Understanding Preferential Trapping

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Preferential Trapping on Tree Structures

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Complex Systems

- Energy over State Space depicted as Mountainous Landscape
- Barriers can not be overcome below certain Temperature
- ➤ Broken Ergodicity
- Significant Decisions at Critical Saddle-Points
- ➤ Preferential Trapping

Important Problem $\Rightarrow$ Applications in
- Protein Folding
- Simulated Annealing
- Cluster Formation
- ...

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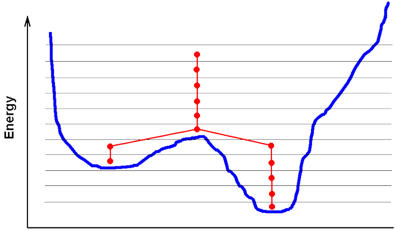
Simplified Approach

Energy Landscape Clipping



- Only one Saddle Point
- Connecting two Valleys
- Embedded in a Super-Valley

Distilling Tree Model by Coarse Graining and Slicing Energy

- Energy Level
- Density of States
- Connectivity

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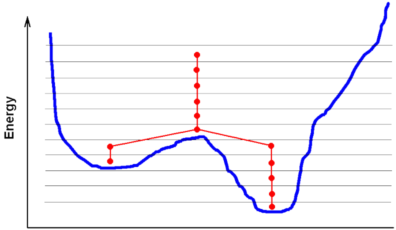

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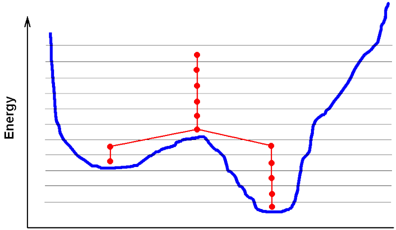

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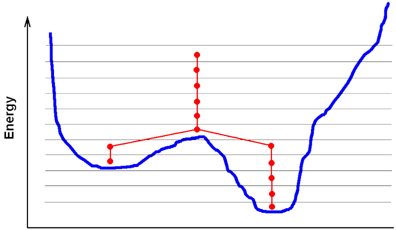

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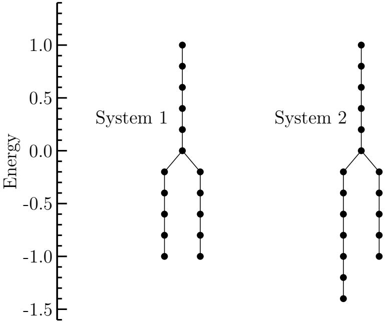
State Space Model

Two Alternative Systems



Valley's Energy Depth

- Equal
- Different

Density of States Growth

- Exponential
- Power-Law like

➤ Different Connectivities at the Saddle-Point

➤ Competing Effects in Attraction

State Space Model

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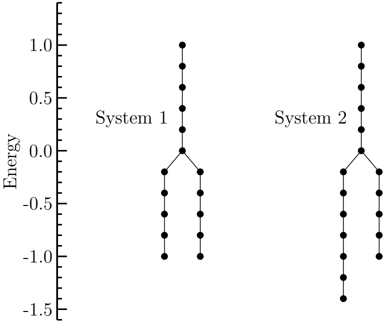

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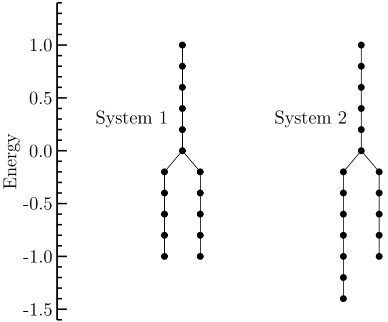

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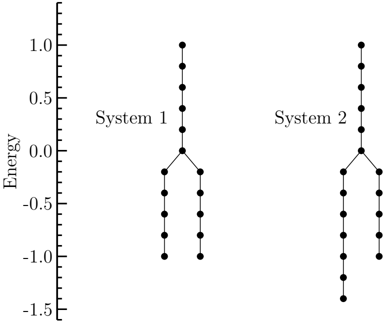

