Generalised Ensembles for Full Counting Statistics in Open Quantum Systems

Robert Turner
University of Nottingham

Collaborators:
J.P. Garrahan and A.A. Budini

Overview

- Full Counting Statistics
  - Use in studying 'dynamical' phases, so-called “thermodynamics of trajectories”
  - S-ensemble
- Generalised Ensembles
  - 'X-ensemble'
- Numerical Simulation
  - Reconstruct ensembles using Transition Path Sampling

Full Counting Statistics - S-ensemble

- Time record of some event, K – e.g. photon emissions from an atomic source
- Probability of observing K events:

$$P_t(K) = Tr\left[\rho^{(K)}(t)\right]$$

which, for large times, has a Large Deviation (LD) form:

$$P_t(K) \approx e^{-t\varphi(K/t)}$$

- Can obtain the moment generating function:

$$Z_t(s) \equiv \sum_{K=0}^{\infty} P_t(K) e^{-sK} \approx e^{t\theta(s)}$$

- θ and φ related by a Legendre transform:

$$\theta(s) = -min_{K/t}\left[\varphi(K/t) + sK/t\right]$$

J.P Garrahan and I. Lesonovsky, Phys. Rev. Lett. **104**, 160601 (2010)

P. Zoller, M. Marte, and D. F. Walls, Phys. Rev. A **35**, 198 (1987)

Full Counting Statistics - S-ensemble

- Open quantum systems described by a Lindblad master equation
  - Can extract θ(s) directly from its largest eigenvalue:

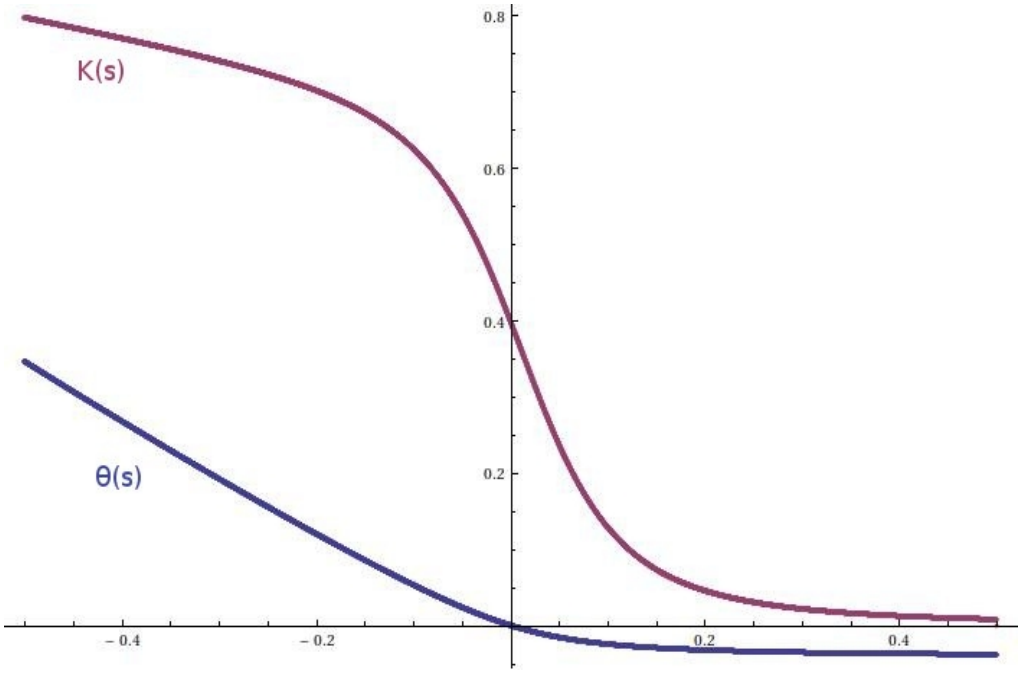
$$\frac{d}{dt}\rho_s(t) = W_s(\rho_s) = -i[H,\rho] + e^{-s} L_1 \rho L_1^\dagger + \sum_{i=2}^{N_L} L_i \rho L_i^\dagger - \frac{1}{2}\sum_{i=1}^{N_L} \{L_i^\dagger L_i, \rho\}$$

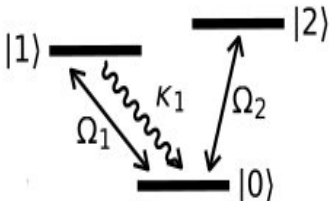
- Activity of the system, k(s), follows from definition:

