Spin-Glass Bottlenecks in Quantum Annealing

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I A R P A

BE THE FUTURE

Quantum Adiabatic Annealing

- Heuristic algorithm for tackling NP-complete problems.

Kadowaki & Nishimori, PRE '98
Farhi *et al.*, Science '01

$$H = \underbrace{-\frac{1}{2}\sum_{i,k} J_{ik}\sigma_i^z\sigma_k^z - \sum_i h_i\sigma_i^z}_{\text{objective function}} - \Gamma(t)\sum_i \sigma_i^x$$

spin-flip dynamics

- Transverse field $\Gamma(t)$ slowly decreased to zero.
- Ground state interpolates from $|\Psi(0)\rangle = \frac{1}{2^{N/2}}\sum_{s\in\{\pm 1\}^N} |s\rangle$ to $|\Psi(T)\rangle = |s_{\mathrm{min}}\rangle$

Adiabatic condition

$$\mathrm{d}\Gamma/\mathrm{d}t \ll \Delta E \cdot \Delta\Gamma$$

- For Landau-Zener crossing $\Delta E \sim \Delta\Gamma$
- Gap closes at QCP in thermodynamic limit.
- Finite-size scaling gives average-case complexity.
- Example: 1st order phase transition in REM $\Delta E_c \sim 2^{-N/2}$

Continuous Phase Transition

- Critical scaling at 2nd order QCP

Normalized GSE (singular component): $E_0^{(sing)}/N \sim |\gamma^a|$

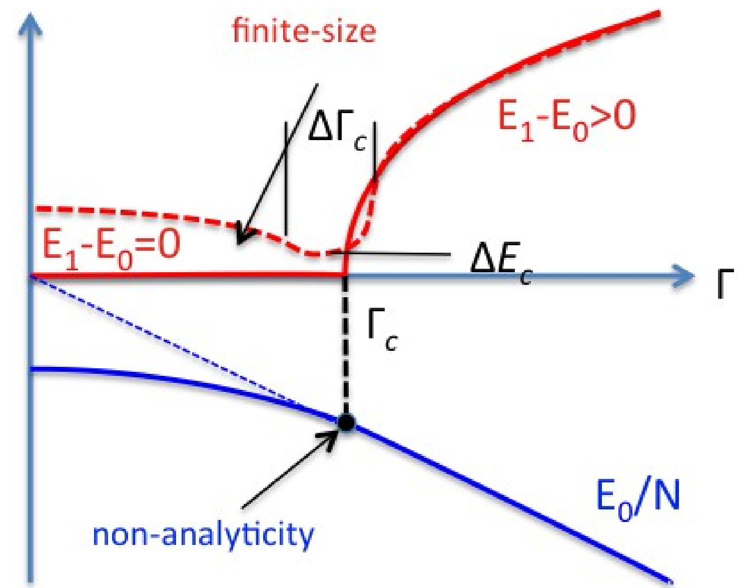
Gap in PM phase: $E_1 - E_0 \sim \gamma^b$

- Finite-size scaling:

$\boxed{\gamma = \Gamma - \Gamma_c}$

$$\Delta E_c \sim N^{-\frac{b}{a-b}}$$

$$\Delta \Gamma_c \sim N^{-\frac{1}{a-b}}$$



- Polynomial annealing rate avoids QCP bottleneck.

$$\xi \sim L = N^{1/d} \Rightarrow \begin{array}{l} \Delta \Gamma_c \sim \xi^{-1/\nu} \sim N^{-1/(d\nu)} \\ \Delta E_c \sim \xi^{-z} \sim N^{-z/d} \end{array}$$

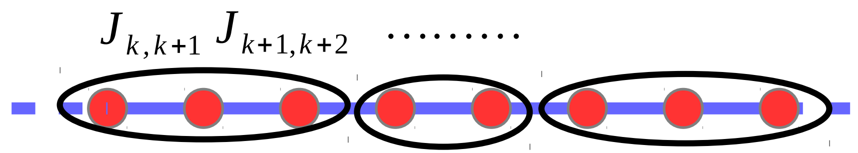
$$a = 2 - \alpha = (d+z)\nu$$

$$b = z\nu$$

Exceptions to Polynomial Scaling

Disorder

1D chain with i.i.d. random $J_{k,k+1}$



"Finite-size" critical field $\Gamma_c \approx \left(J_{12} J_{23} \cdots J_{n-1,n}\right)^{\frac{1}{n-1}}$