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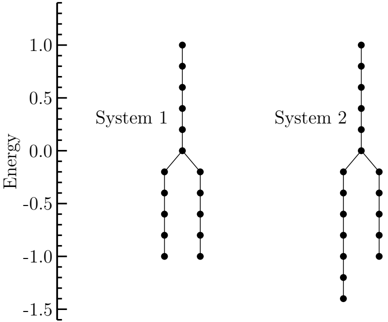

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Numerical Setup

Exponential DoS

$$g^{(i)}_{\text{exp}}(E) = g^{(i)}_{\text{min}} \exp\left[\frac{E - E^{(i)}_{\text{min}}}{T^{(i)}}\right]$$

Power-Law DoS

Transition Rates

Master Equation

Numerical Setup

Exponential DoS

$$g_{\mathrm{exp}}^{(i)}(E) = g_{\mathrm{min}}^{(i)} \exp\left[\frac{E - E_{\mathrm{min}}^{(i)}}{T^{(i)}}\right]$$

Power-Law DoS

$$g_{\mathrm{pow}}^{(i)}(E) = g_{\mathrm{min}}^{(i)} \left(\frac{E - E_{\mathrm{min}}^{\mathrm{global}} + \Delta E}{E_{\mathrm{min}}^{(i)} - E_{\mathrm{min}}^{\mathrm{global}} + \Delta E}\right)^{\gamma}$$

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Transition Rates

$$\begin{aligned} f_{\mathrm{up}} &= f_{\mathrm{kin}}\ \kappa\ \exp\left[-\Delta E / T^{(k)}\right] \\ f_{\mathrm{down}} &= f_{\mathrm{kin}} \end{aligned}$$

Master Equation

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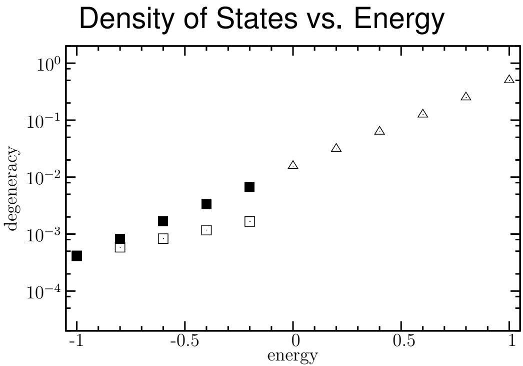
Master Equation

$$P_i^{(t+1)} = \sum_{j=1}^{n} \Gamma_{ij}\left(T^{(t)}\right) P_j^{(t)}$$

Exponentially Growing Density of States



△ Super-Valley $T_{\text{trap}}^{(SV)} = 0.29$

⊡ Valley 1 $T_{\text{trap}}^{(1)} = 0.58$

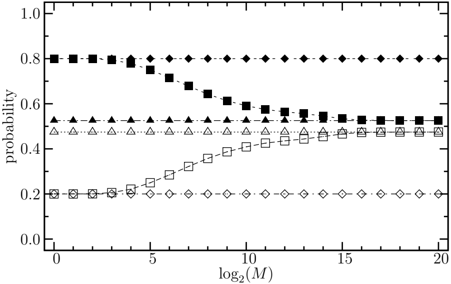
■ Valley 2 $T_{\text{trap}}^{(2)} = 0.29$

- System 1 — Equal Energy Depth

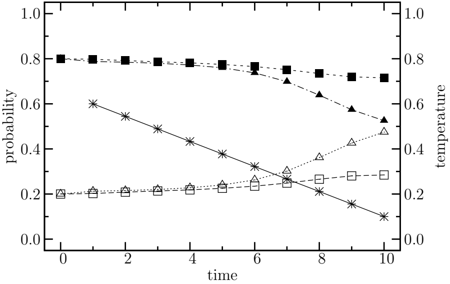
[Hoffmann & Schön, FPL 18(2)2005, 171–182]

