations $y = 1, \ldots, 3^{N-1}$ into thirds as just described. These generalize (2.1) and (2.2).

Within any one of the three blocks along the main diagonal of either $\boldsymbol{\Lambda}$ or $\bar{\boldsymbol{\Lambda}}$ the bond variable j_l has a fixed value: 1,0 or -1. Therefore the non-zero off-diagonal elements $\Lambda_{y'y}$ and $\bar{\Lambda}_{y'y}$ in those blocks are associated only with transitions $y \to y'$ in which neither repton l nor repton $l+1$ moves, since such a move by either of those reptons necessarily causes j_l to alter its value. According to the rules of construction of the $\boldsymbol{\Lambda}(q)$, then, none of those elements carries a factor e^{iq} or e^{-iq}. But it is only in the number and location of the factors $e^{\pm iq}$ that $\boldsymbol{\Lambda}$ and $\bar{\boldsymbol{\Lambda}}$ differ, so we again conclude that

the three blocks along the main diagonal of $\bar{\Lambda}$ are identical to those in Λ. Similarly, the farthest off-diagonal blocks in both Λ and $\bar{\Lambda}$ consist entirely of zeros, just as in (2.1) and (2.2), because those elements would correspond to transitions $y \to y'$ in which j_l changed from $+1$ to -1 or the reverse, and there is no allowed move by any repton that can change the value of any bond variable by more than one unit. Therefore, as in (2.1) and (2.2), Λ and $\bar{\Lambda}$ differ only in their blocks that lie immediately above and below the main diagonal of blocks. Thus, Λ and $\bar{\Lambda}$ have the same structures as in the special case $N = 3$ in (2.3) and (2.4), but with $\boldsymbol{O}$ and the various $\boldsymbol{L}_{mn}$ and $\bar{\boldsymbol{L}}_{mn}$ now $3^{N-2} \times 3^{N-2}$ sub-matrices.

Where the move rules allow the transition $y \to y'$ the corresponding elements in Λ and $\bar{\Lambda}$ are B, B^{-1}, $B\mathrm{e}^{-iq}$, or $B^{-1}\mathrm{e}^{iq}$; where the move rules do not allow that transition the corresponding elements are 0. The elements of $\boldsymbol{L}_{12}$ and $\bar{\boldsymbol{L}}_{12}$ all correspond to transitions $y \to y'$ in which the bond variable j_l would change from 0 to $+1$. That change requires either that repton l move $\downarrow$ or that repton $l+1$ move $\uparrow$. If $y \to y'$ is an allowed transition in which repton l moves $\downarrow$ the corresponding element $\Lambda_{y'y}$ in $\boldsymbol{L}_{12}$ is $B^{-1}\mathrm{e}^{iq}$ (because l is the marker repton in Λ) while in $\bar{\boldsymbol{L}}_{12}$ it is just B^{-1}; whereas if $y \to y'$ is an allowed transition in which repton $l+1$ moves $\uparrow$ the corresponding element $\Lambda_{y'y}$ in $\boldsymbol{L}_{12}$ is B while in $\bar{\boldsymbol{L}}_{12}$ it is $B\mathrm{e}^{-iq}$ (because $l+1$ is the marker repton in $\bar{\Lambda}$). Thus, each non-zero element of $\bar{\boldsymbol{L}}_{12}$ is e^{-iq} times the corresponding element of $\boldsymbol{L}_{12}$; and since that is also true of the 0 elements, we have

$$\bar{\boldsymbol{L}}_{12} = \mathrm{e}^{-iq}\boldsymbol{L}_{12}\,, \tag{3.1}$$

just as in the $N = 3$ case.

In the allowed transitions that correspond to the non-zero elements in $\boldsymbol{L}_{23}$ and $\bar{\boldsymbol{L}}_{23}$ the bond variable j_l changes from -1 to 0, which again means either that repton l moves $\downarrow$ or that repton $l+1$ moves $\uparrow$. Then, just as with $\boldsymbol{L}_{12}$ and $\bar{\boldsymbol{L}}_{12}$ in (3.1), every element of $\bar{\boldsymbol{L}}_{23}$ is e^{-iq} times the corresponding element of $\boldsymbol{L}_{23}$,

$$\bar{\boldsymbol{L}}_{23} = \mathrm{e}^{-iq}\boldsymbol{L}_{23}\,. \tag{3.2}$$

In the allowed transitions corresponding to $\boldsymbol{L}_{21}$, $\bar{\boldsymbol{L}}_{21}$, $\boldsymbol{L}_{32}$ and $\bar{\boldsymbol{L}}_{32}$ the bond variable j_l decreases by one unit, thus entailing a move $\uparrow$ by repton l or $\downarrow$ by repton $l+1$; so by the same argument that led to (3.1) and (3.2) we have also

$$\bar{\boldsymbol{L}}_{21} = \mathrm{e}^{iq}\boldsymbol{L}_{21} \tag{3.3}$$

and

$$\bar{\boldsymbol{L}}_{32} = \mathrm{e}^{iq}\boldsymbol{L}_{32}\,. \tag{3.4}$$

From (2.3), (2.4), and (3.1)–(3.4), therefore, it follows that Λ and $\bar{\Lambda}$ for general N are still related by the similarity transformation (2.5), where now $\boldsymbol{S}(q)$ is the $3^{N-1} \times 3^{N-1}$ diagonal matrix the first third of whose elements are e^{-iq}, the middle third 1, and the last third e^{iq}, just as in (2.6).

Taken together with the remarks at the beginning of this section, this completes the demonstration that the transition-rate matrices Λ and $\bar{\Lambda}$ for *any* two choices of marker repton are related by similarity transformation.

4. Summary

It is required on physical grounds that the eigenvalues of the q-dependent transition-rate matrix $\Lambda(q)$ of the Rubinstein–Duke model be independent of the choice of marker. That is not immediately obvious from the structure of $\Lambda(q)$ itself, which depends on the choice of marker; but we have shown that the matrices $\Lambda(q)$ and $\bar{\Lambda}(q)$ for any two such choices are related by a similarity transformation and therefore do indeed have the same eigenvalues.

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