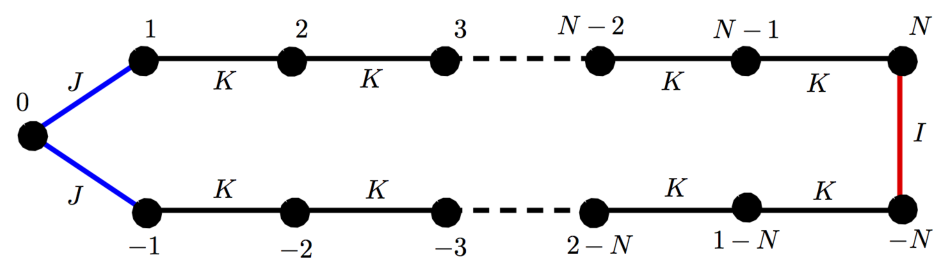
$$\Delta E_c \sim \mathrm{e}^{-c\sqrt{N}}$$

- Different parts of the system become critical at different times
- Slow dynamics as clusters of spins are flipped

- Not an issue with all-to-all connectivity
- "Fixable" by synchronizing phase transitions with local Γ_i

Frustration

1D loop with odd number of antiferromagnetic couplings



$I < J < K \qquad J^2 < IK$

- "Competition" between solutions
- Develops exponentially small gap in the ordered phase, $\Gamma < \Gamma_c$

Polynomial gap at $\Gamma_c = K$

Exponential gap at $\Gamma_* = \dfrac{1}{I} \dfrac{\left(K^2 - J^2\right)\left(J^2 - I^2\right)}{I^2 + K^2 - 2J^2}$

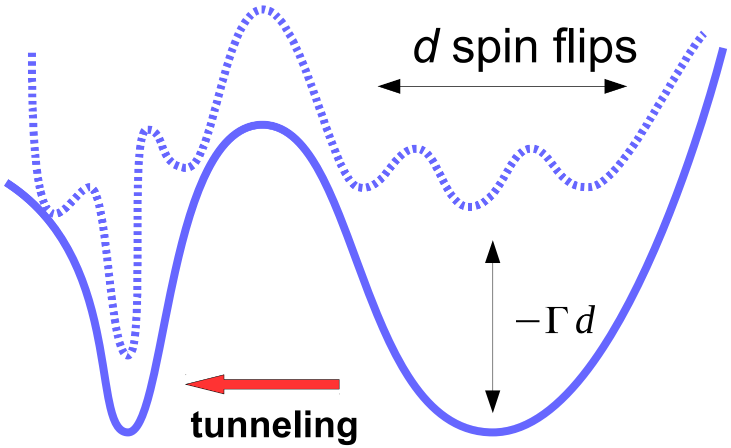
Spin-Glass Bottlenecks

- Spin-glass phase characterized by many valleys
- Energy levels "reshuffled" as Γ changes
- But: Ground state is less sensitive (extreme value)

Santoro *et al.*, Science '02
Altshuler *et al.*, PNAS '10
Farhi *et al.*, PRE '12

Effect of the Transverse Field

- "Smoothes out" energy landscapes on scales ~Γ
- Lowers energy of wide valleys
- Deep-and-narrow and shallow-and-wide valleys can come into resonance



Fractal Energy Landscapes

- No intrinsic scale $(\Gamma \ll \Gamma_c)$
- Expected # of hard bottlenecks

$$N_{h.b.}[\Gamma_1, \Gamma_2] = f(\Gamma_2/\Gamma_1)$$

- Additivity: $N_{\mathrm{h.b.}}[\Gamma_1;\Gamma_2] = N_{\mathrm{h.b.}}[\Gamma_1;\Gamma'] + N_{\mathrm{h.b.}}[\Gamma';\Gamma_2]$

$$N_{\mathrm{h.b.}} = \alpha \ln \frac{\Gamma_c}{\Gamma_{\min}}$$

$$\Gamma_c \sim 1 \qquad \Gamma_{\min} \sim \frac{1}{N^{\delta}}$$

Associative Memory: Hopfield Network

Nishimori & Nonomura, JPSJ '96

- Craft Hamiltonian encoding *p* \`patterns'

