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Conservation laws in stochastic deposition–evaporation models in one dimension

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Abstract. An infinite number of conservation laws is identified for a stochastic model of deposition and evaporation of trimers on a linear chain. These laws can be encoded into a single nonlocal invariant, the irreducible string, which uniquely lables an exponentially large number of kinetically disconnected sectors of phase space. This enables the number and sizes of sectors to be determined. The effects of conservation laws on some thermodynamic properties are studied.

Keywords. Conservation laws; stochastic processes; deposition-evaporation models; slow kinetics.

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Conservation laws are known to play a very important role in determining the behaviour of systems which evolve by stochastic dynamics. In this paper, we identify and study an infinite number of conservation laws for a recently introduced model of deposition and evaporation of trimers on a lattice [1, 2]. These laws have a number of interesting and useful consequences. They provide a labelling scheme to uniquely identify each of an exponentially large number of dynamically disconnected sectors of phase space; they clarify why steady states differ from the Gibbs state for a simple lattice gas, even though the transition rates satisfy the detailed balance condition for the lattice gas; and they shed light on the time-dependence of correlation functions.

The model is defined as follows. At each site i of a chain of L sites, there is a variable n_i which takes two possible values, say a if the site is occupied, and b if it is empty. The time evolution is Markovian: In a small time dt any three adjacent empty sites become occupied with a probability εdt (trimer deposition). Any three adjacent occupied sites become unoccupied with a probability $\varepsilon' dt$ (trimer evaporation). If three consecutive sites are not all empty, or all full, no deposition or evaporation takes place on those three sites. Note that the model allows for free reconstitution of trimers. If $\varepsilon' = 0$ (irreversible deposition only), the process reduces to the well-studied problem of random sequential adsorption [3, 4]. The higher-dimensional generalizations of this model are also of interest [5], but we restrict ourselves to the one-dimensional case in this paper. For simplicity, we consider open boundary conditions throughout.

It is natural to think of the line as made of three sublattices, A, B and C. If M_A, M_B and M_C are the numbers of occupied sites on each sublattice, it is clear that $(M_A - M_B)$ and $(M_B - M_C)$ are conserved under the stochastic dynamics [1, 2]. These conservation laws imply that the state-space breaks up into many disconnected sectors; evidently, the number of sectors increases at least as fast as L^2 for large L. As a matter of fact, however, the number increases much faster—exponentially with L [1, 2]. The additional conservation laws responsible for this further break up into smaller sectors in this model are not immediately obvious, and form the subject of this paper.

A configuration of the chain is specified by giving an L-bit string composed of letters a and b. We define a *reduction rule* for a string by looking for the occurrence of any triplet aaa or bbb. If any such triplet occurs, it is replaced by the null string ϕ, reducing the length of the string by 3 bits. This reduction procedure is applied repeatedly, until we are left with a string that cannot be further reduced. We call such a string *irreducible*. The irreducible string corresponding to the string S is denoted by $I(S)$. For example, $I(aabaab) = aabaab$, $I(abbbba) = aba$ and $I(abbbaa) = \phi$, the null string. The key observation that allows us to construct an infinite number of conservation laws corresponding to trimer dynamics is the following: If S is the string specifying a configuration of the chain, and S' is another string obtained by a time evolution of S, then $I(S) = I(S')$. This is because the elementary Markovian step of deposition or evaporation does not change I. Also, if two strings S and S' correspond to the same irreducible string, then it can be shown [6] that S can be obtained from S' in a finite number of steps using the rules of trimer dynamics, i.e. $aaa \to bbb$ and $bbb \to aaa$. Thus, treated as a dynamical variable, the irreducible string is a constant of motion and provides a unique label for each invariant subspace of the stochastic dynamical evolution operator.