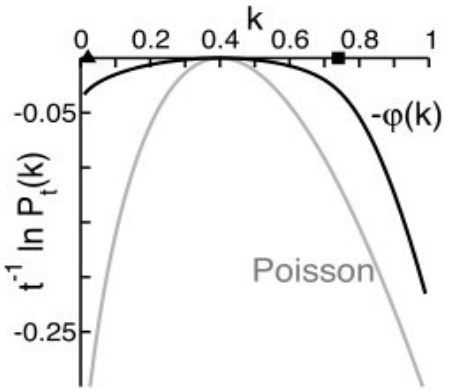
$$k(s) \equiv \frac{\langle K \rangle_s}{t} = \frac{1}{t Z_t(s)} \sum_K K P_t(K) e^{-sK} = -\theta'(s)$$

Full Counting Statistics - S-ensemble

- Physical dynamics takes place at S=0, but the behaviour away from s=0 provides insights into the tails of the distribution







J.P Garrahan and I. Lesonovsky, Phys. Rev. Lett. **104**, 160601 (2010)

Generalised Ensembles

- S-ensemble: Fixed time, fluctuating event numbers
  - Time ~ “Volume”
  - K ~ “Particle Numbers”
  - $\Phi(K/t)$ ~ “Entropy density”
  - $\theta(s)$ ~ ”(minus) Free Energy”
  - S ~ “Chemical Potential”

Generalised Ensembles - X-ensemble

- X-Ensemble: Fix event numbers, K, allow time to fluctuate
  - Probability that observing K events takes a time t:

$$P_K(t) \approx e^{-K\psi(t/K)}$$

  - Moment Generating Function

$$Z_t(s) \equiv \int_{t=0}^{\infty} P_K(t)\, e^{-xt} \approx e^{Kg(x)}$$

  - Again, ψ and g are related by a Legendre transformation:

$$g(x) = -min_{t/K}\left[\psi(t/K) + xt/K\right]$$

  - Moreover g and θ can be related

$$g(x) = -\theta^{-1}(-x) \qquad \theta(s) = -g^{-1}(-s)$$

Generalised Ensembles

- S-ensemble: Fixed time, fluctuating event numbers
  - Time ~ “Volume”
    - fixed
  - K ~ “Particle Numbers”
    - fluctuates
  - $\Phi(K/t)$ ~ “Entropy density”
  - $\theta(s)$ ~ ”(minus) Free Energy”
    - “Helmholtz Free Energy”
  - S ~ “Chemical Potential”
- X-ensemble: Fixed event numbers, fluctuating time
  - Time
    - fluctuates
  - K
    - fixed
  - $\Psi(t/K)$
  - g(x)
  - X ~ “Pressure”

Vectorial Case

- This can be generalised to cases where more than one kind of event is counted
  - S becomes a vector $\vec{s} = \{s_1, s_2 \ldots, s_n\}$
    where s_n is the field conjugate to event K_n
- Of particular interest, one can reconstruct $\theta(s_1)$ of one jump only from the X-ensemble:

$$P_K(t, K_1) \approx e^{-K\psi\left(\frac{t}{K}, \frac{K_1}{K}\right)}$$

$$Z_K(x, s_1) \equiv \sum_{K_1} \int_{t=0}^{\infty} P_K(t, K_1) e^{-s_1 K_1} e^{-xt} \approx e^{Kg(x, s_1)}$$

$$\Rightarrow g(x, s_1) \rightarrow g(x) + s_1 K_1$$

Reconstructing θ(s1) from the X-ensemble

- Can imagine some 2-dimensional space {x(s_1),s_1}

$$g(x,s_1) \rightarrow g(x) + s_1 K_1$$

- θ(s) will be given by the curve where g(x,s_1) = 0
- However, we know g(x=0,s_1=0) = 0 to ensure probability conservation

$$\frac{d}{ds_1} g(x(s_1),s_1) = \partial_{s_1} g(x(s_1),s_1) + \partial_x g(x(s_1),s_1)\, x'(s_1) = 0$$

$$\Rightarrow \delta s_1 \frac{\langle K_1 \rangle}{K} + \delta x \frac{\langle t \rangle}{K} = 0 \quad \Rightarrow \quad \delta x = \delta s \frac{\langle K_1 \rangle}{\langle t \rangle}$$

Numerical simulation

- Motivation:
  - Reconstruct moments from simulations
- Open quantum systems are easily simulated using continuous time Monte Carlo
- Transition Path Sampling can be applied to generate non-equilibrium trajectories

Dellago, C., Bolhuis, P. G. and Geissler, P. L. (2003) Transition Path Sampling, in Advances in Chemical Physics, Volume 123 (eds I. Prigogine and S. A. Rice), John Wiley & Sons, Inc., Hoboken, NJ, USA.