Exponentially Growing Density of States

Probability vs. Annealing Speed



Time Development



- System 1 — Equal Energy Depth
- Linear Temperature Schedule

[Hoffmann & Schön, FPL 18(2)2005, 171–182]

Exponentially Growing Density of States

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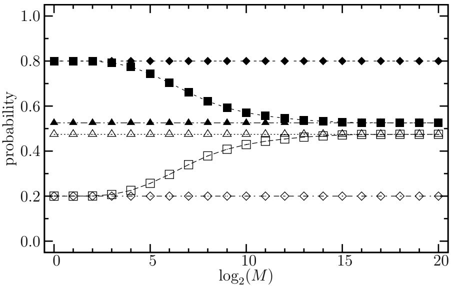

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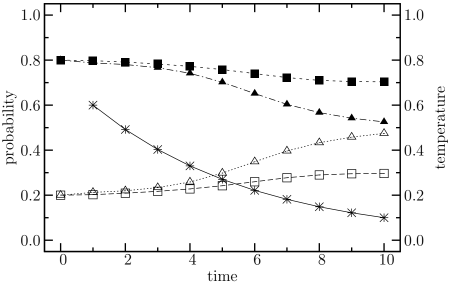

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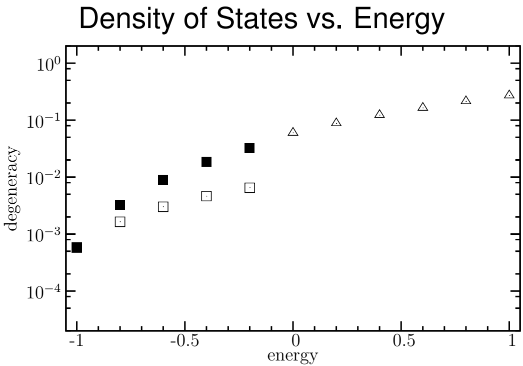
Power-Law like Growing Density of States



△ Super-Valley
$\gamma^{(SV)} = 2.5$

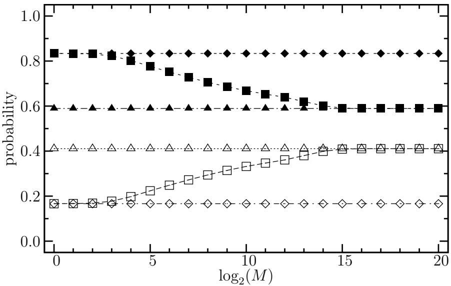
⊡ Valley 1
$\gamma^{(1)} = 1.5$

■ Valley 2
$\gamma^{(2)} = 2.5$

- System 1 — Equal Energy Depth

Power-Law like Growing Density of States

Probability vs. Annealing Speed



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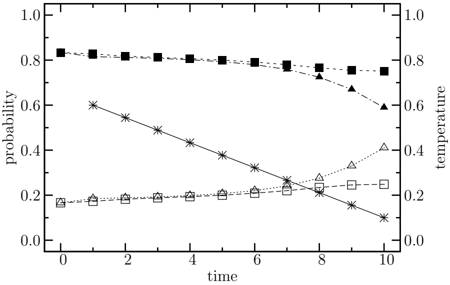
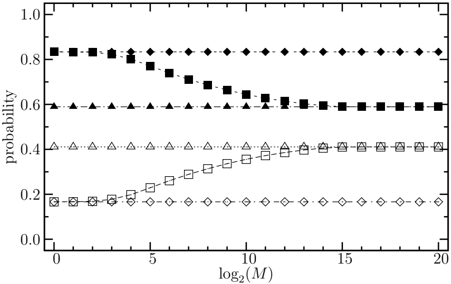