The number N_L of distinct sectors is thus the number of distinct irreducible strings I obtainable from all possible L-bit strings. First consider strings S containing no triplets aaa or bbb, for which $I(S)$ is also of length L. These configurations are totally jammed, and cannot evolve at all. As shown earlier [1, 2], their number is $2F_L$, where F_L are the Fibonacci numbers defined by $F_1 = 1$, $F_2 = 2$, $F_{k+2} = F_{k+1} + F_k$, for $k \geqslant 1$. Thus F_L increases as μ^L, where μ is the golden ratio $(\sqrt{5}+1)/2 \approx 1{\cdot}618$. Since all possible irreducible strings I obtainable from strings of length L are either of length L or obtainable from strings of length $(L-3)$, the total number of sectors N_L corresponding to length L satisfies the recursion relation $N_L = N_{L-3} + 2F_L$. This has the solution

$$N_L = \sum_{m=0}^{[L/3]} 2F_{L-3m} \tag{1}$$

where $[x]$ is the largest integer less than x. Thus N_L also grows as μ^L for large L, and the ratio N_L/F_L tends to $2(1-\mu^{-3})^{-1} \approx 2{\cdot}618$. As a consequence, the number of unjammed sectors $(N_L - F_L)$ (for which only numerical results were available earlier [1, 2]) grows as μ^L as well.

Next we characterize the sizes of sectors. Let $D(I, L)$ be the size of sector (I, L), i.e. the number of L-site configurations in a sector labelled by the irreducible string I. It is convenient to introduce the generating function

$$g(I, x) = \sum_{L=l}^{\infty} x^L D(I, L) \tag{2}$$

where l is the length of the irreducible string I. First consider the sector Φ, which is comprised of all configurations which are reducible to the null string ϕ. (The all-sites-empty configuration clearly belongs to this sector.) It is useful to define a formal series $G(\phi)$ which is a sum over all distinct strings (of arbitrary length) which are reducible to ϕ. Thus

$$G(\phi) = \phi + aaa + bbb + aaaaaa + abbbaa + aaabbb + \cdots \tag{3}$$

A string S is said to be *indecomposable* if $I(S) = \phi$, and one cannot find strings $t_1, t_2 \neq \phi$ such that $s = t_1 \cdot t_2$ and $I(t_1) = I(t_2) = \phi$. For example, the string *aabbba* is indecomposable while *aaabbb* is decomposable. Then any string S which is reducible to ϕ has a unique decomposition of the form $S = t_1 \cdot t_2 \cdot t_3 \cdots t_r$, where $t_1, t_2, \cdots t_r$ are indecomposable substrings, and the product of strings is understood as the standard concatenation operation. If $G_{\text{in}}(\phi)$ is the sum over all non-null indecomposable substrings reducible to ϕ, equation (3) can be rewritten as

$$G(\phi) = \frac{\phi}{1 - G_{\text{in}}(\phi)} \tag{4}$$

where the right hand side of (4) is defined by its binomial expansion. If $G_a(G_b)$ consists of a sum over all non-null indecomposable strings which reduce to ϕ and start with the letter $a(b)$, then we have $G_{\text{in}}(\phi) = G_a + G_b$ and

$$G_a = a \frac{1}{1 - G_b} a \frac{1}{1 - G_b} a \tag{5a}$$

$$G_b = b \frac{1}{1 - G_a} b \frac{1}{1 - G_a} b. \tag{5b}$$

Equations (4) and (5) determine $G(\phi)$. The generating function $g(\phi, x)$ for sector sizes is obtained from the formal string sum $G(\phi)$ by substituting $\phi \to 1$, $a \to x$, $b \to x$ in the latter and treating the result as an ordinary polynomial. Under these substitutions, both G_a and G_b reduce to the same function $h(x)$, which, in view of (5), satisfies

$$h(1 - h)^2 = x^3. \tag{6}$$

Further, G_{in} reduces to $2h(x)$, so eq. (4) becomes

$$g(\phi, x) = \frac{1}{1 - 2h(x)}. \tag{7}$$

Of the three solutions of the cubic equation (6), the branch on which $h \to 0$ as $x \to 0$ is the physical branch. In view of (2) and (7), the rate of growth of $D(\phi, L)$ with L is governed by the singularities of $h(x)$ closest to the origin in the complex x^3-plane. This occurs when two roots of the cubic equation (6) coincide, i.e. when $h = 1/3$, corresponding to $x_c^3 = (4/27)$. Thus for large L, the size of null sector grows as $L^{-3/2}(27/4)^{L/3}$—an exponentially small fraction of the total number of configurations, 2^L.