Transition Path Sampling

- Biased random walk through the space of trajectories generates non-equilibrium trajectories
- Generic Algorithm:
  - Generate a trajectory and count the number of events that occur, Y(K)
  - Propose new trajectory Y'(K')
  - Compare event numbers ΔK = K' – K
  - Calculate the acceptance probability for the proposed trajectory from the bias:

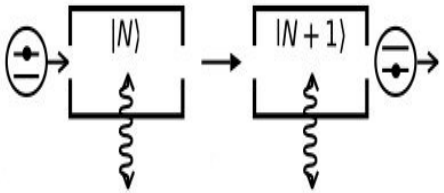
    $P_{accept} = min\{1, e^{-s\Delta K}\}$ for the S-ensemble or $P_{accept} = min\{1, e^{-x\Delta t}\}$ for the x-ensemble
- Continuous time Monte Carlo lends itself to fixed number of events rather than fixed total time => x-ensemble is much more efficient for such systems

Example: MicroMaser

- Excited two-level atoms pumped into a cavity one at a time
  - Events are recorded when an outgoing atom is in the ground state
- Four Lindblad terms:

$$L_1 = \sqrt{r}\sin\frac{\left(\varphi\sqrt{aa^\dagger}\right)}{\sqrt{aa^\dagger}}a \qquad L_2 = \sqrt{r}\cos\left(\varphi\sqrt{aa^\dagger}\right)$$

$$L_3 = \sqrt{\kappa}\,a \qquad L_4 = \sqrt{\gamma}\,a^\dagger$$

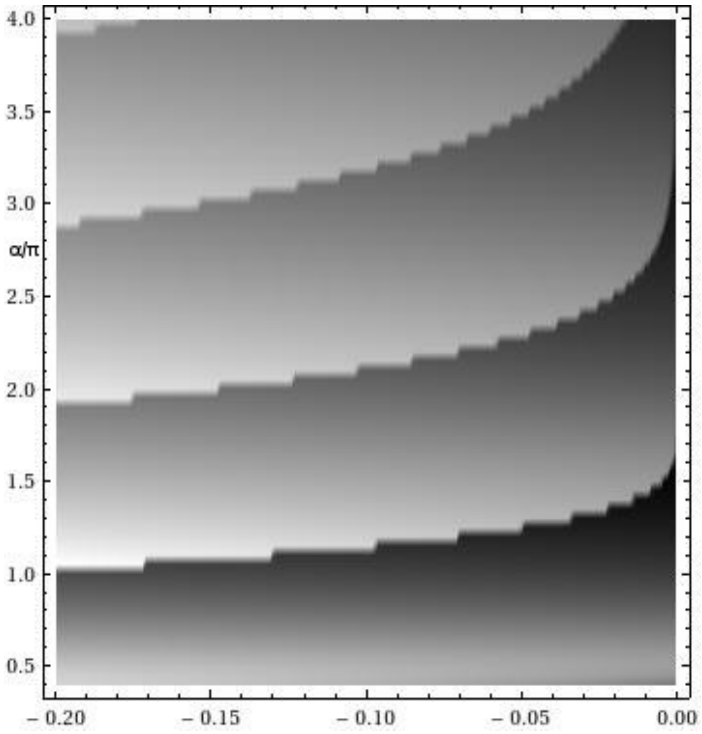


- Can be parameterised by a single “pump parameter”:

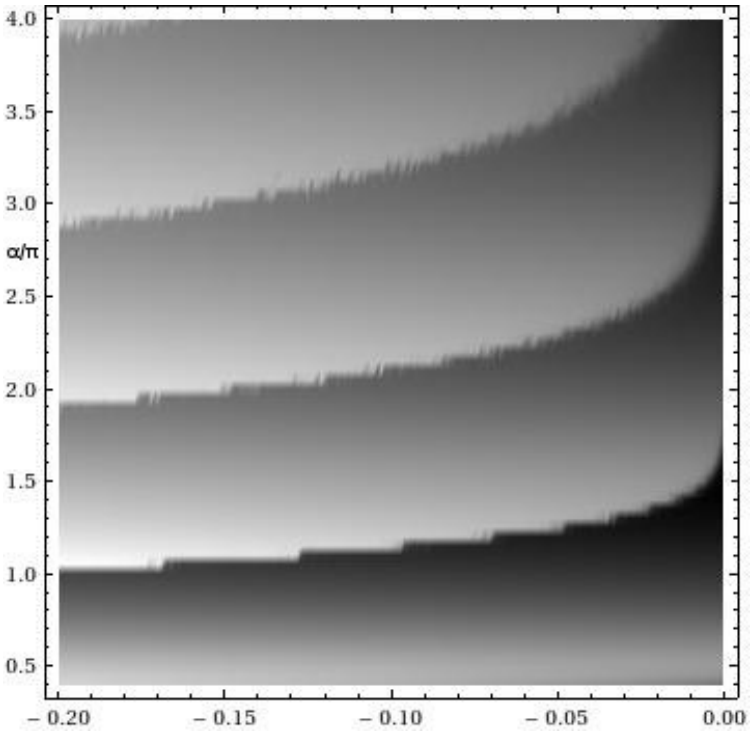
$$\alpha \equiv \varphi\sqrt{r/(\kappa-\gamma)}$$

