Project and Paper

60% of module mark -

__New deadline Feb 3, 2025, 3pm__

Quality and style of presentation = 50%

Content and understanding = 50%

Submission via Moodle

3 page paper

Style of Physical Review Letters (typeset in LaTeX)

All programming in **Python**

Neural network packages **not allowed**

Code submitted together with the paper

(paper and code go through TurnitIn)

Example in Moodle (from arXiv:2108.11418)

Finite time large deviations via matrix product states

Mari Carmen Bañuls, Luke Causer, and Juan P. Garrahan

Recent work has shown the effectiveness of tensor network methods for computing large deviation functions in constrained stochastic models in the infinite time limit. Here we show that these methods can also be used to study the statistics of dynamical observables at *arbitrary finite time*. This is a harder problem because, in contrast to the infinite time case where only the extremal eigenstate of a tilted Markov generator is relevant, for finite time the whole spectrum plays a role. We show that finite time dynamical partition sums can be computed efficiently and accurately in one dimension using matrix product states, and describe how to use such results to generate rare event trajectories on demand. We apply our methods to the Fredrickson-Andersen (FA) and East kinetically constrained models, and to the symmetric simple exclusion process (SSEP), unveiling dynamical phase diagrams in terms of counting field and trajectory time. We also discuss extensions of this method to higher dimensions.

Introduction.– Large deviation (LD) theory provides a powerful framework to investigate the statistical fluctuations of time-averaged observables in stochastic systems (for reviews, see e.g. Refs. [1–4]). At long times (assuming finite correlation times) the probabilities of such observables obey a LD principle, and the corresponding scaled cumulant generating function (SCGF, see below) can be retrieved from the leading eigenvalue of the *tilted* (or deformed or biased) generator [1]. For large systems, estimating this eigenvalue is difficult, so one resorts to sampling the corresponding biased trajectory ensemble via numerical methods such as trajectory importance sampling [5–8], population dynamics [9–11], optimal control [12–18], or machine learning approaches [19–24]. For lattice models, recent work has focused on the use of tensor network (TN) techniques to approximate the leading eigenvector of the titled generator through variational means [25–27] or power methods [28].

A harder problem is that of computing the statistics of time-averaged observables for *finite time*. The reason is that away from the long time limit the corresponding dynamical partition sums (i.e., moment generating functions) do not obey a LD principle in time - only obeying an LD principle in space for large sizes - and as a consequence they are not determined only by the leading eigenvalue of the tilted generator, but by their whole spectrum. If time is very short, one can get away with direct sampling, but for intermediate times the usual sampling approaches fall short [29]. Here we develop a scheme to study these rare events by implementing well-developed TN techniques to simulate time evolution. This allows us to calculate dynamical partition functions for trajectories of arbitrary time extent. Furthermore, we show how to use the results here to directly simulate stochastic trajectories in finite-time tilted ensembles at small computational cost, thus generalising the method of Ref. [29].

We focus for concreteness on one dimensional kinetically constrained models (KCMs) - often used in the modelling of structural glasses [2, 30–32] - specifically the Fredrickson-Andersen (FA) [33] and the East [34] models, and on the symmetric simple exclusion process (SSEP). Both KCMs and SEPs display phase transitions in their dynamical LDs in the long-time limit [35–41]. With the methods developed here we are able to construct the dynamical phase diagram both as a function of counting field and of trajectory time, determining finite time scaling of active-inactive phase transitions in these models, and uncovering the emergence with time of the correlated structure of the active phase in the East model and the SSEP.

Models.– The three models we consider live in a one dimensional lattice of N sites, with binary variables $n_j = 0, 1$ for each $j = 1 \cdots N$, evolving under continuous-time Markov dynamics with local transitions. The probability for each configuration $|x\rangle = |n_1 \cdots n_N\rangle$ at time t, encoded in a vector $|P(t)\rangle = \sum_x P(t,x)\,|x\rangle$, evolves deterministically via a Master equation, $\partial_t\,|P(t)\rangle = \mathbb{W}\,|P(t)\rangle$, where $\mathbb{W}$ is the Markov generator. Being a stochastic operator $\mathbb{W}$ has a structure $\mathbb{W} = \mathbb{K} - \mathbb{R}$, with an off-diagonal matrix of transition rates $\mathbb{K}$, and a positive diagonal matrix of escape rates $\mathbb{R}$.

For the KCMs the generator reads

$$\mathbb{W}^{\mathrm{KCM}} = \sum_i f_i \big[c\sigma_i^+ + (1-c)\sigma_i^- - c(1-n_i) - (1-c)n_i \big], \qquad (1)$$

where $c \in (0, 1/2]$ defines the site occupation at equilibrium, and $\sigma_i^{\pm}$ are the Pauli raising and lowering operators at site i. Spin flips are only permitted if the kinetic constraint, f_i, is satisfied. We consider two paradigmatic KCMs, the Fredrickson-Andersen (FA) [33] model and the East [34] model. They are defined by the respective constraint functions

$$f_i^{\mathrm{FA}} = n_{i-1} + n_{i+1}, \;\; f_i^{\mathrm{East}} = n_{i-1}. \qquad (2)$$

We consider lattices with open boundary conditions (OBC) to allow for efficient tensor network contractions. For numerical convenience, we choose the fixed boundaries $n_1 = n_N = 1$ for the FA [42] model and $n_1 = 1$ for the East model. The corresponding stationary states are

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Recent work has shown the effectiveness of tensor network methods for computing large deviation functions in constrained stochastic models in the infinite time limit. Here we show that these methods can also be used to study the statistics of dynamical observables at *arbitrary finite time*. This is a harder problem because, in contrast to the infinite time case where only the extremal eigenstate of a tilted Markov generator is relevant, for finite time the whole spectrum plays a role. We show that finite time dynamical partition sums can be computed efficiently and accurately in one dimension using matrix product states, and describe how to use such results to generate rare event trajectories on demand. We apply our methods to the Fredrickson-Andersen (FA) and East kinetically constrained models, and to the symmetric simple exclusion process (SSEP), unveiling dynamical phase diagrams in terms of counting field and trajectory time. We also discuss extensions of this method to higher dimensions.