Now consider non-null sectors, labelled by a given irreducible string $I = \alpha_1 \alpha_2 \alpha_3 \cdots \alpha_l$, where l is the length of I, and α_i are letters taking values a and b. Analogously to (4) and (5) we have

$$G(I) = \frac{1}{1 - H(\alpha_1)} \alpha_1 \frac{1}{1 - H(\alpha_2)} \alpha_2 \frac{1}{1 - H(\alpha_3)} \alpha_3 \cdots \alpha_l G(\phi) \tag{8}$$

where $H(a) = G_b$ and $H(b) = G_a$. As a result, we find

$$g(I, x) = \left[\frac{x}{1 - h(x)}\right]^l \frac{1}{1 - 2h(x)}. \tag{9}$$

Note that the only dependence of the generating function on the irreducible string I is through l, the length of I. So long as l is finite, $D(L, I)$ increases as $(27/4)^{L/3}$ as $L \to \infty$. If, however, l/L tends to a finite limit λ as $L \to \infty$, then $D(L, I)$ increases as $[\kappa(\lambda)]^L$ where $\kappa(0) = (27/4)^{1/3}$ and $\kappa(1) = 1$. The growth constant $\kappa(\lambda)$ can be determined explicitly for arbitrary λ, and is found to be

$$\kappa(\lambda) = 3[(1 - \lambda)^{1 - \lambda}(2 + \lambda)^{2 + \lambda}]^{-1/3}. \tag{10}$$

For a random string of length L, the corresponding irreducible string has an average length $\lambda_0 L$ where $\lambda_0 = 1 - 3\mu^{-2}/2$.

In random sequential adsorption (which is the $\varepsilon' = 0$ case of our model) it is known that the final state is not described by an equilibrium ensemble of a simple local Hamiltonian, and it is worthwhile to investigate whether this is true also of the dynamical steady state when both deposition and evaporation are allowed. In particular, consider the sector Φ, and let $W(S_1)$ and $W(S_2)$ be the steady state weights of configurations S_1 and S_2, where S_1 is obtained from S_2 by the deposition of a single trimer. Detailed balance then implies $W(S_1)/W(S_2) = \varepsilon/\varepsilon' \equiv z^3$ where z is the single a-particle fugacity. This condition is the same as would hold for a simple lattice gas with no constraint other than single occupancy of sites. The question is then whether thermodynamic properties of our model are the same as the lattice gas. The partition function associated with sector Φ is

$$Z_{L,\Phi} = \sum{}' z^{N_a(S)} \tag{11}$$

where the prime indicates that the sum is over all strings of length L which can be reduced to the null string ϕ, and $N_a(S)$ is the number of a's in S. The transform $\Sigma_L x^L Z_{L,\Phi}(z)$ can be found on making the substitutions $a \to xz$, $b \to x$ in (4) and (5). Then Z is found on inverting the transform, and the mean density n_a of a sites is obtained by differentiating with respect to z. In the low-density limit, the result [6] is $n_a \approx 2^{-1/3} z$. The significant point is that this differs from the answer which would result from the Gibbs state characterized just by fugacity z (as for the lattice gas) for which $n_a \approx z$ in the low density limit. Of course, there is no contradiction; we have demonstrated only that the constraints implied by the conservation laws for trimer dynamics restrict the ensemble to such a small portion of the full phase space that averages over this ensemble differ from those in the canonical ensemble.

It is clear that the construction of the irreducible string for a given configuration is a non-local operation, and three sites well-separated from each other may or may not form a reducible triplet depending on the substrings in between. However, it is possible to reexpress the constant of motion given by the irreducible string in a form which appears more local. To this end, we define two 2×2 complex matrices $A(0, x)$ and $A(1, x)$ depending on a real parameter x by

$$A(n, x) = \begin{pmatrix} \omega & nx \\ \bar{n}x & \omega^* \end{pmatrix}, \quad n = 0, 1 \tag{12}$$

where $\bar{n} = 1 - n$, and ω is a complex cube root of unity. It is easily checked that