Micromaser: Analytics vs Numerics

- Analytics:
  - Negative s



- X-ensemble Numerics:
  - Negative s:



Micromaser: Analytics vs Numerics

- Analytics:
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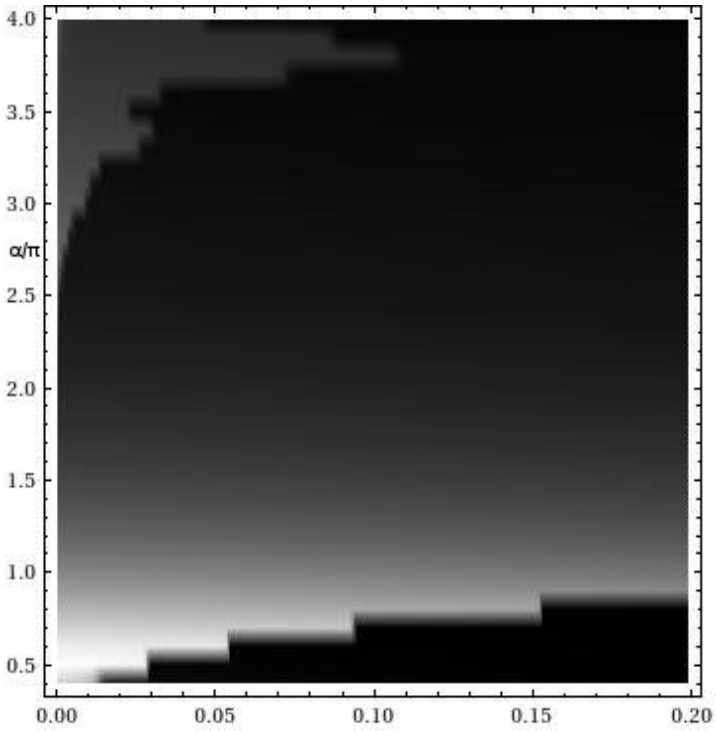
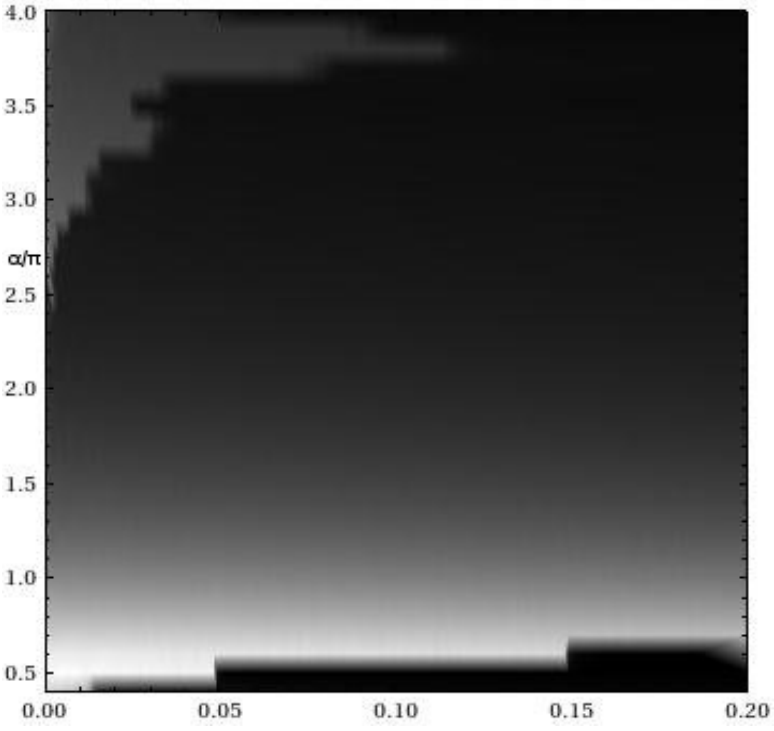
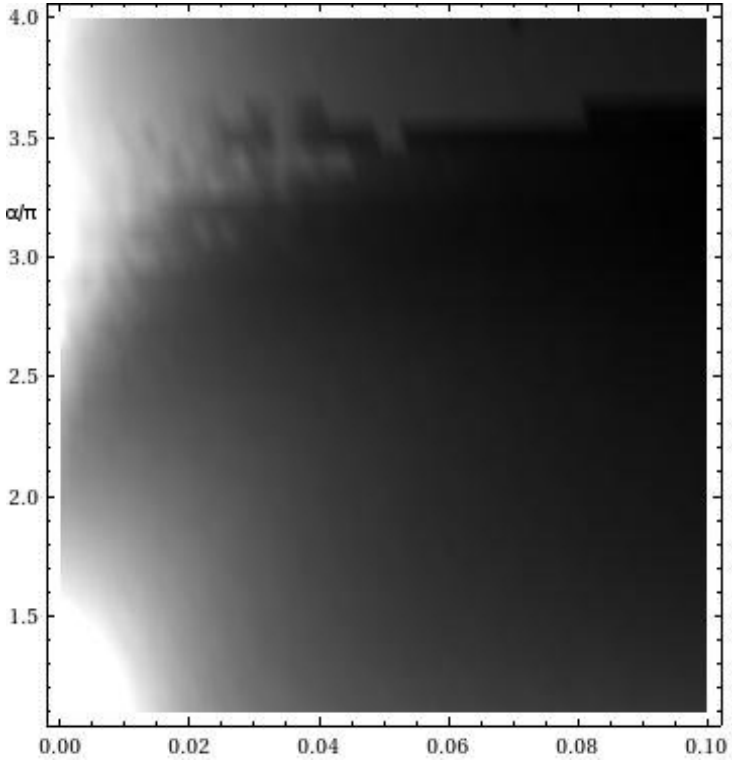


