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In collaboration with

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Statistical Physics of Systems out of Equilibrium, IHP Paris, October 2007

qpzx-oscillator: one-dimensional heat conduction

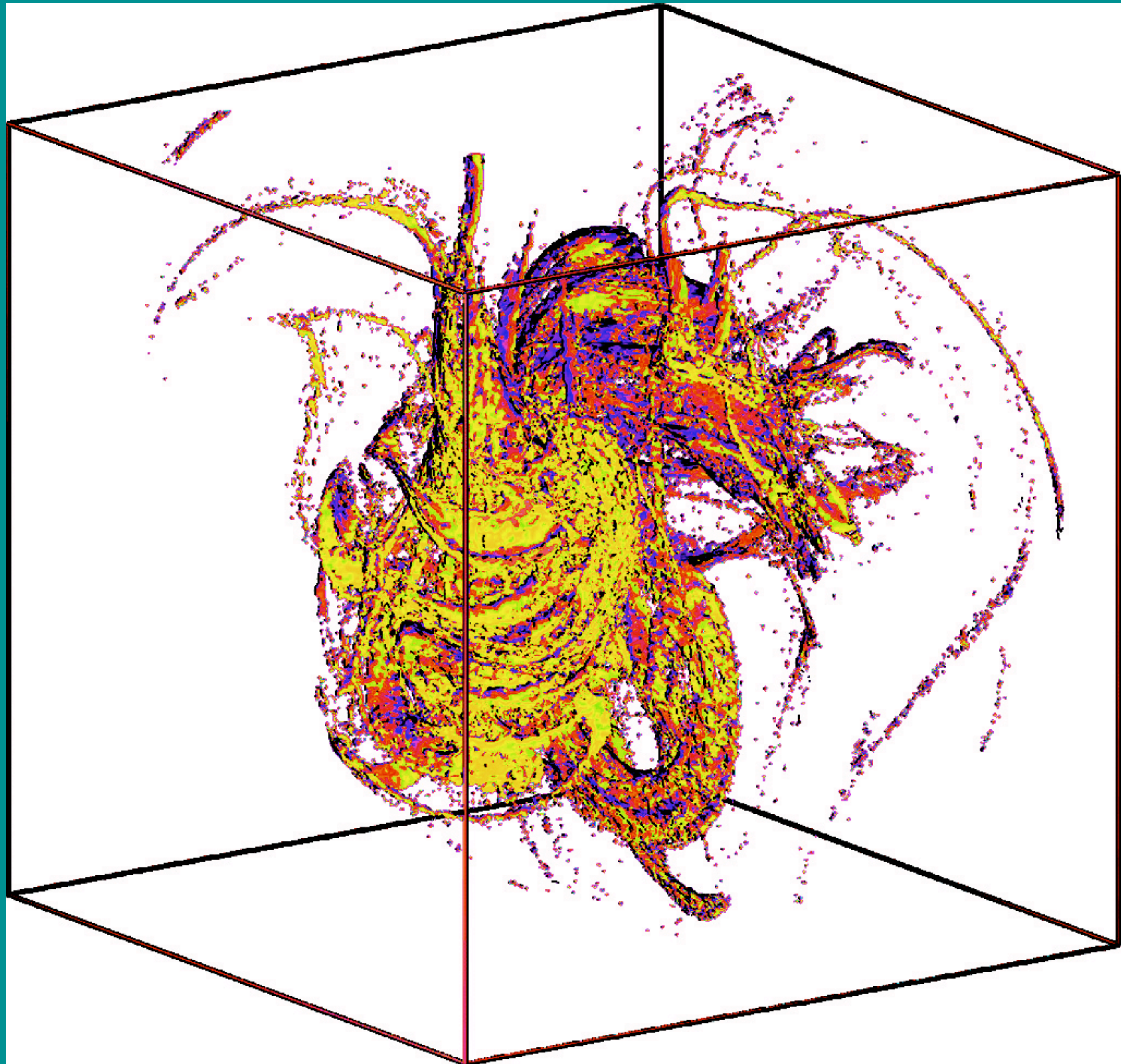
$$\dot{q} = p/m$$

$$\dot{p} = -q - zp$$

$$\dot{z} = p^2 - T(q) - xz$$

$$\dot{x} = z^2 - T(q)$$

$$T(q) = 1 + \epsilon \tanh(q)$$



The New York Times
nytimes.com

July 7, 2005

Finding Design in Nature

By CHRISTOPH SCH÷NBORN

But this is not true. The Catholic Church, while leaving to science many details about the history of life on earth, proclaims that by the light of reason the human intellect can readily and clearly discern purpose and design in the natural world, including the world of living things.

Evolution in the sense of common ancestry might be true, but evolution in the neo-Darwinian sense - an unguided, unplanned process of random variation and natural selection - is not. Any system of thought that denies or seeks to explain away the overwhelming evidence for design in biology is ideology, not science.

Emergence of Order in quasi-species evolution: classical and quantum

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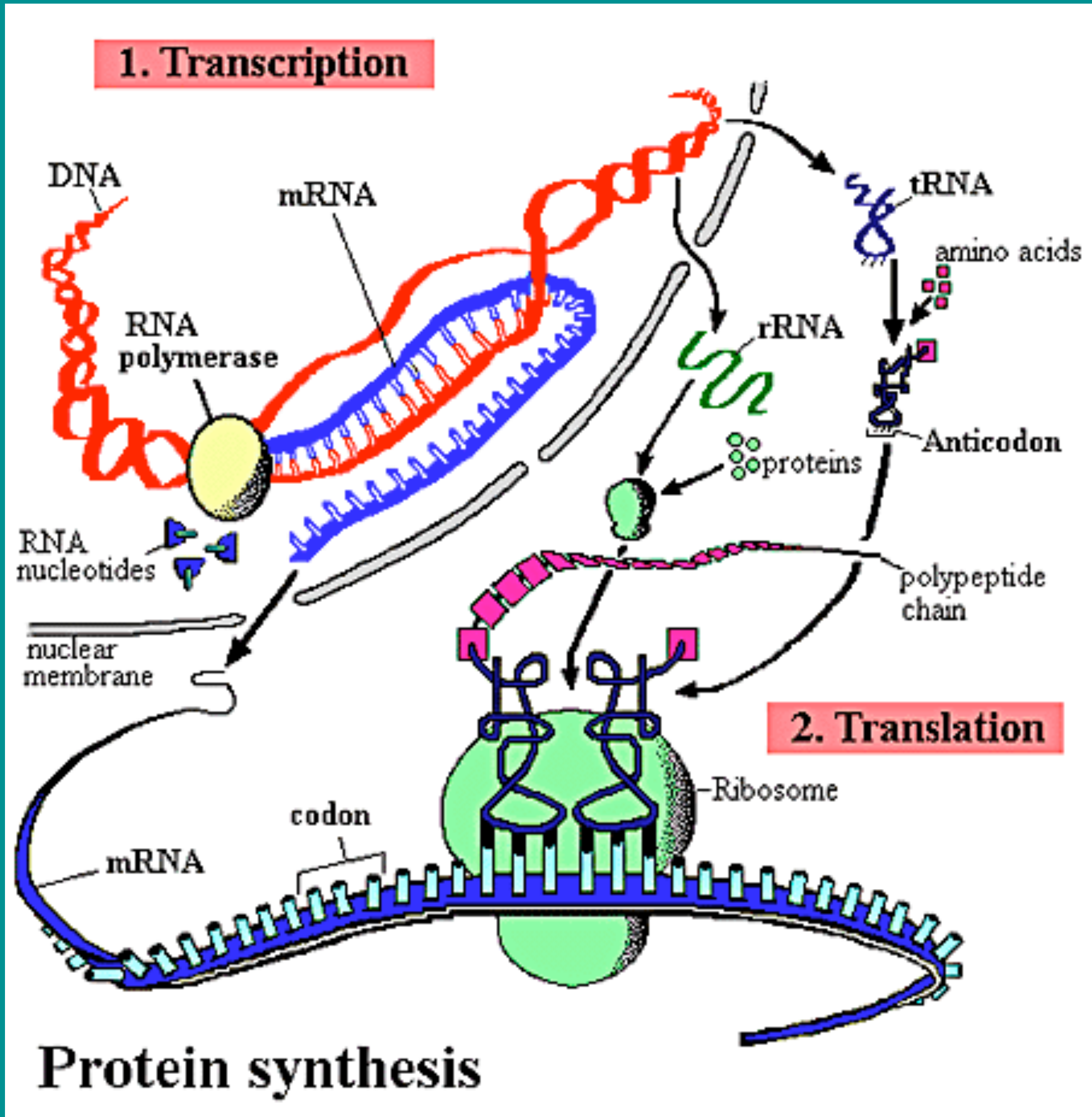
Outline