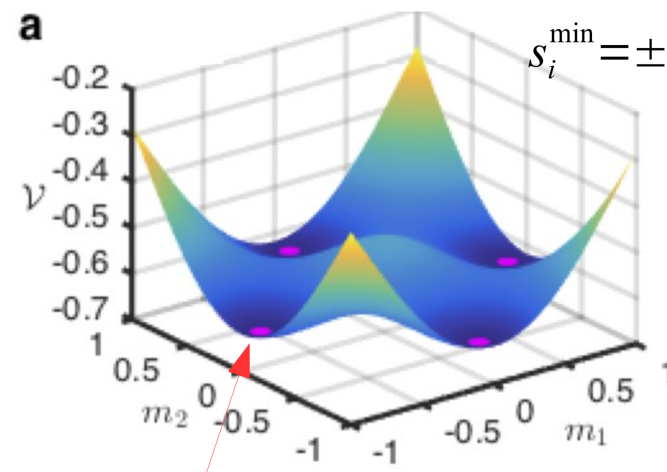
$$\xi_i^{(1)}=\{1,-1,-1,\ldots,1\}$$
$$\xi_i^{(2)}=\{-1,1,-1,\ldots,-1\}$$
$$\ldots\ldots\ldots\ldots\ldots$$

$$J_{ik}=\frac{1}{N}\sum_{\mu=1}^{p}\xi_i^{(\mu)}\xi_k^{(\mu)}$$

- Small *p*: \`project' onto patterns

$$\vec{m}=\frac{1}{N}\sum_i \vec{\xi}_i\langle\hat{\sigma}_i^z\rangle$$

$$s_i^{\min}=\pm\xi_i^{(\mu)}$$



attractors, $\pm O(1)$

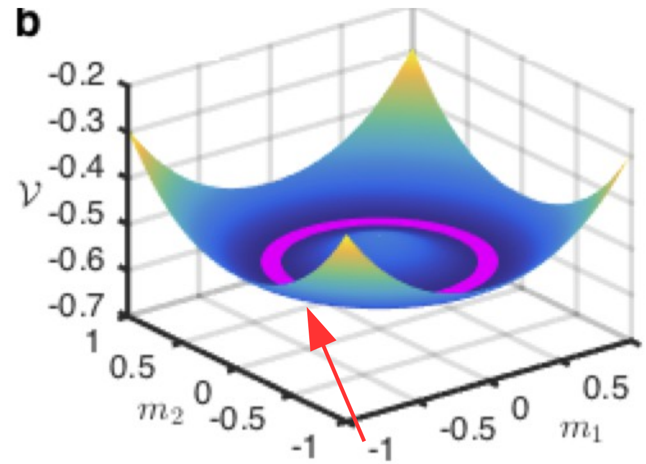
- Barriers are *O*(*N*)
- Classical (Γ=0) gap is *O*(1)
- QCP is the only bottleneck: $\Delta E_c \sim N^{-1/3}$, $\Delta\Gamma_c \sim N^{-2/3}$

Capacity limit: *p*=*O*(*N*)

- Spurious states become globally stable: $s_i^{\min}=\pm\mathrm{sgn}\sum_{\mu}\alpha_\mu\xi_i^{(\mu)}$
- Smaller barriers; classical gap vanishes asymptotically

Hopfield Model with Gaussian Patterns

- Spurious states appear for *p*≥2
- Classical gap is $O(1/N)$
- Barriers are $O(\sqrt{N})$



degenerate to *O*(*N*)

Mean Field Theory

- Finite-temperature partition function

$$Z(\beta)=\sum_{[\{s_i(t)\}]} e^{\frac{1}{2}\int_0^{\beta}(\sum_i \vec{\xi}_i s_i(t))^2 \mathrm{d}t+\sum_i K[s_i(t)]}$$

$$(\text{\# of kinks})\times\frac{1}{2}\ln\tanh(\Gamma\Delta t)$$

$$J_{ik}=\frac{1}{N}\vec{\xi}_i\vec{\xi}_k$$

- Rewrite as a path integral using Hubbard-Stratonovich

$$Z(\beta)=\int[\mathrm{d}\vec{m}(t)]\mathrm{e}^{-\frac{N}{2}\int_0^{\beta}\vec{m}^2(t)\mathrm{d}t+\sum_i \ln Z_i}$$

$$\mathrm{e}^{\frac{1}{2}(\sum_i \vec{\xi}_i s_i)^2}\propto\int \mathrm{d}\vec{m}\,\mathrm{e}^{-\vec{m}^2/2+\vec{m}\vec{\xi}_i s_i}$$