- System 1 — Equal Energy Depth
- Linear Temperature Schedule

Power-Law like Growing Density of States

Probability vs. Annealing Speed



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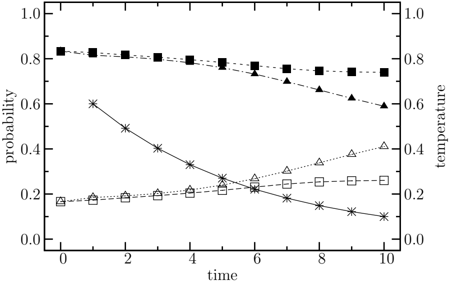
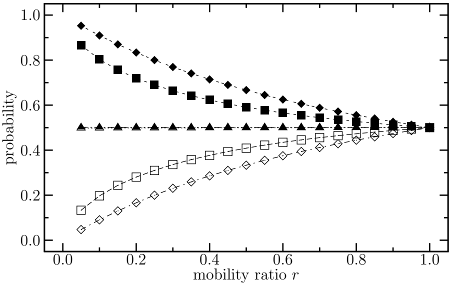


- System 1 — Equal Energy Depth
- Exponential Temperature Schedule

Probability vs. Mobility Ratio



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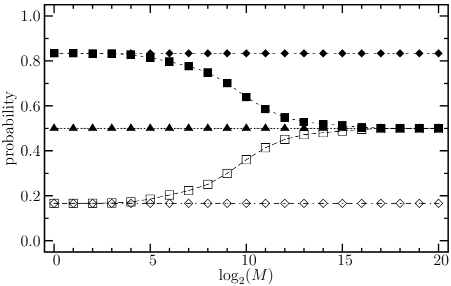
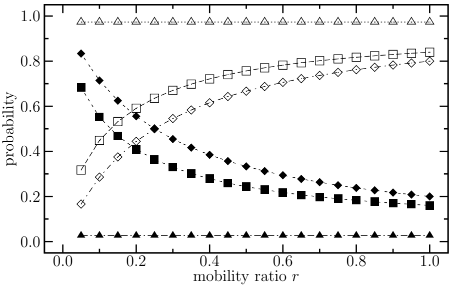


- System 1 — Equal Energy Depth
- Linear Temperature Schedule
- $r = f^{(1)}_{\text{kin}} / f^{(2)}_{\text{kin}}$

Probability vs. Annealing Speed



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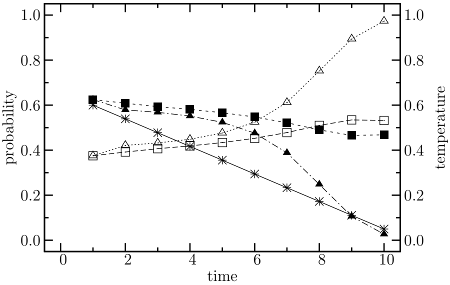
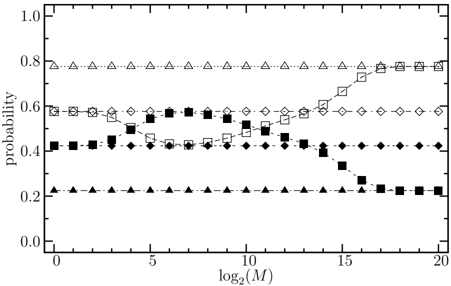


- System 2 — Different Energy Depth
- $T^{(all)}_{\text{trap}} = 0.29$
- Linear Temperature Schedule

