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APPLICATIONS OF TRIDIAGONAL MATRICES IN NON-EQUILIBRIUM STATISTICAL PHYSICS*

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Abstract. One dimensional stochastic problems on a finite lattice that model the time dependence of epidemics, particle deposition and voter influence can easily be cast into a simple form $dV/dt = MV$, where V is a vector with components representing the average occupation of the i-th cell and M is a matrix with coefficients drawn from the equations that give rates of evolution of a particular cell's occupation due to its dependence upon other cells. These matrices are often in tridiagonal form (the only non-zero elements are along the main diagonal and the two diagonal rows to its right), or can be transformed via a unitary transformation into this form. In the tridiagonal form, eigenvalues and eigenvectors can be extracted via straightforward techniques, and the inverse of the matrix of eigenvectors can be inverted (in arbitrary finite dimension) so as to enforce the system's initial conditions. Examples of such models are discussed and related to matrix theory.

Key words. Tridiagonal matrices, Determinants, triangular matrices.

AMS subject classifications. 15A15, 15F10.

1. Introduction.

The study of cooperative evolution of multi-agent systems is a part of many sciences, from epidemic dynamics [9] and social sciences [4] to physics, chemistry and engineering [11]. The methods of statistical physics are often employed, and simple models are the building blocks in this quest to understand complexity. The goal of statistical physics is to predict the behavior of the collective, based on the microscopic interactions of its constituents. This problem is solved for systems in thermal equilibrium using the Boltzmann-Gibbs theoretical framework. However, in nature, most phenomena are not in equilibrium, and to understand their dynamics, other tools must be employed.

Simple non-equilibrium physics models are the forerunners in the race for fundamental understanding of underlying mechanisms that govern complex systems driven far from thermal equilibrium [18]. The key challenge is to create a comprehensive theoretical framework that predicts macroscopic observables from the microscopic dynamics of statistical systems, similar to the Gibbs ensemble theory for equilibrium systems. Despite the simplicity of these models, finding exact solutions can be challenging. Exact solutions are invaluable as they shed light on some general properties of related, more complex, systems [20].

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This paper has two objectives. The first is to introduce the linear algebra community to the field of non-equilibrium statistical physics. The second is to present two classes of non-equilibrium models that can be solved using matrix theory and to point out related unsolved problems involving special matrices.

2. The master equation. One avenue of study in non-equilibrium statistical physics is the so called "kinetic approach". Since there is no equivalent to Gibbs ensemble theory for non-equilibrium systems, macroscopic observables cannot be computed without explicit reference to the imposed dynamics, generally described by the master equation.

The master equation is a balance (continuity) equation which expresses conservation of configurational probabilities. In general, we define $P_r(t)$ as the probability that a system is in state r at time t. The equation governing the time evolution of P_r is:

$$\frac{dP_r}{dt} = \sum_s P_s W_{sr} - \sum_s P_r W_{rs}. \tag{2.1}$$

Showing that the probability of state r increases with time due to all states that evolve into it, and decreases with time due to states into which it evolves. Knowledge of W (transition rates to and from state r) allows one to calculate all probabilities P_r as a function of time.

This equation can be recast in matrix form,

$$\frac{dP}{dt} = MP,$$

In a system with N distinct configurations, P is an N-component column vector with components P_s, and M is an $N \times N$ array known as the transition matrix. The elements of the transition matrix are real, and its dimension large but finite. The master equation can be easily solved numerically for small N, but as the system size increases the direct approach becomes impractical. For example, a system of n spins, each with two possible orientations (up or down), has $N = 2^n$ configurations, so even relatively small spin systems lead to extremely large transition matrices. We present below some particular models for which the master equations can be solved exactly for any finite N, leading to a wealth of information about the physical properties of the system.