- Single-site partition function

$$Z_i=\sum_{[s(t)]}\mathrm{e}^{\int_0^{\beta}h_i(t)s(t)\mathrm{d}t+K[s(t)]}=\mathrm{Tr}\,\mathrm{T}\,\mathrm{e}^{\int_0^{\beta}(h_i(t)\hat{\sigma}^z+\Gamma\hat{\sigma}^x)\mathrm{d}t}$$

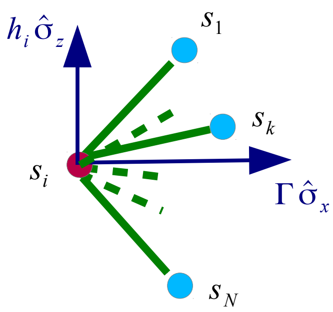
$$h_i(t)=\vec{\xi}\vec{m}(t)$$

Mapping to Ordinary Quantum Mechanics

- Saddle-point solution is stationary

$$\vec{m}=\frac{1}{N}\sum_i \vec{\xi}_i \frac{h_i}{\sqrt{\Gamma^2+h_i^2}} \qquad h_i=\vec{\xi}_i \vec{m}$$

replace sum by
disorder average



- Finite-N corrections: path integral is dominated by $\vec{m}(t)\approx m_\Gamma \begin{pmatrix} -\sin\vartheta(t) \\ \cos\vartheta(t) \end{pmatrix}$
- $\vartheta(t)$ is slow-varying

$$\ln Z_i=\int_0^\beta \left(\sqrt{\Gamma^2+h_i^2(t)}+O\left(\left(\mathrm{d}h_i/\mathrm{d}t\right)^2\right)\right)\,\mathrm{d}t$$

non-adiabatic
corrections

- Disorder realization – dependent partition function

$$Z(\beta)=\mathrm{e}^{-N\beta\langle F\rangle}\int[\mathrm{d}\vec{\vartheta}(t)]\,\mathrm{e}^{-\int_0^\beta \left(M(\mathrm{d}\vartheta/\mathrm{d}t)^2/2+V_\Gamma(\vartheta)\right)\mathrm{d}t}$$

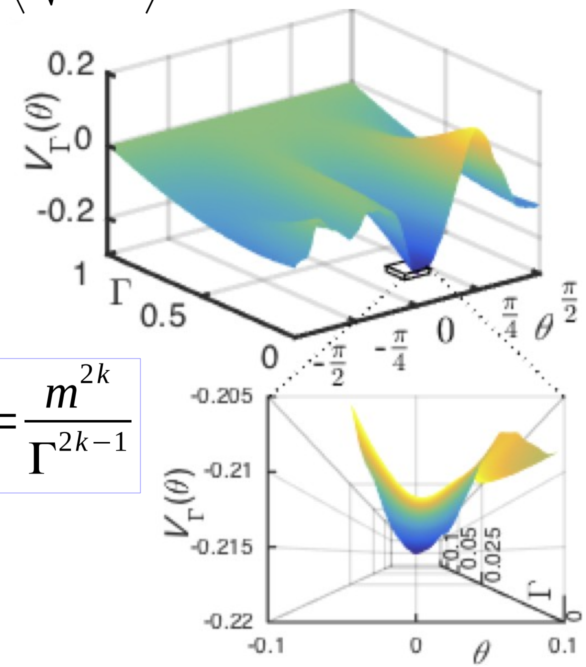
- Low energy spectrum is equivalent to that of a particle on a ring

$$V_\Gamma(\vartheta)=-\sum_i \sqrt{\Gamma^2+m_\Gamma^2\xi_i^2\sin^2(\vartheta-\theta_i)}+N\langle\sqrt{\cdots}\rangle$$

$$\boxed{\vec{\xi}_i=\xi_i\begin{pmatrix}\cos\theta_i\\ \sin\theta_i\end{pmatrix}}$$