- Introduction to quasispecies theory
- Fermi (quadratic) entropy
- Classical quasispecies evolution
- Results for typical ensembles
- The two-dimensional case
- Quantum quasispecies evolution (QS)
- Alternative quasispecies evolution (AQS)
- Lindblad dynamics

Evolutionary dynamics

- Evolution of populations involves reproduction, MUTATION, SELECTION, random drift, spatial movement
- Quasi-species: population of genomes subject to mutation and selection
- Human genome (DNA): sequence of 3 x 10^9 nucleotides (A,T,C,G). Three consecutive nucleotides (reduntantly) define an amino acid, which are the building blocks of proteins in the cell.
- Sequence space of proteins of length L (M. Smith): high dimension, small distanc; each sequence of amino acids defines a lattice point
- Fitness landscape (M. Eigen, P. Schuster): rate of reproduction
- Genotype -> phenotype -> fitness

Protein synthesis



Mutation and selection of an infinitely large population on a constant fitness landscape: Quasi-species equation

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \sum_{j=1}^{d} q_{ij} f_j p_j - p_i \sum_{k=1}^{d} f_k p_k$$

- $q_{ij} \geq 0$: Mutation probability from j to i:

$$\sum_{i=1}^{d} q_{ij} = 1$$

- $f_j > 0$: Fitness of j

$$q_{ij} f_j = \alpha_{ij}$$

M.Eigen, J.McCaskill and P. Schuster, Adv. Chem.Phys. 75,149 (1989);
M.A. Nowak, “Evolutionary Dynamics“ (2006).

Classical quasi-species evolution

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = \sum_{j=1}^{d} \alpha_{ij} p_j - p_i \sum_{j=1}^{d} \sum_{k=1}^{d} \alpha_{jk} p_k$$

$$p(t) = \frac{\exp(\alpha t) p(0)}{\sum_{i=1}^{d} [\exp(\alpha t) p(0)]_i}$$

$$\sum_{i=1}^{d} p_i = 1$$

M.Eigen, J.McCaskill and P. Schuster, Adv. Chem.Phys. 75,149 (1989);
M.A. Nowak, “Evolutionary Dynamics“ (2006).

Asymptotic solution

$$\alpha = M^{-1} \sum_j (a_j + S_j) M$$

$$S = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & 0 & \cdots \\ 0 & 0 & 0 & 1 & \cdots \\ . & . & . & . & \cdots \end{pmatrix}$$

$$\alpha v = \lambda v$$

$$\lim_{t \to \infty} p(t) = v \left(\sum_{j=1}^{d} v_j \right)^{-1}$$

Matrix classification

D: $0 \leq \alpha_{ii} \leq D \,;\, 1 \leq i \leq d$

U: $0 < \alpha_{ij} \leq U \,;\, 1 \leq i < j \leq d$

L: $0 < \alpha_{ij} \leq L \,;\, 1 \leq j < i \leq d$

Fermi (quadratic) entropy

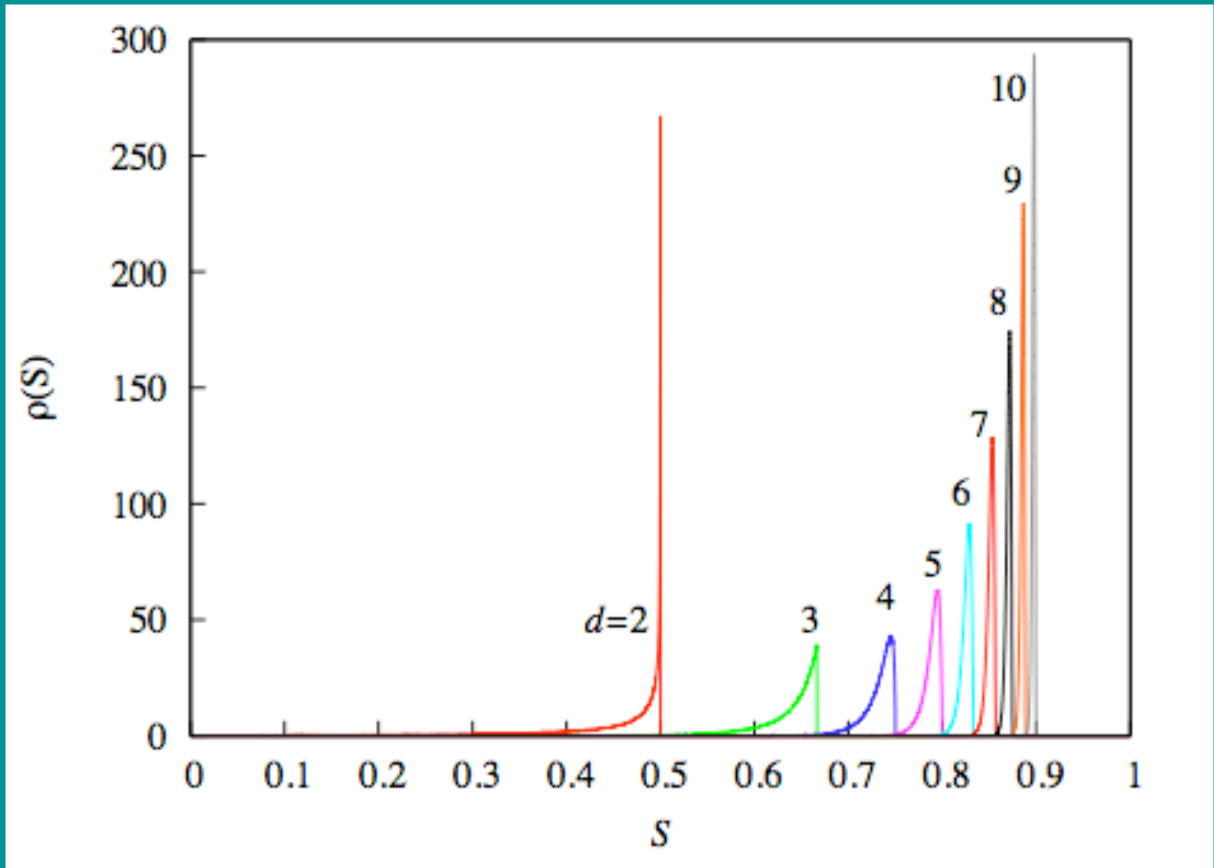
$$p = \{p_i\}, 0 \leq p_i \leq 1;\ i = 1, 2, \ldots, d$$