$A^3(n,x)=I$, for $n=0,1$, for all x. Now, for any configuration $S=\{n_j\}$ on the linear chain, we associate with site i a 2×2 complex matrix $U_i(x)$ which is specified in terms of $\{n_j\}$ by the equation

$$U_i(x)=\prod_{j=1}^{i} A(n_j,x) \tag{13}$$

where the product is ordered so that larger values of j are to the left. Clearly, we can determine the configuration $\{n_i\}$ uniquely if we are given all the matrices U_i. A stochastic evolution of $\{n_i\}$ corresponds to a stochastic evolution of the $\{U_i\}$. While the definition of $\{U_i\}$ in terms of $\{n_i\}$ is non-local, the stochastic evolution rules for updating U_i are local: If $U_i(x)$ and $U_{i+3}(x)$ are equal, then $U_{i+1}(x)$ and $U_{i+2}(x)$ are changed together in a specified way with some given rate, otherwise not. In addition, $U_L(x)$ remains unchanged by the dynamics. If we define $U_{i=0}(x)$ as the identity matrix, the dynamics is tantamount to the stochastic evolution of a 'string' fixed at both ends, the 'displacement' of the string being the matrix variable U_i.

If we expand $U_L(x)$ in a power series in x

$$U_L(x)=\sum_m u_{L,m}x^m, \tag{14}$$

then the conservation of $U_L(x)$ implies that the coefficients $u_{L,m}$ which are functions of the configuration $\{n_i\}$, are constants of motion. This gives us an infinite number of conservation laws. The first member of this family of conserved quantities is $u_{L,1}$, which is of the form $\begin{pmatrix} 0 & V_1 \\ V_2 & 0 \end{pmatrix}$ where V_1 is a complex number given by

$$V_1=\omega^{L+1}\sum_{j=1}^{L} n_j\omega^j. \tag{15}$$

It is easy to see that the conservation of real and imaginary parts of V_1 corresponds to the conservation of M_A-M_B and M_B-M_C.

To identify a sector completely, we have to specify the function $U_L(x)$ for all x, or equivalently an infinite number of coefficients $u_{L,m}$. Let the value of $U_L(x)$ in two configurations C_1 and C_2 be $u_1(x)$ and $u_2(x)$. Let x^* be any transcendental number. Then $u_1(x^*)=u_2(x^*)$ implies that $u_1(x)=u_2(x)$ for all x (otherwise x^* would be the root of a polynomial equation). Thus, the full family of invariants $U_L(x)$ contains no more information than the single invariant $U_L(x^*)$. Indeed, we have seen that a simple integer invariant—the binary representation of which is the irreducible string—already gives the maximal decomposition of phase space into disjoint sectors. This can be understood in terms of a theorem of von Neumann [7, 8] which states that in quantum mechanics, any number of conservation laws can be encoded into a single conservation law which carries the same information. In our case here, the master equation for the evolution of probabilities is the analogue of the Schrödinger equation in quantum mechanics, and conserved quantities are operators which commute with the evolution operator. The single invariant, the irreducible string, here provides a compact representation which, moreover, is quite useful in a practical, computational sense. It is quite possible that similar invariants may also be constructed in other problems with an infinite number of conservation laws.

The existence of these conservation laws implies a slow decay of time-dependent correlation functions in this model. Let the irreducible string be $I = \alpha_1 \alpha_2 \cdots \alpha_l$. Then a general configuration in this sector is of the form $\xi_1 \alpha_1 \xi_2 \alpha_2 \xi_3 \alpha_3 \cdots \alpha_l \xi_{l+1}$, where ξ_i's are substrings reducible to the null string ϕ. If we treat the ξ strings as background, then the time evolution corresponds to a diffusive motion of α_i's on the line. These 'α-particles' cannot cross each other, and in this sense act like hard-core particles. For diffusion of hard core particles on a line, it is well known that with a finite density of particles, density fluctuations decay as $t^{-1/2}$ while the root-mean-square displacement of any given particle varies as $t^{1/4}$ for large times t due to the caging effects of other particles [9]. We have verified in Monte Carlo simulations that the same behavior is obtained for the diffusion of α_i's in our model in several sectors, for t between 10 and 10,000. We also studied the time dependence of the autocorrelation function of density fluctuations in the steady state, and found interesting variations from one sector to another, from power laws with different powers, to stretched exponentials. Details of this work will appear elsewhere [6].

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