Evolution of Random Potential

$$V_\Gamma(\vartheta) = -\sum_i \sqrt{\Gamma^2 + [m_\Gamma \xi_i \sin(\vartheta - \theta_i)]^2} + N\langle\sqrt{\cdots}\rangle$$



Scales as $\sqrt{N}$ (central limit theorem)

Smooth near critical point

$$\frac{1}{\sqrt{N}} V_\Gamma(\vartheta) = C + \sum_k (A_k \cos 2k\vartheta + B_k \sin 2k\vartheta)$$

$$A_k, B_k = \frac{m^{2k}}{\Gamma^{2k-1}}$$

Becomes increasingly rugged for small Γ

Continuous Process

Orthogonalize correlated 2D random process

$$\langle \zeta_n(\theta)\zeta_{n'}(\theta')\rangle = \delta_{nn'}\delta(\theta - \theta')$$

white noise

$$V_\Gamma(\vartheta) = \sum_{n=0}^{\infty} \int f_\Gamma^{(n)}(\vartheta - \theta)\,\zeta_n(\theta)\,\mathrm{d}\theta$$

Choose $f_n(\vartheta)$ to match covariance $\langle V_\Gamma(\vartheta) V_{\Gamma'}(\vartheta')\rangle$

Use orthogonal polynomials (Laguerre) $f_\Gamma^{(n)}(\vartheta) \propto \int_0^\infty \sqrt{\Gamma^2 + \cdots} \times \xi^2 e^{-\xi^2/2} L_n^{(1)}(\xi^2/2)\,\mathrm{d}\xi$

Evolution of Random Potential (cont'd)

$$\frac{1}{\sqrt{N}} V_\Gamma(\theta) \propto (F_\Gamma * \chi)(\vartheta) + \sum_{n=1}^{\infty} (G_\Gamma^{(n)} * \eta_n)(\vartheta) + \mathrm{const}$$

smoothing kernel of width Γ

classical potential

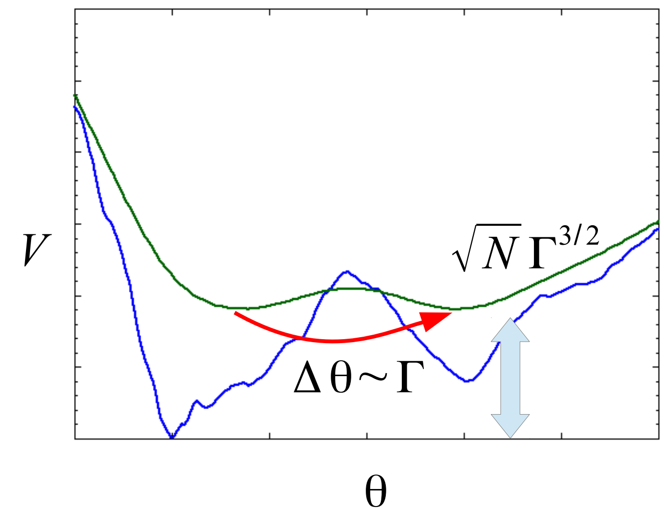
brownian motion

- Convolution with $F_\Gamma(\vartheta)$ raises energy of narrow valleys
- 2nd term vanishes for Γ=0; comparable contribution for Γ>0

Classical potential

Neglect near a global minimum

$$\frac{d^2\chi}{d\vartheta^2} + \cancel{\chi} = \zeta_0(\vartheta)$$



Condition on the fact that $\chi(\vartheta) \geq \chi(\theta_*) = \chi_*$

Without losing generality $\vartheta_* = 0, \chi_* = 0$

Classical Potential near Global Minimum

- Markov process (χ,υ) in `time' $\vartheta$ ($\upsilon=\frac{d\chi}{d\vartheta}$ is the `velocity')

$$\frac{\partial p}{\partial\vartheta}+\upsilon\frac{\partial p}{\partial\chi}-\frac{1}{2}\frac{\partial^2 p}{\partial\upsilon^2}=0$$

- Only include paths with $\chi\geq 0$:

$$\boxed{\lim_{\chi\to+0} p(\theta;\chi,\upsilon)=0 \text{ for } \upsilon>0}$$

- Renormalize probability so that it is conserved

$$q(\vartheta;\chi,\upsilon)\propto p(\vartheta;\chi,\upsilon)\underbrace{\int_{X>0} P(\Theta;X,Y|\vartheta;\chi,\upsilon)\,dX\,dY}_{\text{survival probability } P_\Theta(\chi,\upsilon)}$$