$$S = \sum_{i=1}^{d} p_i (1 - p_i)$$

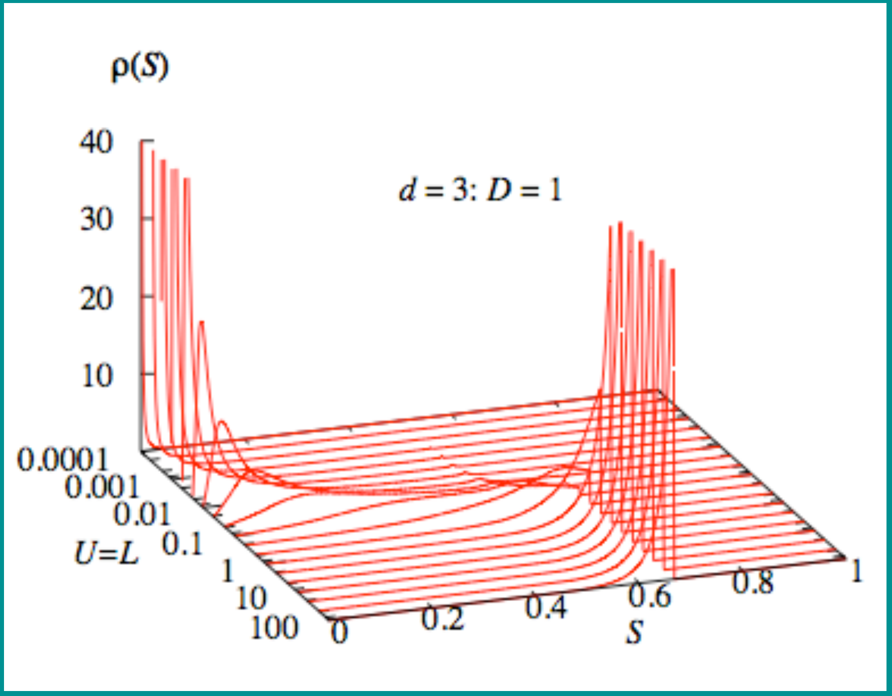
$$0 \leq S \leq \frac{d-1}{d}$$

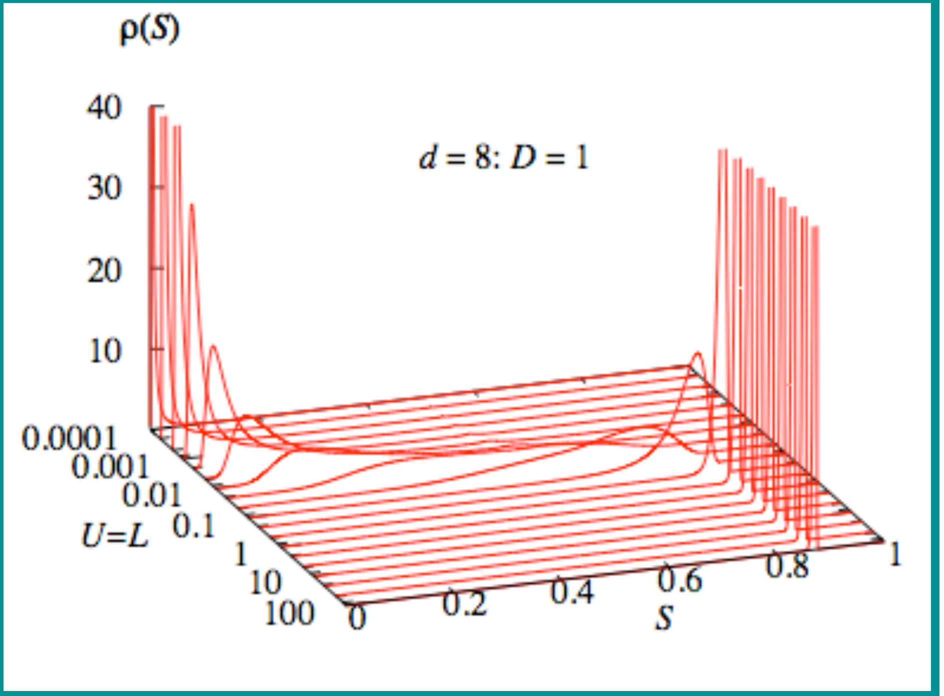
G. Jumarie, “Relative Information“ (Springer, 1990)

The most random case: D = U = L = 1

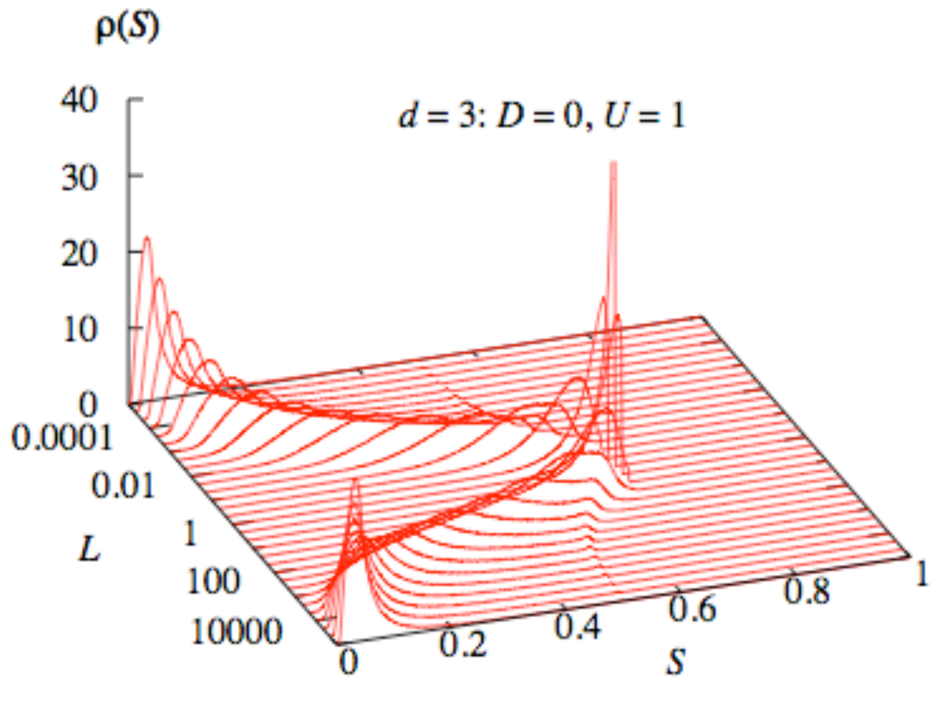


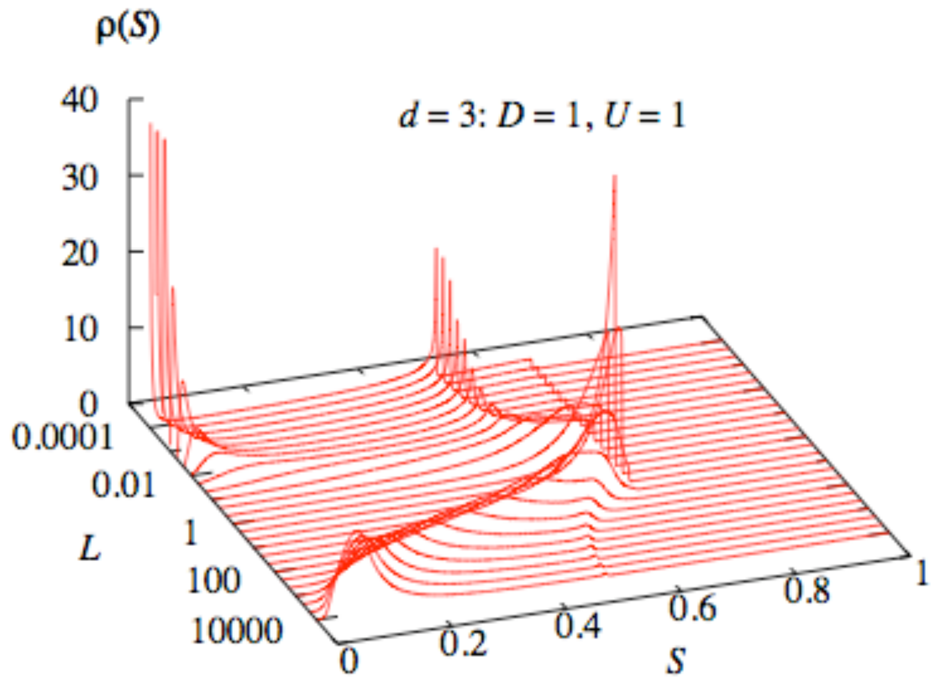
D = 1 and U = L > 0


ρ(S)
40
30
20
10
d = 3: D = 1
0.0001
0.001
0.01
U=L
0.1
1
10
100
0
0.2
0.4
0.6
0.8
1
S

