Numerical Method for Accessing the Universality of the Scaling Function for a Multi-Particle Discrete Time Asymmetric Exclusion Process

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Abstract. – In the universality class of the one dimensional Kardar-Parisi-Zhang surface growth, Derrida and Lebowitz conjectured the universality of not only the scaling exponents, but of an entire scaling function. Since Derrida and Lebowitz's original publication [PRL **80** 209 (1998)] this universality has been verified for a variety of continuous time systems in the KPZ universality class. Here, we present a numerical method for directly examining the entire particle flux of the asymmetric exclusion process, thus providing an alternative to more difficult cumulant ratios studies. Using this method, we find that the Derrida-Lebowitz scaling function properly characterises the large system size limit of a single particle discrete time system, even in the case of very small system sizes. This property serves to further increase the ease and accessibility of our method allowing us to directly study even more challenging dynamics and verify the Derrida-Lebowitz scaling function for the multiple particle discrete time asymmetric exclusion process as well.

Introduction. – The Kardar-Parisi-Zhang (KPZ) equation [1] describes a rich variety of processes such as surface growth [2, 3], directed polymers [4–6], and avalanches [7, 8]. And accordingly, the massive array of literature (see [9–11] and references therein), on the topic of KPZ theory reflects the central role the KPZ equation plays in the study of stochastic dynamic processes. The wide variety of dynamic processes governed by the KPZ equation form the so-called KPZ universality class—a class of seemingly unrelated dynamics whose bulk properties obey, on a course-grained level, this one master equation. One member of the KPZ universality class, the well studied one-dimensional asymmetric exclusion process (ASEP) describes a driven lattice gas with hard core exclusions [12], and has also been applied to studies of highway traffic [13,14], protein synthesis [15], and sequence alignment [16–18]. Characterising the underlying properties of the ASEP promises a greater understanding for these specific studies as well as insights into the broader KPZ universality class. Not surprisingly, much effort has been spent calculating some of the many properties of the ASEP such as the density profile, steady states, mass gaps, and diffusion constants [19–28]. Though many questions still remain, these myriad studies have helped to uncover a great deal of insight into the ASEP.

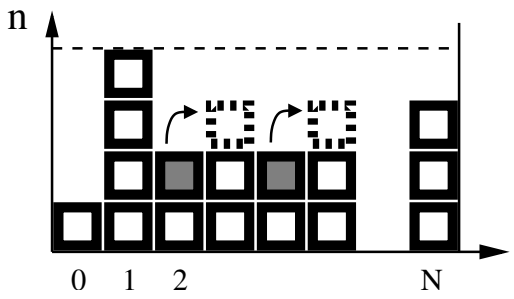

Fig. 1 – Diagram of our discrete time asymmetric exclusion process. The diagram shows an even time where only particles on even sites are considered for hopping. Notice that the particle at site 0 cannot move because site 1 is already at maximum occupancy. However, for sites 2 and 4, the shaded particles can hop to the right with a probability q, as shown by the boxes with dotted outlines.

In their study of the ASEP, Derrida and Lebowitz [29] extended the Bethe Ansatz approach of Gwa and Spohn [23] in order to solve the totally ASEP for particle displacement in the asymptotic limit of large system size [29]. One of the most interesting aspects of their solution involves the scaling function G, describing the non-linear behaviour of the total particle flux. The Derrida-Lebowitz scaling function (DLSF) is independent of any and all of the parameters for the model. Thus, this scaling function was conjectured to be *universal*, i.e., characteristic of all KPZ systems. In a follow-up study, Derrida and Appert analytically continued the Derrida-Lebowitz scaling function (DLSF), successfully completing the solution for all space in the asymptotic limit of large system sizes [30]. Since then, a large number of studies have indeed given strong evidence for the universality of the DLSF. These studies fall into two classes. On the one hand, for a few closely related variants of the totally ASEP [4, 7, 31] the characteristic DLSF behaviour has been analytically verified. All these systems are *continuous* in the time direction. On the other hand, numerical studies have bolstered the universality claim of the DLSF [7, 30–33] for a much broader range of systems including genuinely *discrete* time systems. However, these numerical methods do not directly verify the universality of the DLSF but rather verify the universality of certain cumulant ratios which must be universal if the DLSF is universal [30]. These numerical approaches cannot directly verify the DLSF since they use *sampling* methods that are inherently unable to probe the full DLSF which contains information about *statistically rare* events.