- Before: $p(\Delta\upsilon>0)=p(\Delta\upsilon<0)=1/2$
- After: $p(\Delta\upsilon>0)>1/2>p(\Delta\upsilon<0)$ (the process with $\upsilon'>\upsilon$ more likely to survive)

- Probability is conserved but adds repulsion: $+\frac{\partial}{\partial\upsilon}\left(\frac{1}{P_\Theta}\frac{\partial P_\Theta}{\partial\upsilon}q\right)$

"Stationary" Solution

Green's function satisfies time-reversed PDE

$$P(\Theta;\mathrm{X},\mathrm{Y}|\vartheta;\chi,\upsilon)=P(\vartheta;\chi,-\upsilon|\Theta;\mathrm{X},-\mathrm{Y})$$

Asymptotic form (independent of initial conditions):

$$p(\vartheta;\chi,\upsilon)\sim A\frac{p_*(\chi,\upsilon)}{\vartheta^{\alpha}}$$

Dimensional analysis: $[\chi]=[\vartheta]^{3/2},[\upsilon]=[\vartheta]^{1/2}$

$$p_*(\chi,\upsilon)=\chi^{2\alpha/3}p_*(\upsilon/\chi^{1/3})$$

ODE for $p_*(\nu)$ yields quantized eigenvalues $\alpha=\frac{1}{4}+\frac{3n}{2}$ for $n\geq 0$

- Dimensionless `time' $\mathrm{d}\tau=\chi^{-2/3}\mathrm{d}\vartheta$
- Dimensionless `velocity' $\nu=\upsilon/\chi^{1/3}$
- Dimensionless `coordinate' $\mu=\ln\chi$

Regard $(\vartheta,\chi,\upsilon)$ as a Markov process in `time' τ

Langevin Process

- PDE after the change of variables

$$\frac{\partial \bar{q}}{\partial \tau}+e^{2\mu/3}\frac{\partial \bar{q}}{\partial \vartheta}+\nu\frac{\partial \bar{q}}{\partial \mu}-\frac{\partial}{\partial \nu}\left(\frac{\partial U}{\partial \nu}\bar{q}\right)-\frac{1}{2}\frac{\partial^2 \bar{q}}{\partial \nu^2}=0$$

$$\boxed{U\sim\frac{\nu^3}{9}-\ln p_*(-\nu)}$$

- Describes a solution to a stochastic differential equation

$$\frac{d\nu_\pm}{d\tau}=-U'(\nu)\,\mathrm{sgn}(\tau)+\zeta(\tau)$$

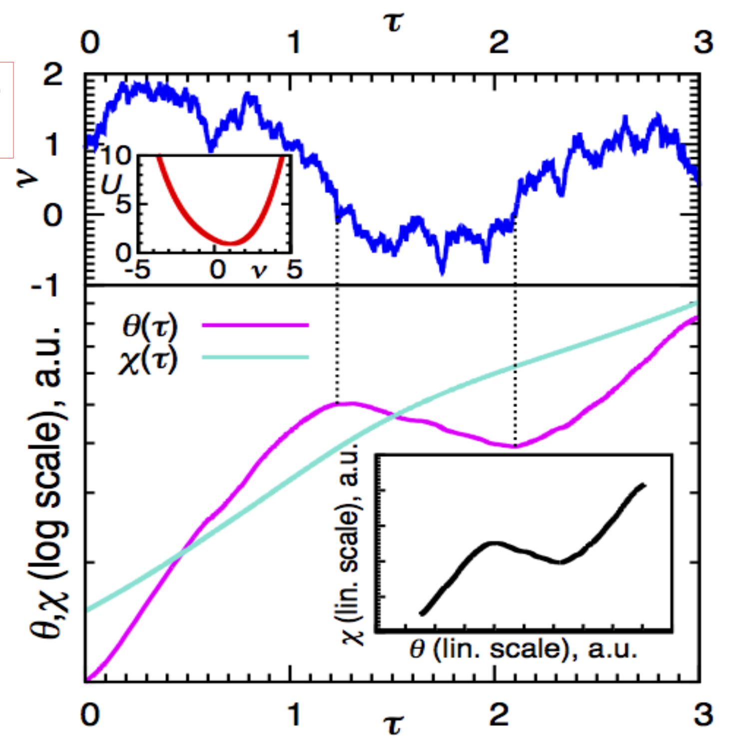
$$\boxed{\rho(\nu(0))\sim e^{-2U(\nu)}}$$