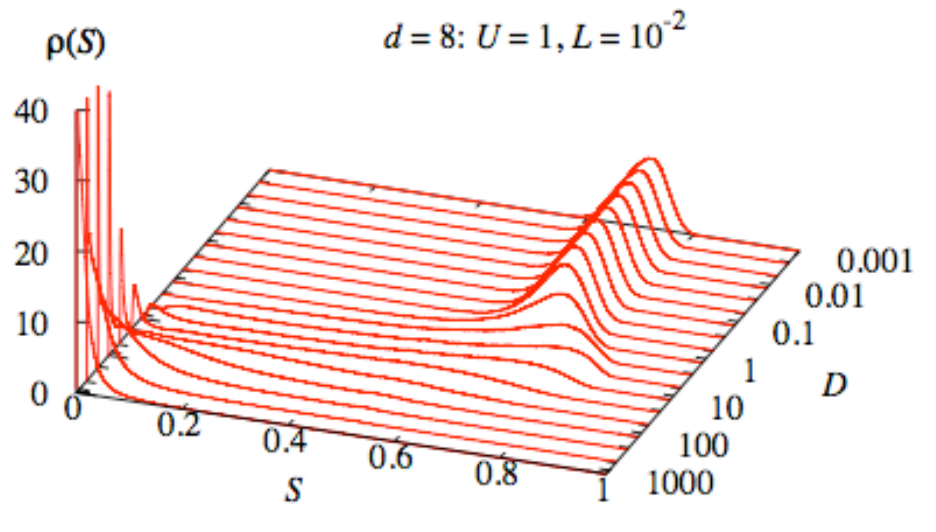

ρ(S)
40
30
20
10
d = 8: D = 1
0.0001
0.001
0.01
U=L
0.1
1
10
100
0
0.2
0.4
0.6
0.8
1
S

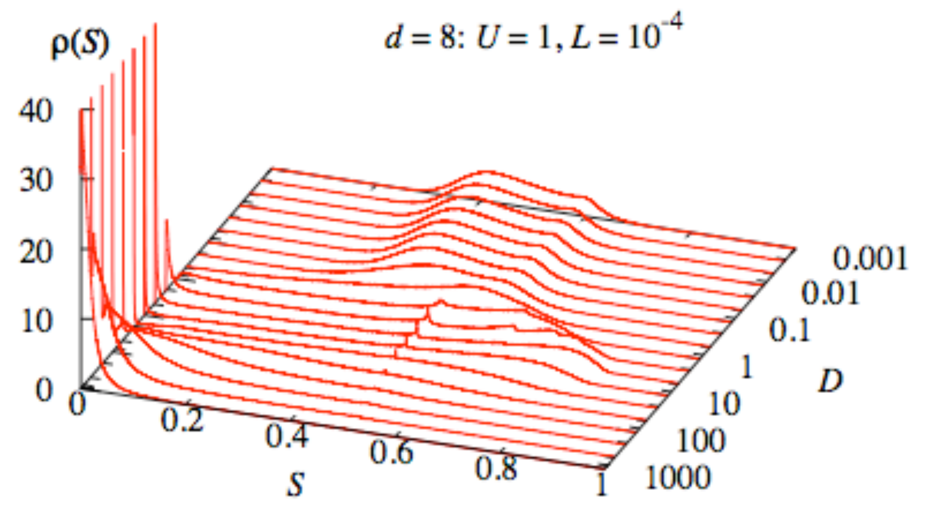
Strong asymmetry: dependence on D and L for U=1

