Density-matrix renormalization-group approach to large deviations and dynamical phase transitions

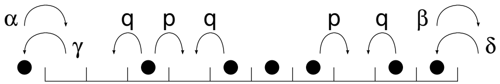
Mieke Gorissen and Carlo Vanderzande

Hasselt University - Belgium

Lyon - 12 June 2012

Current fluctuations in exclusion processes

- The (a)symmetric exclusion process (ASEP) with open boundaries (N sites)



- Densities of reservoirs at the boundary

$$\rho_a = \frac{\alpha}{\alpha + \gamma} \qquad \rho_b = \frac{\delta}{\beta + \delta}$$

- Each realisation of the stochastic process can be characterised by the total number of particles Q_T passing through the system for $T \gg 1$.

Current fluctuations in exclusion processes

- The average and fluctuations of Q_T can be determined from the cumulant generating function

$$\mu(s,L) = \lim_{T\to\infty} \frac{1}{T} \ln\langle e^{sQ_T}\rangle$$

by taking derivatives at $s = 0$.

- Thermodynamics of histories or s-ensemble - Weight histories of the process with e^{sQ_T}
  1. $s = 0$: typical histories
  2. $|s| \gg 1$: histories with a very large current

By tuning s we can study rare events

The symmetric exclusion process

- For the symmetric exclusion process ($p = q = 1/2$) one has [1]

$$\mu(s, L) = \frac{1}{N} M(s) + \frac{1}{8N^2} \mathcal{F}(-4M(s)) + \frac{1-a-b}{N^2} M(s) + \mathcal{O}(N^{-3})$$

1. $M(s)$ is a known analytical function [2]
2. $\mathcal{F}$ is a universal function with a singularity at $\pi^2/2$
3. The third term is non-universal ($a = 1/(\alpha+\gamma),\ b = 1/(\beta+\delta)$)

- The singularity of $\mathcal{F}$ is reached when $M(s) < -\pi^2/8$
- For the SSEP the singularity is never reached - no dynamical phase transition
- No exact results for $q \neq p$ and open boundaries $\rightarrow$ need for a numerical approach that can reach large N-values and gives precise results

[1] A. Imparato, V. Lecomte and F. van Wijland, PRE **80**, 011131 (2009)

[2] B. Derrida, B. Douçot and P.-E. Roche, J. Stat. Phys. **115**, 717 (2004)

DMRG-approach

- Markov evolution $P(C,t)$

$$\partial_t P(C,t) = \sum_{C'} H(C,C')P(C',t)$$

- The generator H of the ASEP can be mapped onto a quantum spin chain (XXZ-model).
- The stationary state corresponds to the ground state of $-H$.
- The stationary state of one-dimensional stochastic many particle systems is a matrix product state (MPS).
- The density matrix renormalisation group (DMRG) (White, 1992) is the most precise numerical technique to determine ground state properties of quantum (spin) chains.
- It corresponds to a variational optimisation over MPS-states (Dukelsky *et al.*, 1998).
- First applications of DMRG to stochastic problems: Hieida (1998), Carlon *et al.* (1999).

DMRG-approach

- Cumulant generating function

$$\boxed{\mu(s,N) = \lambda(s,N)}$$

where $\lambda(s,N)$ is the largest eigenvalue of a generalised generator

$$H_s(C,C') = H(C,C')e^{s\alpha(C,C')} \qquad C \neq C'$$

and $\alpha(C,C') = +1(-1)$ if a particle leaves (enters) the system on the right when $C' \to C$.

- Expectation values like the density ρ_i at site i

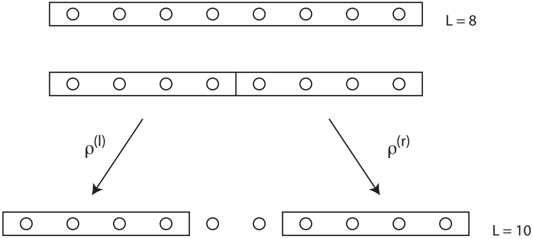
$$\boxed{\rho_i(s,N) = \langle L_0|\hat{n}_i|R_0\rangle}$$

with $\langle L_0|$ and $|R_0\rangle$ the left and right eigenvector associated to the largest eigenvalue of H_s

- First application of DMRG to current/activity fluctuation: M. Gorissen, J. Hooyberghs and C.V., PRE **79**, 020101 (2009).