- Further integrated twice

$$\frac{d(\ln\chi)}{d\tau}=\pm\nu_\pm \qquad \frac{d\vartheta}{d\tau}=\pm\chi^{2/3}$$

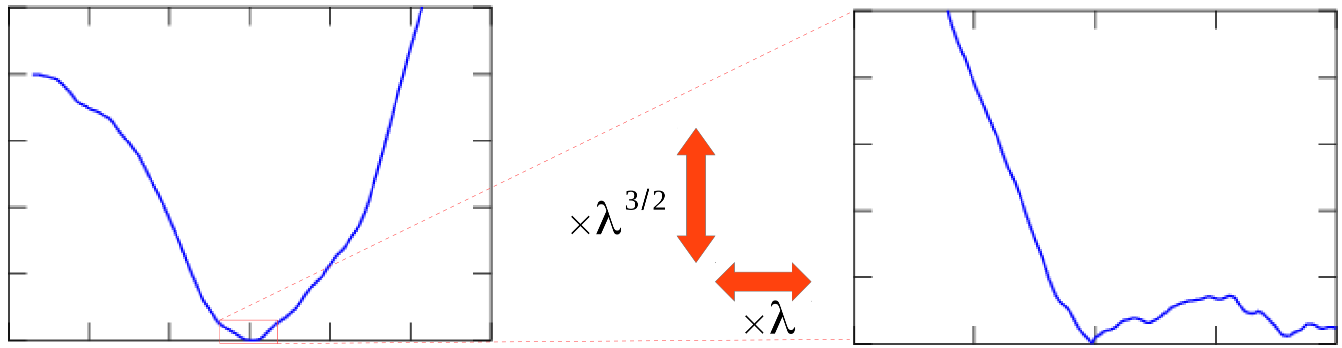
- To yield a parametric representation $(\chi(\tau),\vartheta(\tau))$ of function $\chi(\vartheta)$

- $\chi\sim\vartheta^{3/2}$ but can drop by arbitrarily large percentage

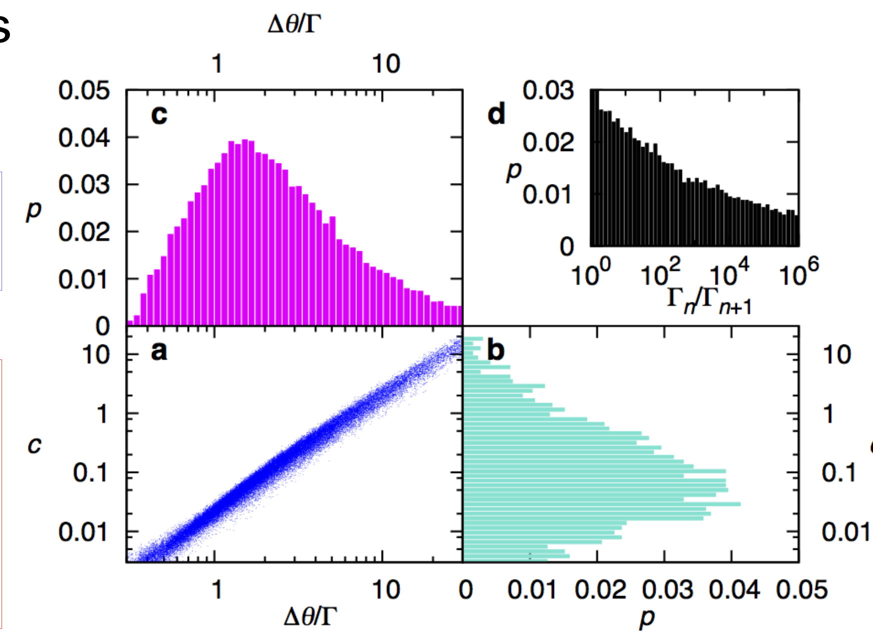


Results

- Energy landscape is a self-similar random process (every realization happens on some scale)