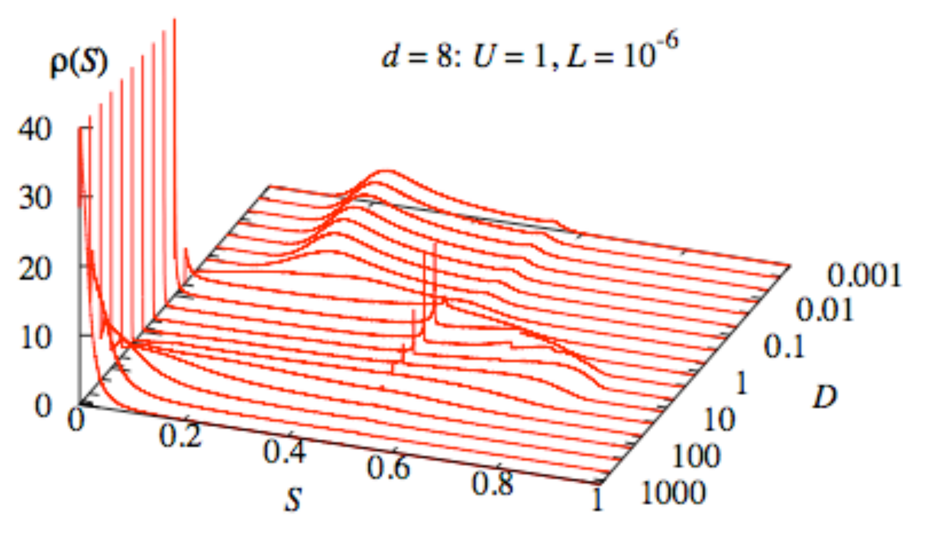


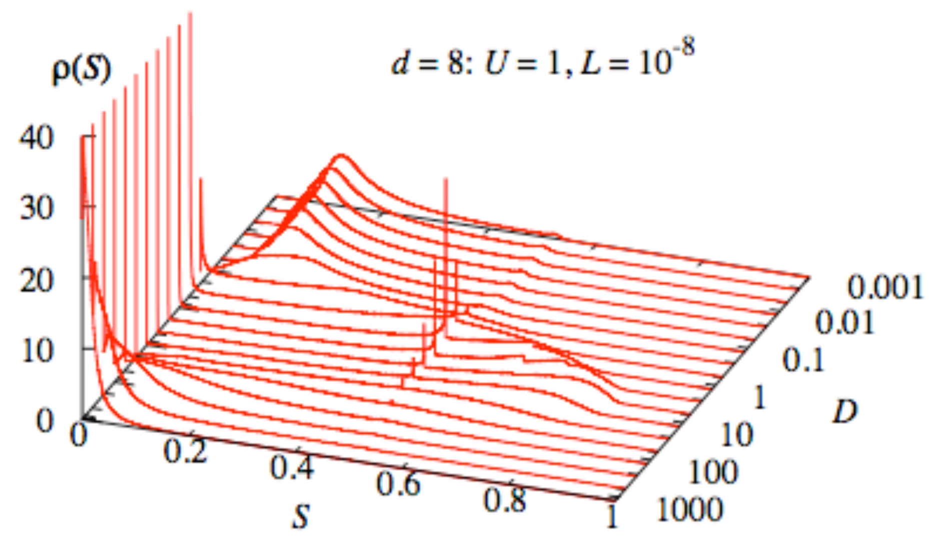


Dependence on D for given U and L

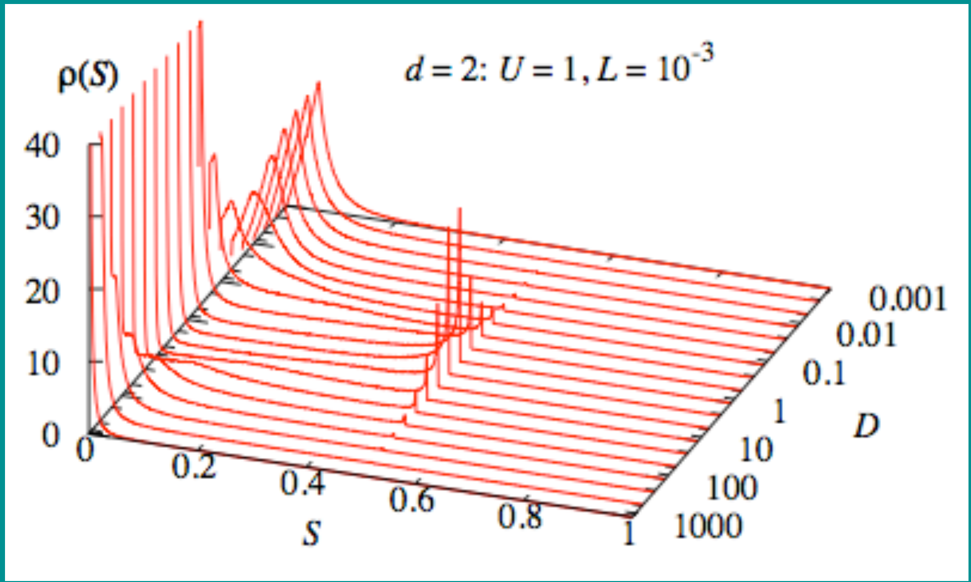


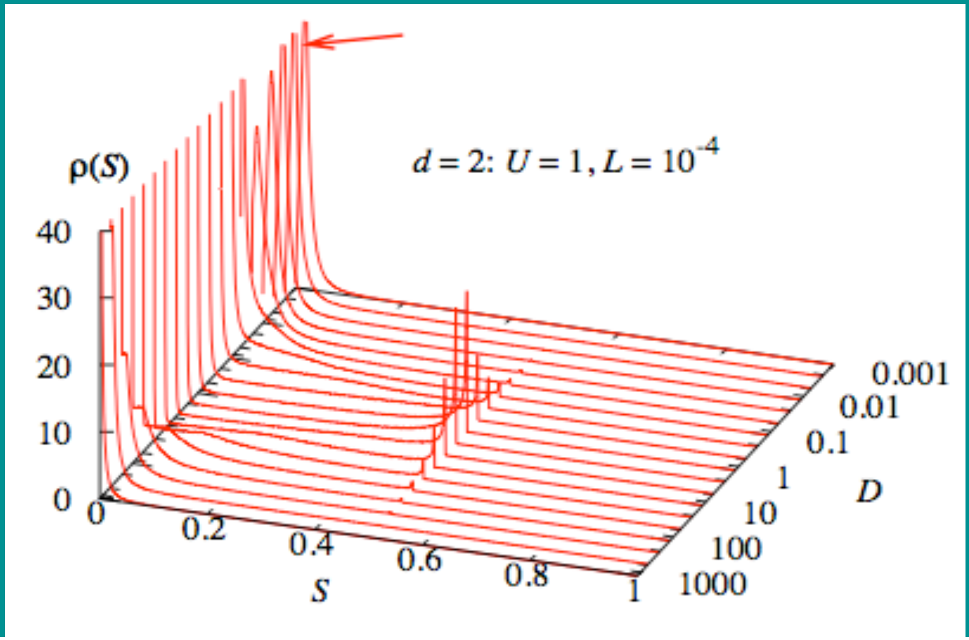






Simplest example: d = 2





Exact solution for d = 2

$$\alpha = \begin{pmatrix} a & b \\ c & d \end{pmatrix}; \quad 0 < \{a, d\} < D\,;\ 0 < b < U\,;\ 0 < c < L.$$

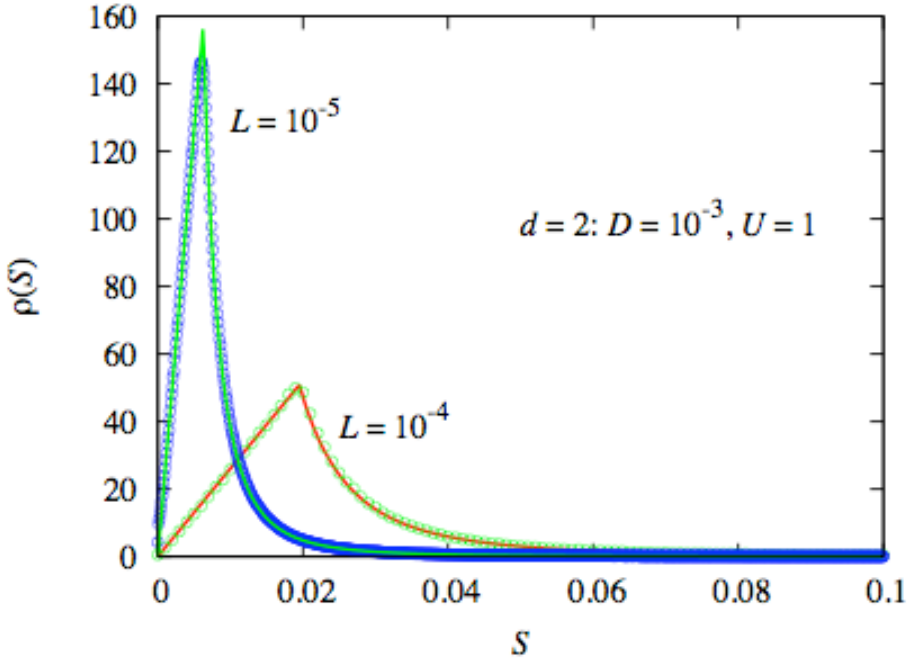
$$r \equiv \frac{p_1}{p_2} = \frac{1}{c}\left[\sqrt{\beta^2 + bc} + \beta\right]; \quad \beta = (a-d)/2$$

$$\pi(\beta) = \frac{2}{D}\left(1 - \frac{2}{D}|\beta|\right); \quad -D/2 < \beta < D/2$$

$$S(r) = \frac{2r}{(1+r)^2} = S\left(\frac{1}{r}\right)$$

$$\rho(S) = \frac{\bar{\rho}(r(S))}{|dS(r)/dr|}$$

$$\bar{\rho}(r) = \frac{1}{UL}\int_0^U db \int_0^L dc \int_{-D/2}^{D/2} d\beta\, \pi(\beta)\, \delta\left(r - \frac{\sqrt{\beta^2 + bc} + \beta}{c}\right)$$



Result for the classical quasi-species evolution

The matrix space is spanned by three parts, the diagonal matrices (D), and the upper (U) and lower (L) triangular matrices. Matrices taken from solely one of these subalgebras give a purifying dynamics, but admixture of a small fraction of another part renders the dynamics mixing. Since zero is not a random number, these subalgebras are never pure, but we may keep the admixtures so small such that they do not matter.