DMRG-approach

- Problem Dimension of vector space $= 2^N$ - puts a limit to system size that can be studied by exact diagonalisation
- DMRG technique
  1. RG-idea: eliminate variables $\rightarrow$ "choose" m $(< 2^N)$ vectors and project H (Hamiltonian, generator) in space spanned by these vectors
  2. How to choose these m vectors : use the density-matrix



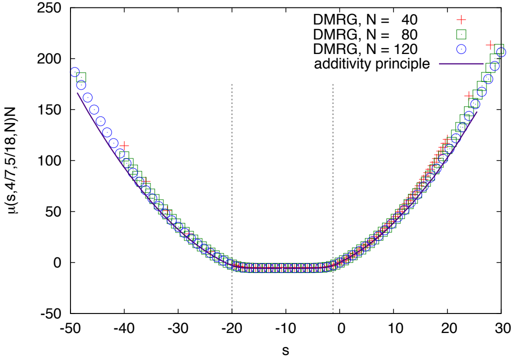
DMRG-algorithm

1. Take a system with N even, "Hamiltonian" H_N: calculate ground state $|\psi_0\rangle$ - density matrix $\rho = |\psi_0\rangle\langle\psi_0|$
   For stochastic systems: symmetric combination of projection on left and right eigenvectors
2. Construct left and right reduced density matrices
   $$\rho^{(l)} = \text{Tr}'_r\ \rho \qquad\qquad \rho^{(r)} = \text{Tr}'_l\ \rho$$
3. Take the m eigenvectors of $\rho^{(l)}$ ($\rho^{(r)}$) with largest eigenvalue: $|\varphi^l\rangle_1, \ldots, |\varphi^l\rangle_m$ $\;(|\varphi^r\rangle_1, \ldots, |\varphi^r\rangle_m)$
4. Add two extra sites i and $i+1$ in the middle of the system: project H_{N+2} in the space spanned by $\{|\varphi^l\rangle_1, \ldots, |\varphi^l\rangle_m, |\pm\rangle_{N/2+1}, |\pm\rangle_{N/2+2}, |\varphi^r\rangle_1, \ldots, |\varphi^r\rangle_m\}$

   Reduction of "number of degrees of freedom" : $2^{N+2} \rightarrow 4m^2$

Results I : The weakly asymmetric exclusion process

- $p = 1/2 + \nu/(2N)$, $q = 1/2 - \nu/(2N)$ $(\nu > 0)$: diffusive model
- We determined $M(s)$ using the additivity principle [3]
- Comparison with DMRG results for N up to 120.

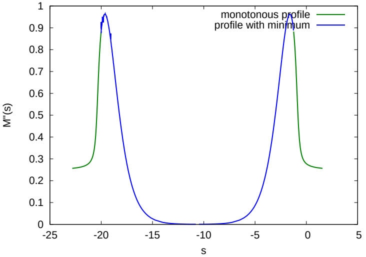


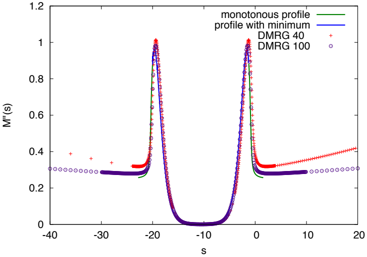
$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18$$

[3] Bodineau and Derrida, PRL **92** 180601 (2004)

Results I : The weakly asymmetric exclusion process

- Is there a dynamical transition?

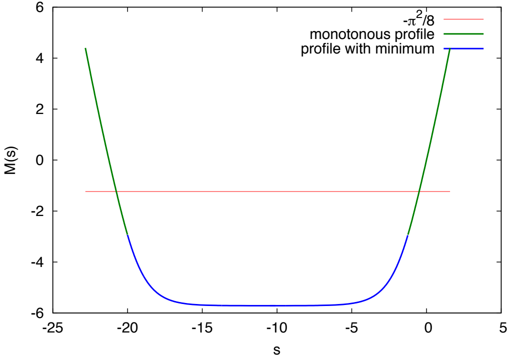




$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18$$

- No dynamical transition for parameter values investigated.

- Is the universal function $\mathcal{F}$ appearing in this diffusive model ?

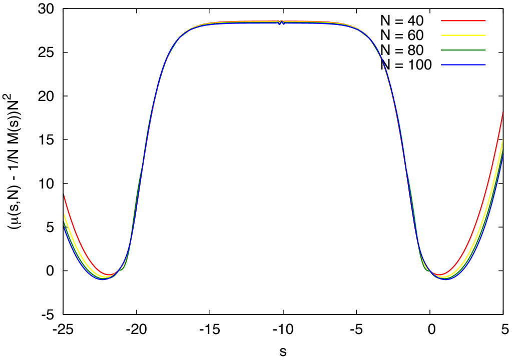


$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18$$

- Finite size corrections are not described by the universal function $\mathcal{F}$.