In this work, we *directly* measure the DLSF for a *discrete time* ASEP with multiple particles per site without the use of stochastic sampling. Our results show that the particle hopping under any parameter choice within our discrete time system is characterised by the same DLSF conjectured to be universal for all processes within the KPZ universality class.

Discrete Time Asymmetric Exclusion Process. – In the following, we present our numerical solution of the DLSF for the discrete time totally ASEP using the sublattice-parallel update scheme [13]. In our totally ASEP, we consider a periodically bound system of size N where M particles can only move to the right. During each odd time interval t, the positions with odd numbers are evaluated for transitions. Particles can hop only if available space exists to the right for the particle to move, i.e., only if the site does not already contain the maximum number of allowed particles n. For allowed transitions, particles hop with probability q and stay put with probability $1 - q$. If there is more than one particle on a site only one particle is considered for hopping. For even time intervals, the exact same dynamic occurs

at the even numbered positions. Notice that in order to use this sublattice-parallel update scheme the number of sites N must be even. For this system, we solve via a transfer matrix method described below for the exponential term, λ, of the generating function, Z, of the total particle flux per site, y_t, in the large time limit, $t \to \infty$. Let us first define this generating function as

$$Z_{t,N}(\gamma;\Omega) \equiv \langle \exp[\gamma y_t] \rangle \tag{1}$$

where the brackets $\langle\cdot\rangle$ denote the ensemble average and Ω summarises the specific parameters contributing to the evaluation of the particle flux per site y_t, i.e., q, M, and n. For large times, the generating function behaves like

$$Z_{t,N}(\gamma;\Omega) \sim \exp[\lambda_N(\gamma;\Omega)t] \tag{2}$$

where $\lambda_N(\gamma;\Omega)$ is the largest eigenvalue of the characteristic matrix, $\hat{T}_N(\gamma;\Omega)$, the technical details of whose construction will be provided later. For now, suffice it to say that we can extract the leading eigenvalue $\lambda_N(\gamma;\Omega)$ as

$$\lambda_N(\gamma;\Omega) = \lim_{t\to\infty} \frac{1}{t} \ln Z_{t,N}(\gamma;\Omega). \tag{3}$$

Derrida and Lebowitz [29] solve for the scaling in the limit of small γ and large N at constant $\gamma N^{1/2}$ and filling number $M/(nN)$, obtaining the expression

$$\lambda_N(\gamma;\Omega) - \gamma c_\Omega \simeq \frac{a_\Omega G(\gamma N^{1/2} b_\Omega)}{N^{3/2}} \tag{4}$$

where and a_Ω, b_Ω, and c_Ω are non-universal constants that depend on the parameters of the system other than N, represented by Ω, and G represents the characteristic DLSF [30] conjectured to be universal for KPZ dynamics.

Since we will only be able to numerically evaluate $\lambda_N(\gamma;\Omega)$ for relatively small N we will be faced with the problem of having to deal with γ's that are still too large in spite of the fact that we are interested in the scaling limit of constant $\gamma N^{1/2}$ and $N \to \infty$. Thus, we have to modify Eq. (4) to include higher powers of γ. Toward this end, we introduce the function $\lambda(\gamma;\Omega)$ describing the infinite size behaviour of the $\lambda_N(\gamma;\Omega)$ as

$$\lambda(\gamma;\Omega) = \lim_{N\to\infty} \lambda_N(\gamma;\Omega). \tag{5}$$

The new scaling form then becomes

$$\lambda_N(\gamma;\Omega) - \lambda(\gamma;\Omega) = \frac{a_\Omega G(\gamma N^{1/2} b_\Omega)}{N^{3/2}} + \frac{a_\Omega (\gamma b_\Omega)^3}{24\pi}. \tag{6}$$