Quantum quasi-species dynamics (QS)

$$d\rho(t)/dt = h\rho(t) + \rho(t)h^{\dagger} - \rho(t)\mathrm{Tr}(h\rho(t) + \rho(t)h^{\dagger})$$

$$\rho(t) = \frac{\exp(ht)\rho(0)\exp(th^{\dagger})}{\mathrm{Tr}[\exp(ht)\rho(0)\exp(th^{\dagger})]}$$

$$\mathrm{Tr}h = 0$$

$$S(t) = \mathrm{Tr}\left[\rho(t)(1 - \rho(t))\right]$$

- Additive generalization to preserve Hermiticity of ρ
- Invariant under $h \mapsto h + c\mathbb{1}$

Pure states: classical vs. quantum

$$\{|i\rangle : i = 1, \cdots, d\}$$

$$\mathbb{1} = \sum_i Q_i;\ Q_i Q_j = \delta_{ij} Q_i;\ Q_i^* = Q_i$$

$$Q_i \equiv |i\rangle\langle i|$$

Classical dynamics:

$$\rho = \sum_i p_i Q_i$$

$$h Q_i = \sum_k \alpha_{ik} Q_k$$

$$\rho \to Q_i$$

Quantum dynamics:

$$|\beta\rangle = \sum_i b_i |i\rangle$$

$$\rho \to P_\beta$$

$$P_\beta = P_\beta^2 = P_\beta^*$$

Quasi-species dynamics is purifying

$$h \in \{A\} = \mathcal{J} : A|\varphi_i\rangle = a_i|\varphi_i\rangle; \quad \langle\varphi_i|\varphi_i\rangle = 1$$

$$|\psi_j\rangle; \quad \langle\varphi_i|\psi_j\rangle = \delta_{ij}$$

$$A = \sum_{i=1}^{d} a_i|\varphi_i\rangle\langle\psi_i|; \quad \sum_i |\varphi_i\rangle\langle\psi_i| = \mathbb{1}; \quad \langle\psi_i|\varphi_i\rangle = 1$$

$$A^2 = \sum_i a_i^2|\varphi_i\rangle\langle\psi_i|; \quad f(A) = \sum_{i=1}^{d} f(a_i)|\varphi_i\rangle\langle\psi_i|$$

$$\rho(t) = \frac{\sum_{j,k}^{d} e^{(a_j+a_k^*)t}|\varphi_j\rangle\langle\psi_j|\rho(0)|\psi_k\rangle\langle\varphi_k|}{\mathrm{Tr}\sum_{j,k}^{d} e^{(a_j+a_k^*)t}|\varphi_j\rangle\langle\psi_j|\rho(0)|\psi_k\rangle\langle\varphi_k|}$$

$$\rho(t) \quad \to_{t\to\infty} |\varphi_j\rangle\langle\varphi_j|$$

Example: two dimensions

$$\rho(t) = \frac{1}{2}(1 + \sigma \cdot n(t)); \quad n \in \mathbb{R}^3; \quad n^2 \leq 1$$

$$\sigma = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}$$

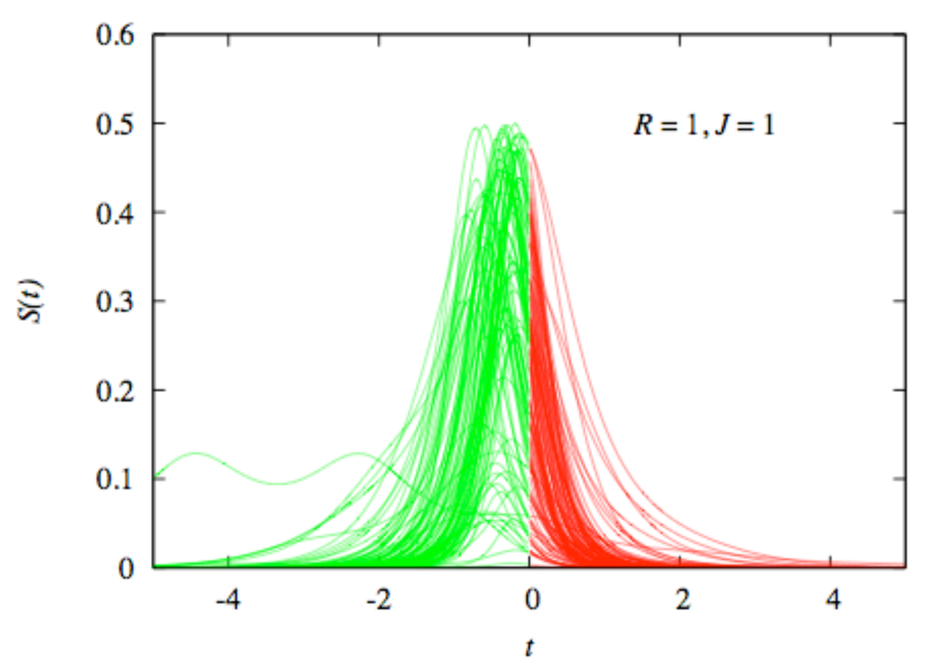
$$h = \sigma \cdot (r + ij); \quad r, j \in \mathbb{R}^3$$

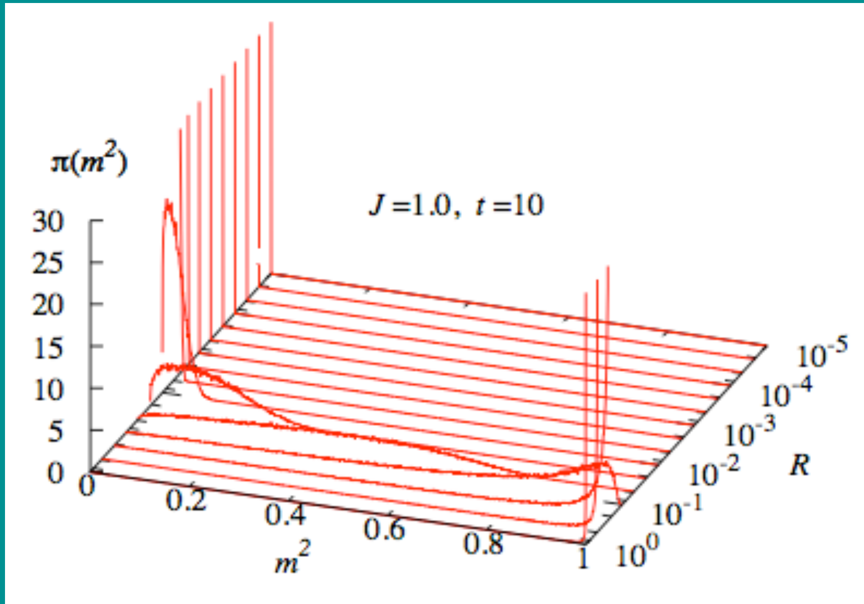
$$M(t) = e^{ht} e^{h^\dagger t} = c(t)(1 + \sigma \cdot m(t)); \quad m^2 \leq 1$$

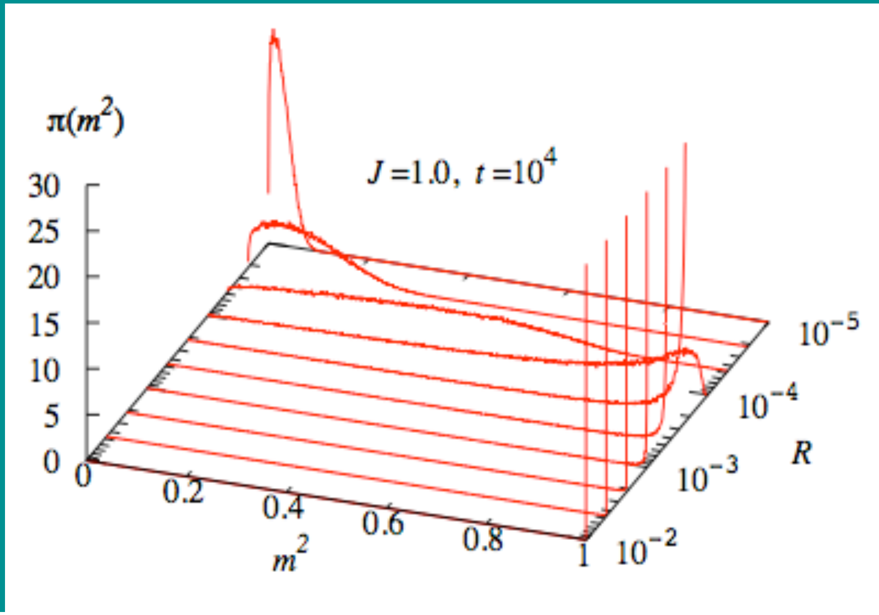
$$S(t) = 1 - \mathrm{Tr}\rho^2(t) = \frac{1}{2} \frac{[1 - m^2(t)][1 - n^2(0)]}{[1 + (m(t) \cdot n(0))]^2}$$

$$r = 0 : h \text{ anti-Hermitian}; \quad m^2(\infty) = 0$$
$$j = 0 : h \text{ Hermitian}; \quad m^2(\infty) = 1$$
$$r, j \neq 0 : h \text{ not Hermitian}, \quad m^2(\infty) = 1$$

