



# The eigenpairs of a Sylvester–Kac type matrix associated with a simple model for one-dimensional deposition and evaporation



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## ABSTRACT

A straightforward model for deposition and evaporation on discrete cells of a finite array of any dimension leads to a matrix equation involving a Sylvester–Kac type matrix. The eigenvalues and eigenvectors of the general matrix are determined for an arbitrary number of cells. A variety of models to which this solution may be applied are discussed.

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## 1. Introduction: the physical model

Consider a set of  $n$  cells, arranged on a  $D$ -dimensional lattice. Each cell of the lattice has two states, empty or filled: empty cells are filled at a rate  $\alpha$ ; filled cells are emptied at a rate  $\beta$ . Let  $Q_k$  represent the time-dependent ensemble average probability that  $k$  cells of the lattice are filled. This satisfies a rate equation:

$$\frac{d}{dt} Q_k = -((n-k)\alpha + k\beta)Q_k + (n-k+1)\alpha Q_{k-1} + (k+1)\beta Q_{k+1}. \quad (1.1)$$

This random sequential model is quite general and versatile, and can be customized to describe a variety of two-state physical systems that exhibit adsorption and evaporation processes. One-dimensional sequential adsorption models have been studied thoroughly in different physics contexts [1,2]. Adsorption in two dimensions is not as well understood, however. There are quite a few computational papers [1] on the topic, but few analytical solutions exist for the general two-dimensional case. The adsorption of particles is exactly solvable in higher dimensions only for tree-like lattices. Recently, analytical results have been reported for the random sequential process [3] and reaction–diffusion processes on Cayley trees and Bethe lattices [4–6]. The standard method used to study these systems is the *empty-interval method* [7]. This mathematical method fails when evaporation is considered. We here demonstrate that a matrix theory approach can lead to exact results for a variety of physical systems.

Two specific experimental topics motivate our paper. One is the self-assembly mechanism of charged nanoparticles on a glass substrate [8]. Known in literature as ionic self-assembled monolayers (ISAM), this technique has been used successfully in making antireflective coatings [9,10]. Physical properties of these coatings depend upon the surface coverage of the

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substrate. The deposition process is stochastic, with particles attaching to and detaching from the substrate, so a random sequential adsorption model with evaporation is appropriate.

The second motivating experimental setting involves properties of synthetic polymers called *dendrimers*, which have potential use as a drug delivery mechanism via drug encapsulation [11]. Dendrimers are physical analogs of Cayley tree structures. They are highly branched, spherical polymers that consist of hydrocarbon chains with various functional groups attached to a central core molecule. The precise control that can be exerted over their size, molecular architecture, and chemical properties give dendrimers great potential in the pharmaceutical industry as effective carriers for drug molecules. The attachment and release of the drug molecules is a stochastic process, and so also can be modeled by a general random sequential model as discussed herein.

The random sequential model can also address other kinds of problems as diverse as voting behavior and the spread of epidemics [12]. Epidemic-type models abound in the literature [13,14], from simple ones that capture only the basic rules of the infection mechanism, to complex models that account for spatial spread, age structure and the possibility of immunization. Epidemic models have been applied successfully in other fields including the social sciences (voter models, rumor spreading models) and computer science (computer virus propagation in a network) [15,16].

## 2. Mathematical model

The rate equation (1.1) easily transforms into an equation for the  $(n + 1)$ -dimensional vector  $Q$  with components  $Q_0, Q_1, \dots, Q_n$  as

$$\frac{dQ}{dt} = MQ,$$

in which  $M$  is the tridiagonal square matrix

$$M = \begin{pmatrix} -n\alpha & \beta & & & \\ n\alpha & -(n-1)\alpha - \beta & 2\beta & & \\ & (n-1)\alpha & -(n-2)\alpha - 2\beta & 3\beta & \\ & & (n-2)\alpha & \ddots & \ddots \\ & & & \ddots & \ddots & n\beta \\ & & & & \alpha & -n\beta \end{pmatrix}. \quad (2.1)$$

The general time-dependent solution for  $Q$  is a linear combination of terms of the form  $u_k \exp(\lambda_k t)$  where  $u_k$  is the  $k$ -th eigenvector of  $M$  and  $\lambda_k$  is the corresponding eigenvalue.

There is a long history of interest in and work on the eigenvalue problem for matrices similar to  $M$ . The  $(n + 1) \times (n + 1)$  Sylvester–Kac matrix is a tridiagonal matrix with zero main diagonal, superdiagonal  $(1, 2, \dots, n)$ , and subdiagonal  $(n, \dots, 2, 1)$ , i.e.,

$$\begin{pmatrix} 0 & 1 & & & \\ n & 0 & 2 & & \\ & n-1 & \ddots & \ddots & \\ & & \ddots & \ddots & n-1 \\ & & & 2 & 0 & n \\ & & & & 1 & 0 \end{pmatrix}.$$

This matrix and its characteristic polynomial were first presented by Sylvester in a short communication in 1854 [17]. It was conjectured that its spectrum is  $2k - n$ , for  $k = 0, 1, \dots, n$ . The first proof of Sylvester's determinant formula is attributed by Muir to Francesco Mazza in 1866 [18, p. 442]. Note that there is a typographical error in this discussion, however. The correct version of the formula that appears on page 442 is

$$\begin{vmatrix} \lambda & a_1 & & & \\ a_n & \lambda & a_2 & & \\ & a_{n-1} & \ddots & \ddots & \\ & & \ddots & \ddots & a_n \\ & & & a_1 & \lambda \end{vmatrix} = \begin{vmatrix} \lambda & a_n \\ a_n & \lambda \end{vmatrix} \begin{vmatrix} \lambda & a_1 & & \\ a_{n-2} & \ddots & \ddots & \\ & \ddots & \ddots & a_{n-2} \\ & & a_1 & \lambda \end{vmatrix},$$

where “ $a_1, a_2, \dots, a_n$  are elements increasing by the common difference  $a_1$ ”. In [18, pp. 432–434] Muir discusses another similar matrix, also of interest.

Only many decades after, these matrices and their eigenvalues were subject of study in a foundational paper of Schrödinger [19], but without a proof (see [20,21]). It appears that Mark Kac [22] in 1947 was in fact the first to prove the formula, using the method of generating functions, and to provide a polynomial characterization of the eigenvectors. Results

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