In comparing (6) to (4), we note that the linear term on the left hand side of (6) corresponds to the first term of the small γ expansion of $\lambda_N(\gamma;\Omega)$. The additional term on the right hand side of Eq. (6) can either be understood as a γ^3 correction to the left hand side or as a correction to the DLSF G, on the right hand side. This term is necessary since for fixed N and $\gamma \to -\infty$, the left hand side of (6) vanishes by definition while at the same time it is known [30] that

$$G(\beta) \simeq -\frac{\beta^3}{24\pi} = -\frac{(\gamma N^{1/2} b_\Omega)^3}{24\pi} \tag{7}$$

in this limit. We note that the γ^3 term is only term that can be interpreted as both a part of the universal scaling function as well as a part of the infinite size solution $\lambda(\gamma;\Omega)$.

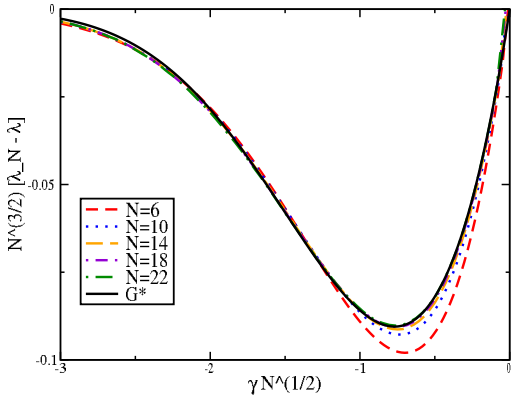

Fig. 2 – The appropriately rescaled and adjusted DLSF (in accordance with the right hand side of Eq. (9)) plotted against the direct measurement of the left hand side of Eq. (9) for $n = 1$, $\rho = M/(nN) = 1/2$ and $q = 3/4$. The left hand side of Eq. (6) has been plotted for $N = 6, 10, 14, 18$, and 22. It becomes difficult to distinguish the values for the larger widths from the adjusted DLSF solved in [30] since they lie in near perfect agreement. This indicates that the proposed universality of the DLSF does hold for this system. The scaling factors a_Ω and b_Ω in Eq. (6), neither of which depends on the finite size effects, are chosen only once for the largest system, $N = 22$, and control the scaling of the adjusted DLSF.

For the specific case in which the allowed number of particles per site equals one, $n = 1$, and the system is half filled, $M = N/2$, there exists an exact analytical solution [16, 17] for $\lambda(\gamma;\Omega)$.

$$\lambda(\gamma;\Omega_{n=1,M=\frac{N}{2}}) = \ln\left(\frac{\sqrt{q}+\exp[-\gamma]}{1+\sqrt{q}\exp[-\gamma]}\right) \tag{8}$$

This, combined with our numerical transfer matrix method for calculating $\lambda_N(\gamma;\Omega)$, allows us to directly measure the left hand side of Eq. (6). Since the DLSF on the right hand side has already been solved, only the scaling coefficients a_Ω and b_Ω are unknown. This allows us to numerically calculate the left hand side of Eq. (6) and use the results to fit a_Ω and b_Ω for one (the largest) system size N. For convenience, here we multiply Eq. (6) by $N^{3/2}$

$$N^{3/2}(\lambda_N(\gamma;\Omega) - \lambda(\gamma;\Omega)) = a_\Omega\left(G(\gamma N^{1/2} b_\Omega) + \tfrac{(\gamma N^{1/2} b_\Omega)^3}{24\pi}\right). \tag{9}$$

and plot the left hand side of Eq. (9) against $\beta \equiv \gamma N^{1/2}$ in Fig. 2 for $N = 6, 10, 14, 18$, and 22. The agreement between the various curves in Fig. 2 gives a good indication that the asymptotic solution for the DLSF indeed applies to our discrete time ASEP.