- X-ensemble Numerics:
  - Positive s:

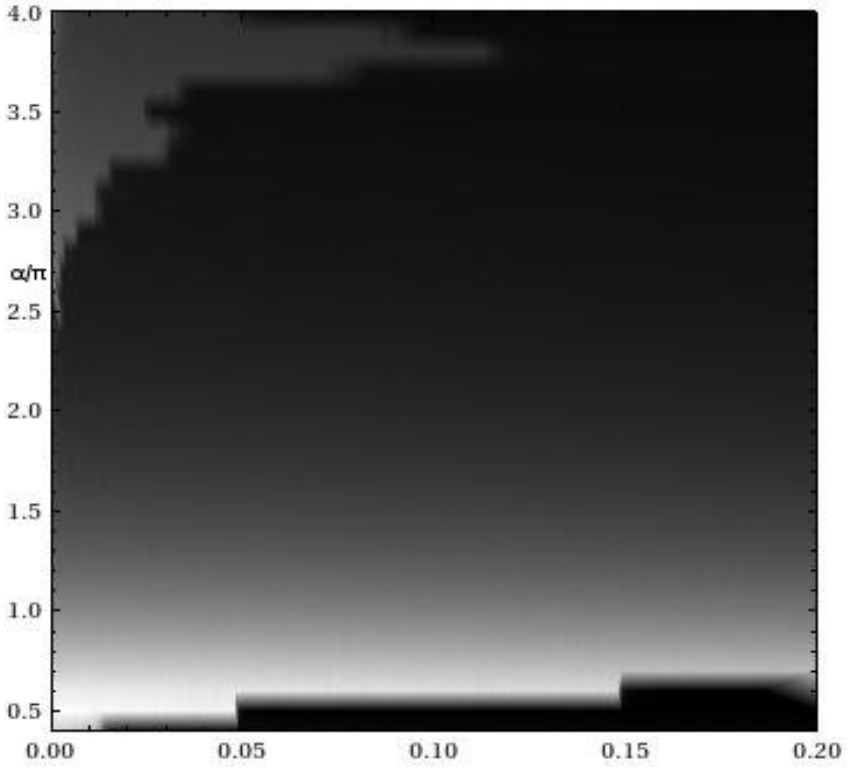


Micromaser: S-ensemble vs X-ensemble

- S-ensemble Numerics:



- X-ensemble Numerics:



Conclusions

- The s-ensemble in the “thermodynamics of trajectories” is one of a set of generalised ensembles
- As in thermodynamics, different ensembles are better suited for different tasks
- In particular, the so-called “x-ensemble” allows far more efficient numerical simullation of non-equilibrium phases in open quantum systems