3. Cooperative sequential adsorption models and related triangular matrices. From the broad category of lattice gas models [21], we focus on one-dimensional sequential adsorption models. These models have been employed successfully in the field of non-equilibrium statistical physics, for modeling surface deposition, polymer chains dynamics and chemisorption on crystal surfaces [12]. One-dimensional sequential adsorption models have been studied thoroughly in different physics contexts [5]. The two basic one-dimensional models are known in literature as RSA (random sequential adsorption) when

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the adsorption sites are chosen randomly, and CSA (cooperative sequential adsorption) when the adsorption mechanism is influenced by the local environment. Despite the large number of studies of one-dimensional models, deposition in two dimensions is not as well understood. There are quite a few computational studies [5] on the matter, but no exact solutions exist for the general two-dimensional case. Recently, some progress was made for the case of a Cayley tree lattice structure [1].

For this set of sequential adsorption models, a linear string of lattice sites changes as each site switches irreversibly from empty to filled. In particular, we consider CSA (cooperative sequential adsorption) in which filling rates are influenced by the local environment [5]. If the incoming particles each can fill a single site (monomers), the density of filled sites increases with time, and the number of vacancies shrinks at an exponential rate. The problem becomes more complex when the incident particles are dimers [17], for example. In this case, the system evolves to a jammed state with vacancies remaining. This class of models, related to parking-type problems, are not new to the mathematical community [15]. Here, we recast such models into a eigenvalue/eigenvector problem.

Our paper was motivated by the process of manufacturing self-assembled antireflective (AR) coatings using silica and titania nanoparticles. The optical properties of the resulting film can be tuned by the choice of nanoparticles and by the number of bilayers deposited. The index of refraction of the coating depends on the surface coverage of the substrate. During the manufacturing process, it is highly desirable to know the analytical relationship between the index of refraction and the particle density of the jammed state to be able to build coatings with variable and controllable indices of refraction.

CSA models can also be used to address other kinds of problems related to voting behavior and the spread of epidemics. Epidemic-type models abound in the literature [13], [14], from very simple ones that capture the basic rules of the infection mechanism, to very complex models that account for spatial spread, age structure and the possibility of immunization. It is interesting to see how some of these epidemic-type models have been applied successfully in other fields as well, such as social sciences (voter models, rumor spreading models) [4] or computer science (the spread of a virus in a computer network) [16].

3.1. General approach to monomer deposition. We assume N sites, initially empty, on a linear chain. A single entity can attach to an empty site with rates α' when two empty sites are adjacent to site to be filled; β' if only one adjacent site is empty; and γ' when both adjacent sites are filled. Walls at $i = 0$ and $i = N + 1$ are treated as initially filled cells.

We define Q_i to be the probability that, through random deposition of monomers into empty cells, there exists a subchain of i empty cells bounded by filled cells. For example Q_1 decreases each time a particle is deposited in the single empty site (rate $-\gamma' Q_1$); increases

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each time a string of two empties has a deposit in either of the empty sites (rate $2\beta' Q_2$); increases by two each time a string of length three has a deposit into its middle empty spot (rate $2\alpha' Q_1$); and increases each time a string of length four or more has a deposit made into a spot leaving a single empty at either end of the original string (rate $2\alpha' Q_i$, for $i \geq 3$). From the master equation follows the rate equation for Q_i:

$$\frac{dQ_1}{dt} = -\gamma' Q_1 + 2\beta' Q_2 + 2\alpha' \sum_{j=3}^{N} Q_j.$$

At this point and henceforth we will simplify the rate equations by redefining our time scale $t \to \alpha' t$, and defining relative rates $\beta \equiv \beta'/\alpha'$ and $\gamma \equiv \gamma'/\alpha'$. This renders the previous rate equation as

$$\frac{dQ_1}{dt} = -\gamma Q_1 + 2\beta Q_2 + 2 \sum_{j=3}^{N} Q_j.$$

By similar logic, the general form for the rate equation for all Q_k, $k > 1$, is seen to be

$$\frac{dQ_k}{dt} = -(2\beta + (k-2)\alpha) Q_k + 2\beta Q_{k+1} + 2 \sum_{j=k+2}^{N} Q_j.$$

A useful simplification comes from the change of variables:

$$R_j = \sum_{n=j}^{N} (n + 1 - j) Q_n.$$

The R_j represent the probability of finding a substring of j (with $1 < j \leq N$) empties that may have particles or empty cells on either end. Using (3.1) one easily finds its inverse:

$$Q_j = R_j - 2R_{j+1} + R_{j+2}.$$

The rate equations now become (for $k > 1$)

$$\frac{dR_k}{dt} = -(2\beta + k - 2) R_k - (2 - 2\beta) R_{k+1};$$

and

$$\frac{dR_1}{dt} = -\gamma R_1 - 2(\beta - \gamma) R_2 - (1 - 2\beta + \gamma) R_3,$$

in agreement with [18].