Discrete Time Multi-Particle Asymmetric Exclusion Process. – In order to further bolster the universality of the DLSF, we also consider an ASEP in which more than one particle is allowed per site. A lattice point with more than one allowed state or highway traffic with more than one lane both provide very good examples of why multiple particle ASEP is important. For $n > 1$, an analytic solution for $\lambda(\gamma;\Omega)$ does not exist. However, we may still test the validity of the DLSF through other means. Since we have a method for obtaining $\lambda_N(\gamma;\Omega)$, we take the difference

$$\lambda_N(\gamma;\Omega) - \lambda_{N-2}(\gamma;\Omega) = \tfrac{a_\Omega G(\gamma N^{1/2} b_\Omega)}{N^{3/2}} - \tfrac{a_\Omega G(\gamma (N-2)^{1/2} b_\Omega)}{(N-2)^{3/2}} \tag{10}$$

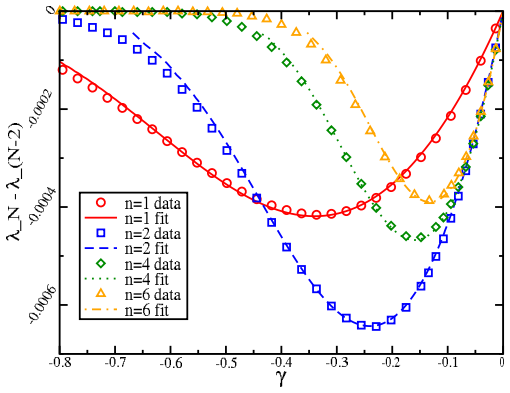

Fig. 3 – Plot of the right hand side of Eq. (10) versus the appropriately fitted left hand side for $q = 3/4$ for various N. This plots shows the excellent agreement between the calculated data and the Derrida *et al.* proposed form of the scaling function under different parameter choices. The total number of particles has been chosen such that $M = Nn/2$, i.e., a half-filled system. For $n = 1$, $N = 22$ was used, for $n = 2$, $N = 14$, for $n = 4$, $N = 10$, and for $n = 6$, $N = 8$.

in order to eliminate the need for the value of $\lambda(\gamma;\Omega)$. Once again, we find the scaling coefficients a_Ω and b_Ω by fitting the right hand side to the left hand side of Eq. (10) for a single N. Fig. 3 shows the right hand side of Eq. (10) for the largest N with the numerically fitted values for a_Ω and b_Ω plotted against the left hand side whose value is obtained using the same transfer matrix method to be described later. While in this approach curves obtained for different N do not overlap each other, we note that we obtain similarly good agreement as in Fig. 3 for small system sizes N *without* refitting the scaling parameters a_Ω and b_Ω (data not shown). This once again results in excellent agreement between our solution for the left hand side and the properly rescaled right hand side for various parameter values Ω including different values for n, q, and N.

Fig. 2 and Fig. 3 each display excellent agreement with established KPZ theory and come without any real adjustment or reformulation of existing theory. They are simply the direct result of studying our multi-particle discrete time ASEP dynamics modelled by a transfer matrix method. In passing, we note that once a_Ω and b_Ω have been determined, their values can be utilised in order to numerically compute the infinite form $\lambda(\gamma;\Omega)$ from $\lambda_N(\gamma;\Omega)$ for even small system sizes by utilising Eq. (6). This fast convergence in N allows for rapid calculation of an entire function $\lambda(\gamma;\Omega)$, an otherwise difficult quantity to compute for most systems. The accessibility of $\lambda(\gamma;\Omega)$ through studies of smaller systems may be put to use in calculating many practical quantities [18].