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product states,

$$|\mathrm{ss}^{\mathrm{FA}}\rangle = |1\rangle \otimes [(1-c)\,|0\rangle + c\,|1\rangle]^{\otimes N-2} \otimes |1\rangle\,, \tag{3}$$

$$|\mathrm{ss}^{\mathrm{East}}\rangle = |1\rangle \otimes [(1-c)\,|0\rangle + c\,|1\rangle]^{\otimes N-1}\,. \tag{4}$$

The third model we consider is the symmetric simple exclusion process (SSEP) whose generator reads

$$\mathbb{W}^{\mathrm{SSEP}} = \frac{1}{2}\sum_i \big[\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+ - (n_i + n_{i+1}) + 2n_in_{i+1}\big] \tag{5}$$

For the SSEP we consider OBC such that particles can come in and out at the boundaries with rate 1/4. The stationary state is $|\mathrm{ss}^{\mathrm{SSEP}}\rangle = 2^{-N}\,|-\rangle = 2^{-N}\sum_x |x\rangle$, with the "flat" state $\langle -|$ being the leading left eigenvector of each generator above.

Dynamical rare events and LDs.– We now consider the ensemble of all possible trajectories $\{\omega_\alpha\}$ with trajectory time t, where $\omega_\alpha = \{x_0 \to x_{t_1} \to \cdots \to x_t\}$ defines

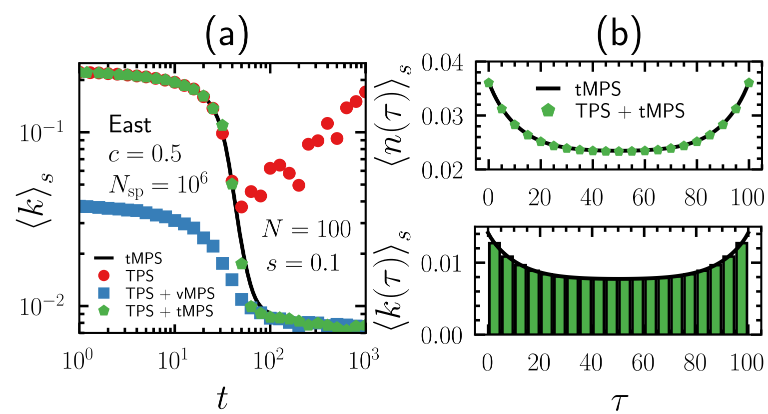

FIG. 1. **Demonstration of the methods.** East model at $c = 0.5$, $N = 100$ and $s = 0.1$. (a) Dynamical activity $\langle k\rangle$ from tMPS (black line), TPS with no auxiliary dynamics (red circles), TPS with the LD eigenvector auxiliary dynamics via vMPS (blue squares), and TPS with a tMPS reference dynamics (green pentagons). (b) Time-dependent occupations (top) and instantaneous activity (bottom) from MPS time-evolution (black line) from direct sampling with a tMPS auxiliary dynamics (green pentagons / bars).

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away from the long time limit. We showed how to directly compute dynamical partition sums, and we derived an efficient sampling scheme for finite-time rare trajectories. A next step would be to extend these ideas to dimensions larger than one. A possibility could be to implement sampling through two dimensional TNs, such as PEPS (e.g. [57, 58]), which have already proven useful in studying the LDs in the long-time limit of two dimensional exclusion processes [28]. While bond dimensions will be limited in this case, using a time evolution scheme like we presented here one could approximate the reference dynamics for the centre of trajectories (i.e. evolve by $e^{t\mathbb{W}_s/2}$) alongside a scheme such as TPS to obtain reliable results. We hope to report on such studies in the near future.

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Project groups

CNeuro MSc

Group A1, Project P1: Johnson, Thomas-Roche, Undelikwo

Group A2, Project P2: Carr, Gunel, Srinivasan

Group A4, Project P4: Broadhurst, Kuntipalo, Su

Group A6, Project P6: Condon, Mathias, Oliver

Group A9, Project P9: Goldsmith, Hardy, Mahmoud

MLiS MSc

Group B1, Project P1: Pan, Xuan, Zhao

Group B2, Project P2: Barrick, Chongsawad, Patil

Group B4, Project P4: Jadhav, Li, Tam

Group B6, Project P6: Liu, Shen, Yan

Group B8, Project P8: Gamston, Rudd, Underdown

Group B9, Project P9: Atkinson, Marshall, Rolfe

Group C1, Project P1: Chandran, Kuatbekov, Lahane

Projects

Unsupervised learning

Project 1: Breast Cancer Tumours

Project 2: Butterfly Species Richness

Supervised learning

Project 4: Classification of Breast Cancer Tumours

Project 6: Changes to Arctic Ice Extent

Reinforcement learning

Project 8: Reinforcement Learning of (stylised) Blackjack

Project 9: Controlling a Drone via Reinforcement Learning

For collaboration we recommend:

Introduction to Git, GitHub and VS Code

Recording of Teams presentation (Jamie Mair)

Source Control Presentation (PDF)

Lecture Recording (Video)