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3.2. Matrix solution to rate equations. We now introduce a column vector $\vec{R}$ with components $R_1,\ R_2,\ , R_3,\ \ldots$ and a matrix M so that the rate equations become

$$\frac{d\vec{R}}{dt} = M\vec{R}, \tag{3.1}$$

with

$$M = \begin{bmatrix} -\gamma & -2(\beta-\gamma) & -(1-2\beta+\gamma) & 0 & 0 & 0 & \cdots \\ 0 & -2\beta & -2(1-\beta) & 0 & 0 & 0 & \cdots \\ 0 & 0 & -(2\beta+1) & -2(1-\beta) & 0 & 0 & \cdots \\ 0 & 0 & 0 & -(2\beta+2) & -2(1-\beta) & 0 & \cdots \\ 0 & 0 & 0 & 0 & -(2\beta+3) & -2(1-\beta) & \cdots \\ 0 & 0 & 0 & 0 & 0 & -(2\beta+4) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}.$$

The general solution to this system of equations is

$$\vec{R}(t) = \sum_{j=1}^{N} c_j \vec{V}_j \exp(\lambda_j t), \tag{3.2}$$

where λ_j is the j-th eigenvalue of M, V_j the corresponding eigenvector of M, and the c_j's are to be determined from the initial conditions, which for an initially empty chain are $R_i(t=0) = N+1-i$.

The eigenvalues of a triangular matrix [2] are its diagonal elements, thus $\lambda_j = -\gamma, -2\beta, -2\beta-1, \ldots, -2\beta-N+2$ for $j = 1, 2, 3, \ldots, N$. We denote the k-th element of the j-th eigenvector as $v_{k,j}$. The eigenvectors can be determined to within a constant multiplicative factor from

$$(M - \lambda_j I)V_j \equiv \mathcal{M}_j V_j = 0. \tag{3.3}$$

Note that $\mathcal{M}_j$ is also upper triangular matrix, with a zero in its j-th diagonal slot. Thus, solutions exist for V_j with $v_{k,j} = 0$ for $k > j$. These are the appropriate physical solutions for which long substrings of empty cells are quickly eliminated in the deposition process.

Without loss of generality, we assume $v_{j,j} = 1$. Proceeding along the diagonal of $\mathcal{M}_j$ up and to the left of the zero value is the sequence of values: $1, 2, \ldots, j-2, -\gamma+2\beta+j-2$. The two-term recursion relation for the eigenvalue elements resulting from (3.3) produces

$$v_{k,j} = \begin{cases} 0 & \text{if } k > j \\ \frac{(2(1-\beta))^{j-k}}{(j-k)!} & \text{if } 2 \le k \le j \\ \frac{(2(1-\beta))^{j-3}(4(1-\beta)(\beta-\gamma)-(j-2)(2\beta-\gamma-1))}{(2\beta-\gamma+j-2)(j-2)!} & \text{if } k = 1. \end{cases} \tag{3.4}$$

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Equation (3.2), at $t = 0$ can be cast as

$$\vec{R}(0) = \mathcal{V}\vec{c},$$

where $\mathcal{V}$ is a matrix with elements $v_{i,j}$. The expansion coefficients c_i can be evaluated in terms of $R_i(0)$ through the inverse matrix $\mathcal{V}^{-1}$.