Trapping Exponential Systems

Probability vs. Annealing Speed



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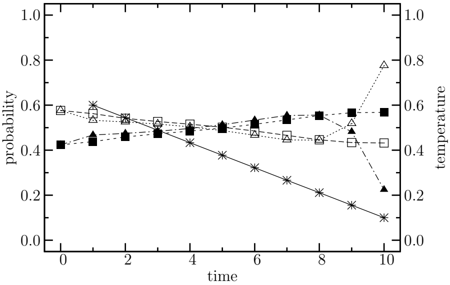
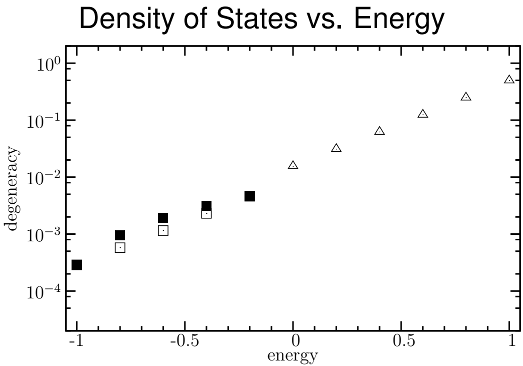


- System 2 — Different Energy Depth
- Linear Temperature Schedule
- ➤ Probability Inversion

Exponential vs. Power-Law Density of States



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$\gamma^{(2)} = \{\textit{fitted}\}$

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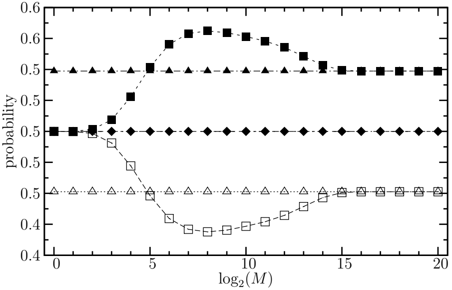
Exponential vs. Power-Law Density of States

Probability vs. Annealing Speed



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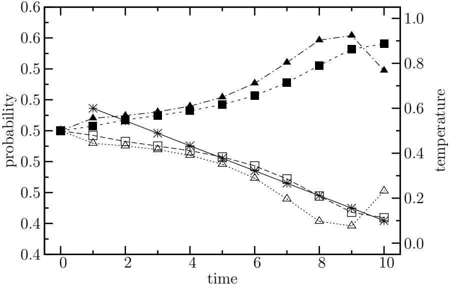
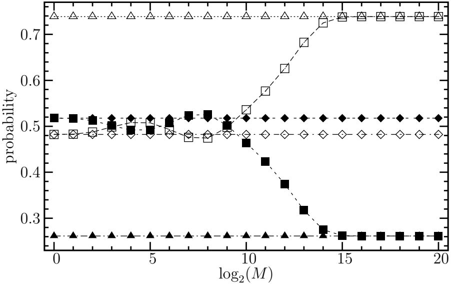


- System 2 — Different Energy Depth
- Linear Temperature Schedule

Trapping Mixed Systems

Probability vs. Annealing Speed



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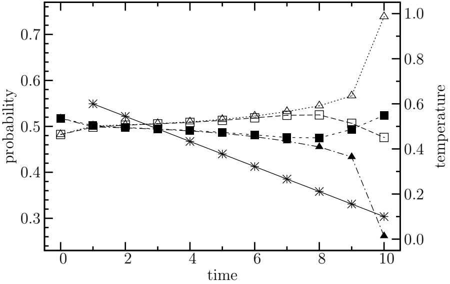

- System 2 — Different Energy Depth
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➤ Multiple Probability Inversions

Exponential vs. Power-Law magnified

Effect of the Vallesys' Volume Ratio:

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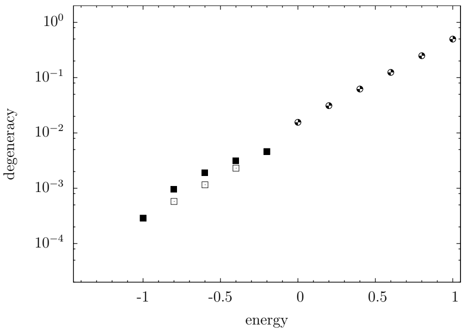
Density of States vs. Energy