Brief Description of Matrix Method. – For the remainder of this letter, we shortly describe how we actually calculate $\lambda_N(\gamma;\Omega)$. In our brand of the ASEP, we use a sublattice-parallel updating scheme where hopping probabilities in even and odd time intervals are evaluated separately. Because our discrete time process may be thought of as a combination of a number of very simple process occurring in some sequential order, we may first examine the base dynamic and expand this into the larger picture. Before examining the movement at all positions, we study the dynamics of a single hopping transition. We first create the transfer matrix $T(\gamma = 0;\Omega)$ describing the transition probabilities for one pair of sites [17] using particle occupancy number d as our basis. Next, we modify this matrix by multiplying

all off diagonal elements by the factor $\exp[-\gamma/N]$. This effectively tags the average number of hops per site. For $n = 2$ particles per site this results in the matrix

$$T(\gamma;\Omega_{n=2}) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & q & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & q & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & z & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & z & 0 & q & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & q & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & z & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & z & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{11}$$

in the basis (00, 01, 02, 10, 11, 12, 20, 21, 22) where $z = (1-q)\exp[-\gamma/N]$.

From this smaller transfer matrix, we may build up this single pair description into the larger N-site picture by taking the tensor product $\hat{T}_N(\gamma;\Omega) = \bigotimes_{k=1}^{N/2} T(\gamma;\Omega)$ eliminating any states that do not contain the right number of particles M. This gives us the matrix that models particle hopping from sites in one time interval. Converting this to the appropriate basis for the next time interval can be done by utilising the translation operator C defined such that $C|d_0 d_1 \ldots d_{N-1}\rangle \equiv |d_1 d_2 \ldots d_{N-1} d_0\rangle$. After exploiting translational invariance and up-down mirror symmetry in order to reduce the size of our state space we obtain the additional identity $C = C^{-1}$ on this reduced state space. Then the matrix product $\hat{T}_{even}\hat{T}_{odd} = \hat{T}_N(C^{-1}\hat{T}_N C) = (\hat{T}_N C)^2$ describes the particle hopping of our discrete time ASEP for all N sites. These dynamics can be viewed as a Markov process on a $(n+1)^N$–dimensional state space of the equal time difference vector $|d(0,t), d(1,t), \ldots, d(N,t)\rangle$. Solving for the largest eigenvalue $\eta_N(\gamma;\Omega)$ of $\hat{T}_N C$ gives us the particle hopping function for finite size [16, 17]

$$\lambda_N(\gamma;\Omega) = \ln \eta_N(\gamma;\Omega). \tag{12}$$

This is the function used in order to produce the results given above. Calculating this largest eigenvalue is somewhat challenging, since this matrix description grows very quickly with N. However, the matrices are very sparse with the number of non-zero matrix elements growing almost linearly with the matrix dimension. This makes it possible to numerically obtain the largest eigenvalue required in Eq. (12) using the implicitly restarted Arnoldi method [34] for matrix dimensions up to around 10^5. This allows us to plot the entire function $\lambda_N(\gamma;\Omega)$ in very reasonable timescales.

Conclusion. – In this letter, we have extended the universality of the Derrida-Lebowitz scaling function to inherently discrete time hopping processes with multiple particles per site by directly measuring the scaling function itself. We have presented a numerical method that allows a direct numerical calculation of the DLSF. In contrast to previous numerical studies our method does not rely on sampling but rather on the exact diagonalisation of sparse modified transfer matrices for finite size systems. Thus, it is able to capture the full information on rare events that the DLSF encodes.

The method we have outlined is applicable to a variety of discrete KPZ systems, including the important open boundary ASEP and the open boundary partially ASEP used for modelling true non-equilibrium driven lattice gas dynamics. In addition to this, the interaction of multiple types of particles can be modelled, a property particularly useful to studies of highway traffic. We also found that the numerically determined scaling function converge toward

the universal scaling function already for relatively small finite systems, a point the deserves further investigation.

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