3.3. Inverse of matrix of eigenvalues. From (3.4), it is seen that $\mathcal{V}$ is an invertible upper-triangular matrix. The inverse of an upper-triangular matrix is itself upper-triangular [2]. The inverse of the leading $n \times n$ submatrix of $\mathcal{V}$ is the leading $n \times n$ submatrix of $\mathcal{V}^{-1}$. We can sequentially find values for off-diagonal elements of $\mathcal{V}^{-1}$ utilizing the expressions that follow from the explicit relationship $\mathcal{V}\mathcal{V}^{-1} = I$:

$$\sum_{k=i}^{j} v_{i,k}v_{k,j} = v_{i,j} + \sum_{k=i+1}^{j-1} v_{i,k}v_{k,j} + v_{i,j} = \delta_{i,j} \tag{3.5}$$

noting that $v_{i,i} = v_{j,j} = 1$. We apply (3.5) sequentially to find all off-diagonal elements of $\mathcal{V}^{-1}$: for $j = i + 1$ it yields $v_{i,i+1} = -v_{i,i+1}$; for $j = i + 2, i + 3, \ldots$ we use $v_{i,j}$ values determined in previous applications. This process is an efficient way to numerically determine all elements of the inverse of $\mathcal{V}$ of arbitrarily large finite dimensions.

The determination of the expansion coefficients c_i makes use of the fact that for physical cases of interest, the size of the systems (N) is large but finite, so that for such cases we can approximate the initial state values $R_i(t = 0) = N + 1 - i \approx N$ for $i << N$. This relates the expansion coefficients to row sums of the matrix $\mathcal{V}^{-1}$:

$$c_i = N \sum_{j=i}^{N} v_{i,j}.$$

In our particular case all row sums after the first are identical, we need only evaluate c_1 and c_2. The fact that these row sums converge quickly compared to the size of N makes our approximation of constant values for $R_i(t = 0)$ quite good.

Results obtained by this method are in complete agreement with previously obtained analytical results for this case. In particular, if one assumes the influence on deposition of two filled neighboring cells to be twice that of only one, $\gamma = 2\beta - 1$, the matrix M is purely bidiagonal, with its sequence of diagonal elements to be $-2\beta + 1. - 2\beta, -2\beta + 1, \ldots$ and all off-diagonal elements equal to $2\beta - 2$. Eigenvector elements are easily expressed, as are the values of the inverse of the matrix of eigenvectors. The value of the methodology comes in the more challenging case of deposition of dimers.

3.4. Dimer deposition. Deposition of entities that occupy two neighboring cells, dimers, can be treated with the same formalism. Defining the R_i's as before, their time

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behavior obeys

$$\begin{aligned}
\frac{dR_1}{dt} &= -2\gamma R_2 - 4(\beta-\gamma)R_3 + 2(2\beta-\gamma-1)R_4;\\
\frac{dR_2}{dt} &= -\gamma R_2 - 2(2\beta-\gamma)R_3 + (4\beta-\gamma-3)R_4;\\
\frac{dR_k}{dt} &= (3-2\beta-k)R_k - 2R_{k+1} + (2\beta-2)R_{k+2}. \qquad (3.6)
\end{aligned}$$

Rewriting as before, in a matricial form,

$$\frac{d\vec{R}}{dt} = M_d\vec{R},$$

with

$$M_d = \begin{bmatrix}
0 & -2\gamma & -4(\beta-\gamma) & 2(2\beta-\gamma-1) & 0 & 0 & 0 & \cdots\\
0 & -\gamma & -2(2\beta-\gamma) & 4\beta-\gamma-3 & 0 & 0 & 0 & \cdots\\
0 & 0 & -2\beta & -2 & 2\beta-2 & 0 & 0 & \cdots\\
0 & 0 & 0 & -(2\beta+1) & -2 & 2\beta-2 & 0 & \cdots\\
0 & 0 & 0 & 0 & -(2\beta+2) & -2 & 2\beta-2 & \cdots\\
0 & 0 & 0 & 0 & 0 & -(2\beta+3) & -2 & \cdots\\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots &
\end{bmatrix}.$$

The time behavior of the system is

$$\vec{R}(t) = \sum_{j=1}^{N} d_j\vec{V}_j \exp(\lambda_j t), \qquad (3.7)$$

in terms of eigenvalues λ_j of M_d and its associated eigenvectors $\vec{V}$.