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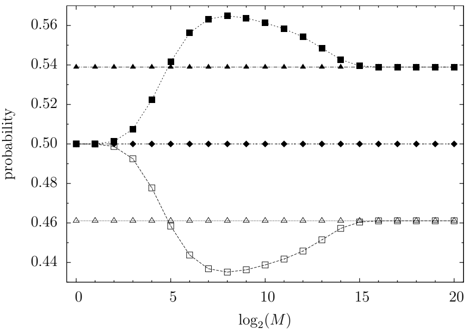
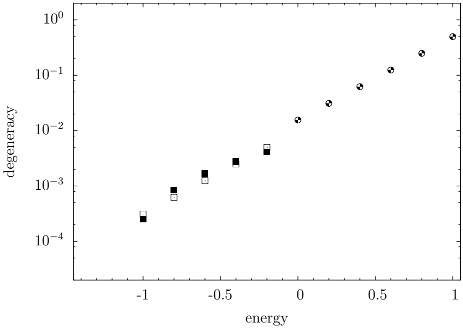


- Competing Valleys — Exponential vs. Power-Law
- Matching Width at Top and Bottom (as before)

Exponential vs. Power-Law magnified

Effect of the Vallesys' Volume Ratio:

Density of States vs. Energy



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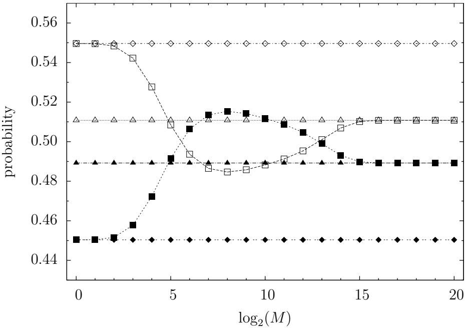

- Competing Valleys — Exponential vs. Power-Law
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Exponential vs. Power-Law magnified

Effect of the Vallesys' Volume Ratio:

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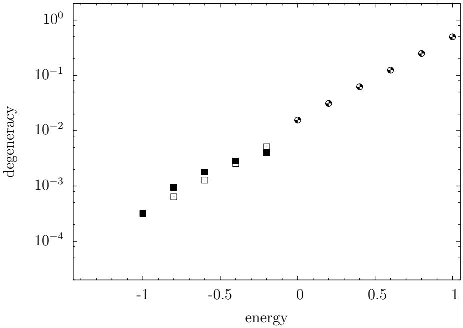

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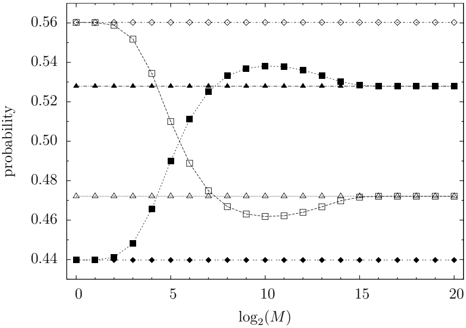
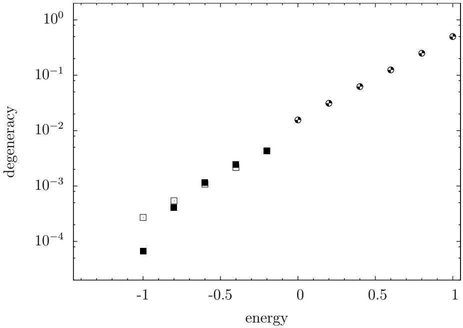


- Competing Valleys — Exponential vs. Power-Law
- Matching Volume and Width at Bottom

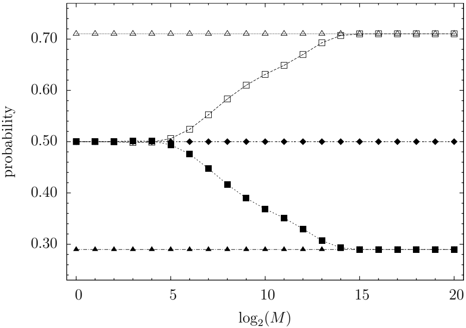
Exponential vs. Power-Law magnified

Effect of the Vallesys' Volume Ratio:

Density of States vs. Energy



Probability vs. Annealing Speed



- Competing Valleys — Exponential vs. Power-Law
- Matching Volume and Width at Top

State Space Dynamics

Systems with *only* Exponential or Power-Law Valleys behave nearly equal.