2d: Convergence of purification







$$0 < r_\alpha < R; \quad 0 < j_\alpha < J; \quad \alpha \in \{1,2,3\}$$

$$0 < n_\alpha(0) < 1, \alpha \in \{1,2,3\}; \quad \sum_{\alpha=1}^{3} n_\alpha^2 < 1$$

Alternative quasi-species evolution (AQS)

$$d\rho(t)/dt = h\rho(t)h^\dagger - \rho(t)\mathrm{Tr}[h\rho(t)h^\dagger]$$

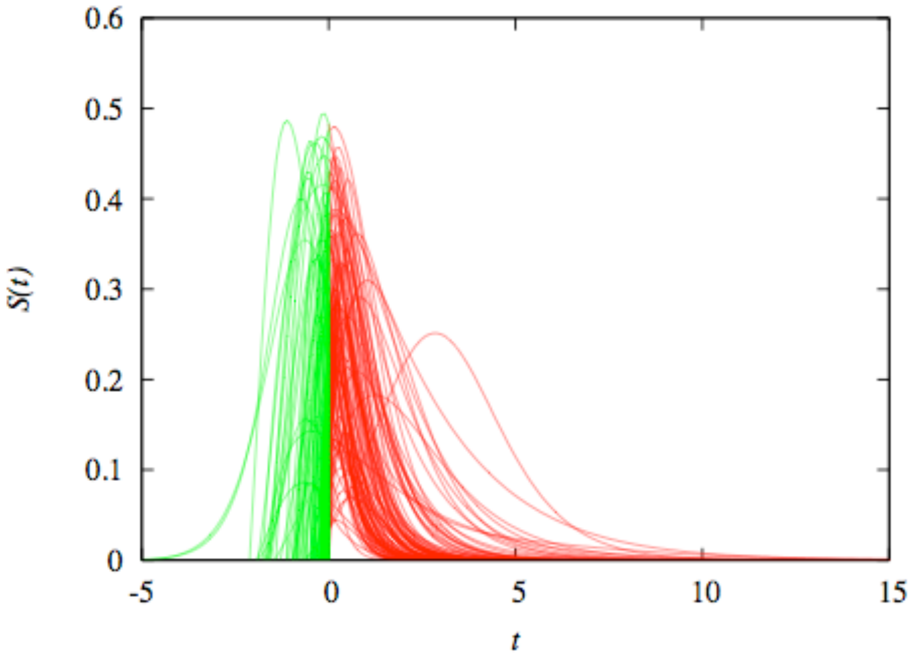
$$\rho(t) = \sum_{k,l} e^{a_k a_l^* t} P_k \rho(0) P_l \,/\, \sum_{k,l} \mathrm{Tr} e^{a_k a_l^* t} P_k \rho(0) P_l$$

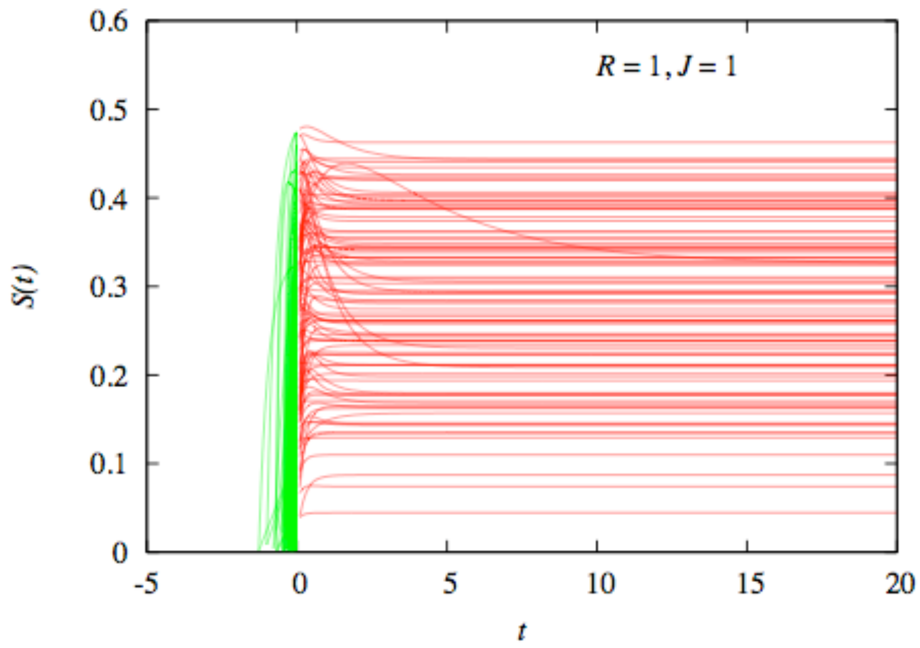
$$P_k = |\varphi_k\rangle\langle\psi_k|$$

$$\rho(t) \rightarrow_{t\rightarrow\infty} |\varphi_k\rangle\langle\varphi_k|$$

- Invariant under $h \mapsto e^{i\gamma}h$, $\gamma \in \mathbb{R}$
- Generates semigroup

AQS-dynamics in 2d





Exceptional case: $|a_1|^2 = |a_2|^2$

$$h = \sigma \cdot (r + ij); \quad 0 < \{r_\alpha, j_\alpha\} < 1$$

Lindblad dynamics

$$d\rho(t)/dt = -i[H,\rho] + \sum_\alpha h^{(\alpha)}\rho(t)h^{(\alpha)\dagger} - \frac{1}{2}\sum_\alpha \left(h^{(\alpha)\dagger}h^{(\alpha)}\rho + \rho h^{(\alpha)\dagger}h^{(\alpha)}\right)$$

$$\dot{\rho} = h\rho h^\dagger - \frac{1}{2}\left(h^\dagger h\rho + \rho h^\dagger h\right)$$