Eigenvalues of this upper triangular matrix are its diagonal elements, all negative and displayed in decreasing order in the diagonal matrix of M_d, from the top to the bottom and from left to right, as long as $2\beta > \gamma$. The zero eigenvalue corresponds to the asymptotic time behavior with some equilibrium number of empty slots of width one. The k-th eigenvector has only its first k elements non-zero, and it is convenient to pick the k-th element to be one. The eigenvector equation for this eigenvector gives recursion relations for remaining nonzero eigenvector components.

The inverse of the upper-triangular matrix of eigenvectors can be evaluated as in the monomer case. Row-sums of the inverse matrix converge quickly, allowing evaluation of expansion coefficients d_i in terms of the initial state characterized by $R_i(0)$.

The agenda for resolution of the dimer deposition problem is thus also set, and straightforward computer code can be written for families of parameter sets worthy of examination.

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4. Multi-temperature kinetic Ising models. In a benchmark paper [8], R. Glauber introduced a stochastic spin system (known in literature as "Glauber model") equivalent to a one-dimensional Ising model. Glauber solved this model exactly, including calculations of the magnetization and the two-point spin correlation functions. Generalizations of this model followed abundantly. The two-temperature kinetic Ising model (KISC) was first introduced by Racz and Zia [19] who calculated exactly the two-point correlation functions for the steady state. Their non-equilibrium model consists of a spin chain in which spins at alternating sites are coupled to thermal baths of two different temperatures.

We present here a more general non-equilibrium Glauber model: a spin chain with every site connected to a different temperature bath. We outline an approach to finding the magnetization dynamics of the model and using matrix theory, in particular tridiagonal matrices. Although particular cases of this model can be solved, the general case remains unsolved, but it is potentially tractable with some additional developments in matrix theory.

The KISC model parallels the one-dimensional Ising model. We treat a lattice of N side-by-side cells, numbered $n = 1, 2, \ldots, N$, with periodic boundary conditions. Each cell has a single degree of freedom with two possible values: -1 ('spin down'); and $+1$ ('spin up'). Each cell interacts with its two nearest neighbors, as well as being in contact with a heat bath with temperature T_n. If at least two of the N temperatures are different, the system cannot achieve equilibrium: each heat bath tries to drive the system towards a different equilibrium state. As a result, energy flows continuously between cells of differing temperatures. Configuration C (a list of the states of the N cells) changes into a configuration C' with generalized Glauber transition rates $\omega\,[C \to C']$. Rate ω is non-zero only if C and C' differ in the spin of a single particle. The rate at which site n has its spin flipped is given by:

$$\omega_n = \frac{1}{2} - \frac{\gamma_n}{4}\sigma_n(\sigma_{n-1} + \sigma_{n+1}), \tag{4.1}$$

where k_B is Boltzmann's constant, the factor γ_n $(0 \leq \gamma_n \leq 1)$ is related to the temperature of cell n by

$$\gamma_n = \tanh(\frac{2}{k_B T_n}) \tag{4.2}$$

and σ_n is the state ($+1$ or -1) of the n-th cell. This rate equation prescribes a spin flip rate for a cell of $1/2$ if cells to the left and right have opposite spins, $(1-\gamma_n)/2$ if adjacent spins are the same and the same as that of cell n, and $(1+\gamma_n)/2$ if adjacent spins are the same and opposite that of cell n. The time scale is arbitrary.

A full description of the state requires knowledge of the time dependence of the probability of each configuration C, namely $P(\sigma_1, \ldots, \sigma_N, t)$. Practically, one seeks the time behavior of certain key macroscopic variables. One such variable is the magnetization, defined as:

$$m_i(t) = \langle \sigma_i(t) \rangle = \sum_{\sigma} \sigma_i P(\sigma_1, \ldots, \sigma_N, t) \tag{4.3}$$

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The equations of motion for the magnetization, derived from the master equation are:

$$\frac{dm_n}{dt} = -m_n + \frac{\gamma_n}{2}(m_{n+1} + m_{n-1}) \tag{4.4}$$

leading, as in Section 3, to a matrix equation with a transition matrix having real non-negative elements:

$$M = \begin{bmatrix} -1 & \frac{\gamma_1}{2} & 0 & \dots & \frac{\gamma_1}{2} \\ \frac{\gamma_2}{2} & -1 & \frac{\gamma_2}{2} & \dots & \\ 0 & \frac{\gamma_3}{2} & -1 & \frac{\gamma_3}{2} & \dots \\ & \vdots & \ddots & & \\ \frac{\gamma_N}{2} & \dots & \dots & \frac{\gamma_N}{2} & -1 \end{bmatrix} \tag{4.5}$$