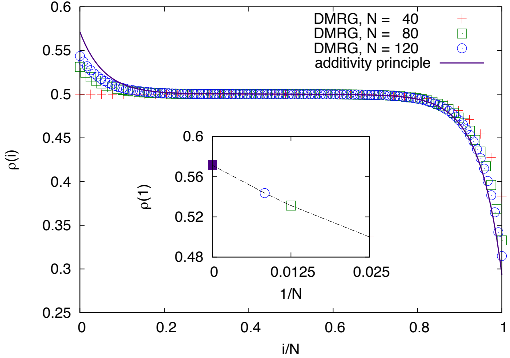
- Corrections are $1/N^2$ as can be expected for a diffusive model

$$\mu(s,N) = \frac{1}{N}M(s) + \frac{1}{N^2}\mathcal{H}(s) + \mathcal{O}(N^{-3})$$



$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18$$

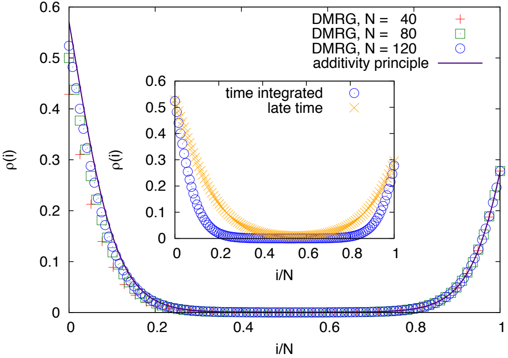
Density profile corresponding to a large current



$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18, j = 5.1214..., s = 10$$

(typical current: $j^\star = 2.5845...$)

Density profile corresponding to a small current



$$\nu = 10, \rho_a = 4/7, \rho_b = 5/18, j = 0.00041..., s = -10$$

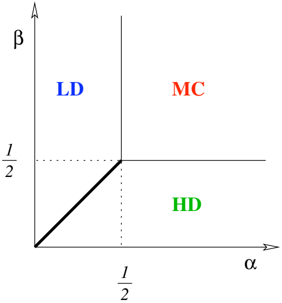
Reference: M. Gorissen and C.V., arxiv.org/abs/1201.6264

Results II: The totally asymmetric exclusion process

- For the TASEP $(p = 1, q = 0)$ numerical results indicate [4]

$$\mu(s, N) = \frac{s}{4} + \frac{1}{N^{3/2}} \mathcal{G}(sN^{1/2}, \Delta\alpha N^{1/2})$$

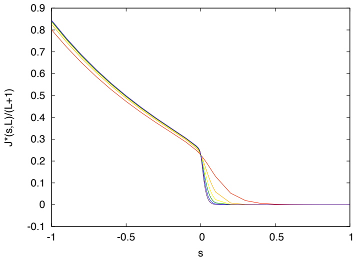
with $\Delta\alpha = \alpha - 1/2$, the distance to the low-density/maximal current phase transition.



[4] M. Gorissen and C.V., J. Phys. A, **44**, 115005 (2011)

Results II: The totally asymmetric exclusion process

- The current shows a dynamical phase transition

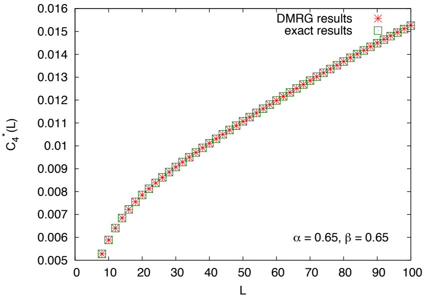


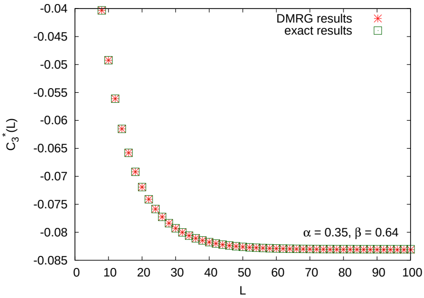
- From the scaling form for $\mu(s,N)$ one finds that the k-th cumulant of the current in the MC-phase scales as

$$\langle Q_T^k \rangle_c \sim N^{k/2-3/2}$$

- Lazarescu and Mallick (J. Phys. A, **44**, 315001 (2011)) have conjectured a parametric representation of the current cumulant generating function for the TASEP.
- Check with DMRG through numerical differentiation of $\mu(s,N)$

Results II: The totally asymmetric exclusion process





Conclusions

- The DMRG is a precise numerical tool that can be used to calculate cumulant generating functions, density profiles, gaps, ... for one-dimensional non-equilibrium models with discrete variables.
- Allows to formulate/verify finite size scaling theories
- Use of tDMRG to investigate time-dependent behavior?