$$d\rho(t)/dt = (\mathrm{AQS}) - \frac{1}{2}(\mathrm{QS})$$

$$(\mathrm{AQS}) = h\rho(t)h^\dagger - \rho(t)\mathrm{Tr}[h\rho(t)h^\dagger]$$

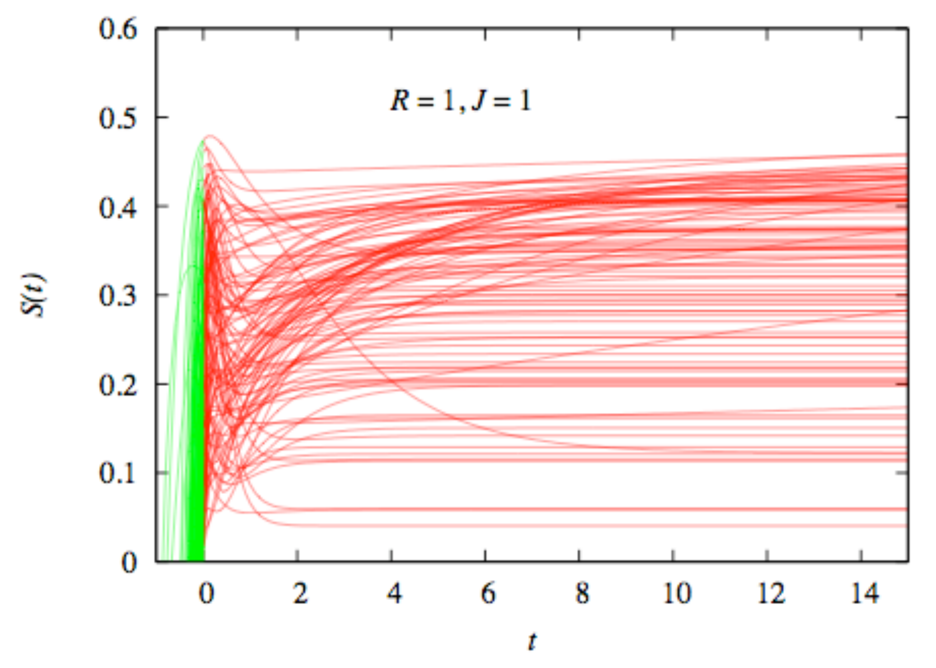
$$(\mathrm{QS}) = h^\dagger h\rho(t) + \rho(t)h^\dagger h - \rho(t)\mathrm{Tr}[h^\dagger h\rho(t) + \rho(t)h^\dagger h]$$

Lindblad dynamics:

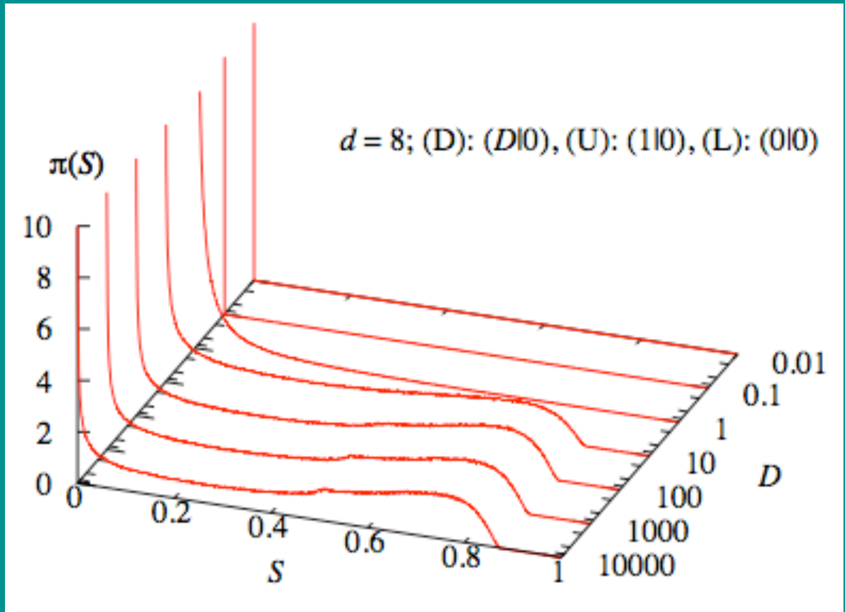
$$\frac{d\rho}{dt} = \mathcal{L}\rho$$

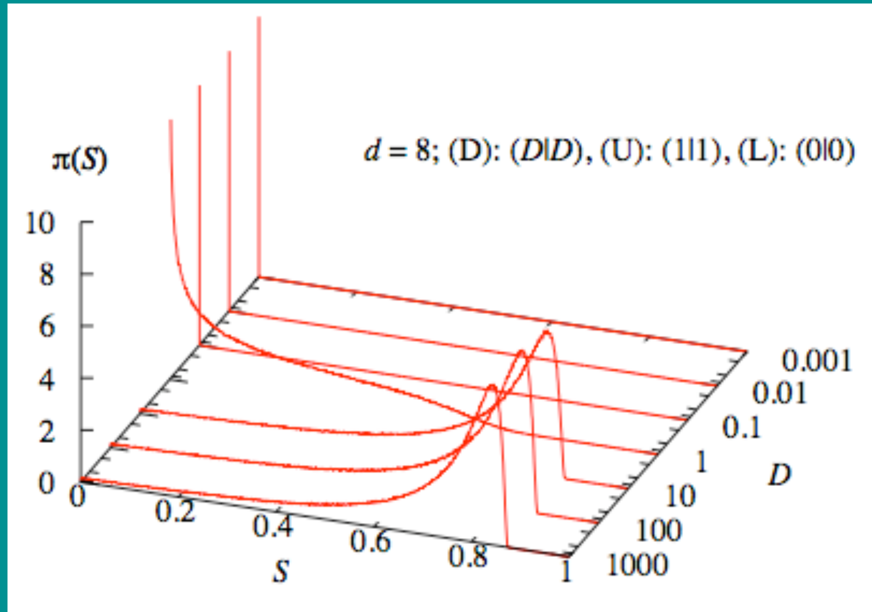
$$\mathcal{L} = h \otimes \bar{h} - \frac{1}{2}(h^\dagger h \otimes \mathbb{1} + \mathbb{1} \otimes \bar{h}h^T)$$

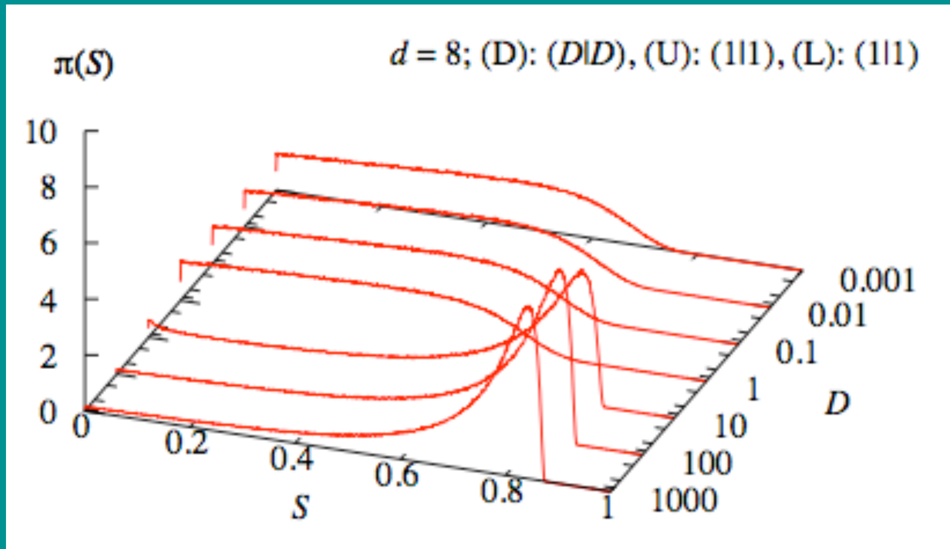
$$\mathcal{L} = \sum_k^{d^2} \lambda_k |\phi_k\rangle\langle\psi_k|$$



Lindblad: entropy distributions in 8d







Summary

The (finite-dimensional) Lindblad equation turns out to be the linear superposition of the quasi-species equation and its alternative formulation.Each of the two sub-processes are purifying by itself, but, in combination, the Lindblad dynamics is partially mixing.

The explanation is found by noting that the two sub-processes generally tend to different pure states and, hence, their combined effort gives a partially-mixing evolution.

Ch. Marx, H.A. Posch and W. Thirring, Phys. Rev. E 75, 061109 (2007)

H. Narnhofer, H.A.Posch and W. Thirring, Phys. Rev. E 76, 041133 2007)

B. Baumgartner, H. Narnhofer and W. Thirring, submitted