Using the following transformed magnetization: $m_n \to \frac{m_n}{\sqrt{\gamma_n}}$, matrix M becomes:

$$M_1 = \begin{bmatrix} -1 & \frac{\sqrt{\gamma_1\gamma_2}}{2} & 0 & \dots & \frac{\sqrt{\gamma_1\gamma_N}}{2} \\ \frac{\sqrt{\gamma_1\gamma_2}}{2} & -1 & \frac{\sqrt{\gamma_2\gamma_3}}{2} & \dots & \\ 0 & \frac{\sqrt{\gamma_2\gamma_3}}{2} & -1 & \frac{\sqrt{\gamma_3\gamma_4}}{2} & \dots \\ & \vdots & \ddots & & \\ \frac{\sqrt{\gamma_1\gamma_N}}{2} & \dots & \dots & \frac{\sqrt{\gamma_{N-1}\gamma_N}}{2} & -1 \end{bmatrix} \tag{4.6}$$

This is a periodic Jacobi matrix. For the general case, the eigenvalues and eigenvectors of this matrix are not known. However, for particular temperature distributions, one can extract information regarding the physical properties of the system from the spectrum analysis of matrix M (or M_1).

For example, assume the first half of the spin chain is at infinite temperature ($\gamma = 0$), and the other half at a finite temperature T. In this case, for matrix M, $N/2$ eigenvalues will be equal to -1. The characteristic equation is reduced to

$$\det(M - \lambda I) = (-1 - \lambda)^{N/2} \det(M_2), \tag{4.7}$$

where M_2 is a tridiagonal symmetric Toeplitz matrix [3] with the elements of the main diagonal equal to $-1 - \lambda$ and the off-diagonal elements equal to $\frac{\gamma}{2}$. The eigenvalues are:

$$\lambda_j = -1 + \gamma \cos(\frac{\pi j}{\frac{N}{2} + 1}), \quad (j = 1, \dots, N/2), \tag{4.8}$$

and the eigenvector for λ_j is $x_j = (x_1^{(j)}, \dots, x_{N/2}^{(j)})^T$ with

$$x_k^{(j)} = \sin(\frac{k\pi j}{\frac{N}{2} + 1}), \quad (j = 1, \dots, N/2) \tag{4.9}$$

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Similarly, there are other temperature patterns for the KISC model that transform the M matrix in special k-matrices with known spectrum and known inverse, such as 2-Toeplitz and 3-Toeplitz matrices [3, 6, 7].

Another approach to simplify the problem is to eliminate the corner elements of the general M matrix by fixing one (or more spins). This method can be motivated by much smaller value of the temperature of the fixed spin (a long time of its relaxation) than the temperature (or temperatures) of the rest of the spins. Such an analog of the two-temperature Ising model (of $\gamma_1 = \gamma_2 = \ = \gamma_{N-1} < 1, \gamma_N = 1$) has been studied in [10].

Finally, an interesting equivalence can be made between the two classes of seemingly unrelated models presented in this paper. In general, the KISC model is mapped onto an equivalent reaction-diffusion model (RDS) with spatially alternating pair creation and annihilation rates in the following way. A dual lattice of N sites is established, in which a site in the dual lattice is associated with the boundary between two sites in the KISC lattice. A pair of adjacent KISC spins with opposite signs is identified with a particle in the dual lattice; adjacent spins with the same sign is identified with the absence of a particle (a hole.) A spin flip in the KISC model translates into either diffusion of particles on the dual lattice with equal left-right rates, or pair creation or annihilation with different rates. Transition rates between configurations in the KISC system become diffusion, pair creation and annihilation rates in the RDS system. In particular, similar dynamical equations to the ones presented in Subsection 3.1 govern the dynamics of multi-spin correlators of such a generalized kinetic Ising model. An example physical system of this type is discussed in Section 4 of [10].

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