➤ Why?

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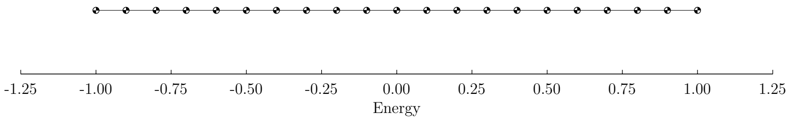
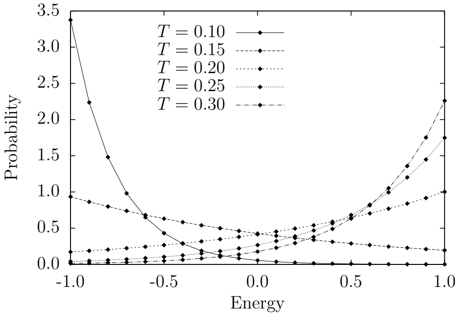
➤ Why?

Test System: A Simple Chain of Ststes

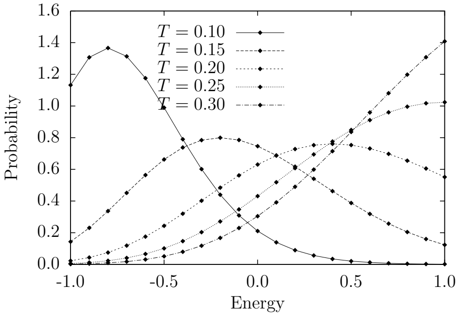


System in Thermal Equilibrium:

Exponential Setup



Power-Law Setup



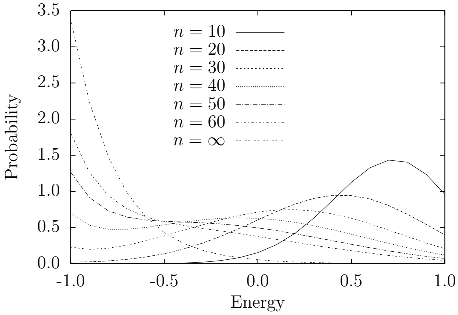
- The System is Stationary
- Increasing/Decreasing Exponential vs. Shiftetd Peak

➤ Different Behavior

State Space Dynamics

Dynamic System in Non-Equilibrium:

Exponential Setup



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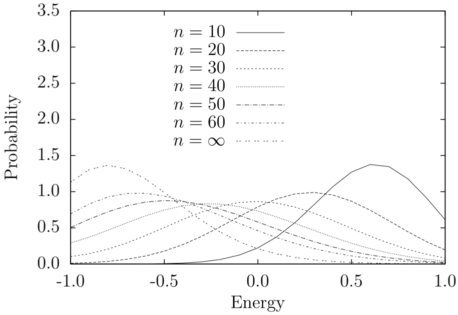

- The System is transported in its State Space
- Both Images show a Shiftetd Peak

➤ Similar Behavior

Conclusions

State Space Dynamics:

- Non-Vanishing Probability Flux occurs
- Equilibrium Considerations often fail in Non-Equilibrium

Trapping:

- Important Feature of Complex Systems
- Observable even at Single Decision Points
- Funneling Controlled by
  - Energy
  - Degeneracy
  - Connectivity
- Decision Influenced by Relaxation Speed

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- Non-Vanishing Probability Flux occurs
- Equilibrium Considerations often fail in Non-Equilibrium

Trapping:

- Important Feature of Complex Systems
- Observable even at Single Decision Points
- Funneling Controlled by
  - Energy
  - Degeneracy
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Questions?