- There will be realizations where two minima compete
- Numerically integrate stochastic equations



Typical gap

$$V(\vartheta) \sim \frac{K}{2}(\vartheta - \vartheta_*)^2$$

$$\Delta E \sim \sqrt{K/M} \sim \frac{\Gamma^{3/4}}{N^{1/4}}$$

Minimum gap

$$K \sim \sqrt{N/\Gamma}$$
$$M \sim N/\Gamma^2$$
$$V \sim \Gamma^{3/2}\sqrt{N}$$
$$\Delta\vartheta \sim \Gamma$$

$$\Delta E \sim \mathrm{e}^{-\sqrt{MV}\,\Delta\vartheta} \sim \mathrm{e}^{-c(\Gamma N)^{3/4}}$$

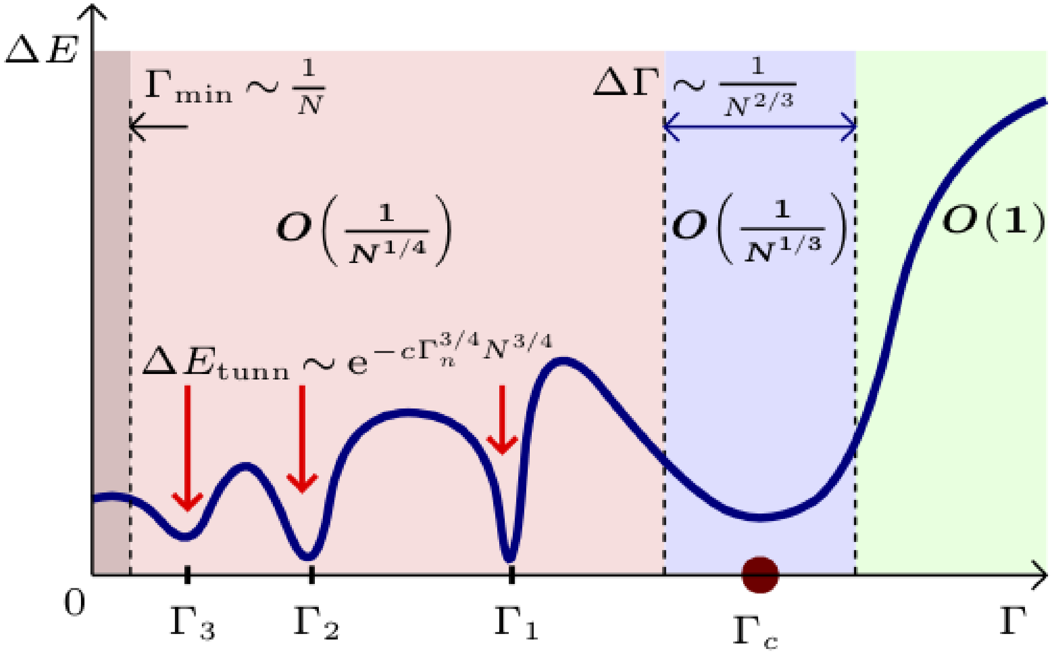
Discussion

- Bottlenecks progressively easier toward the end of the algorithm (problem solved for $\Gamma < 1/N$)

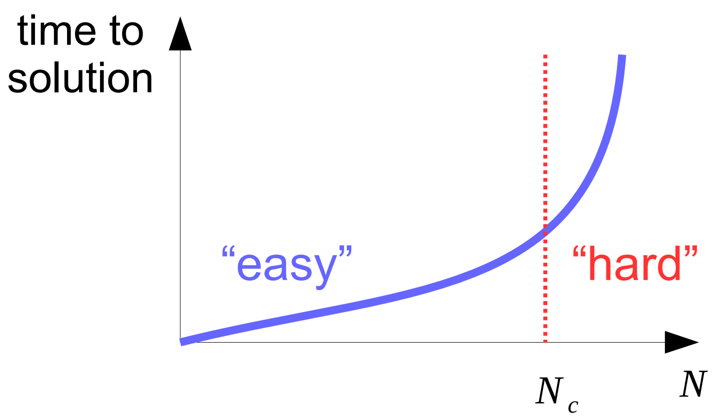
- Only become relevant for large problems

$$N_{\text{h.b.}} \approx \alpha \ln N > 1$$

- Crossover from polynomial to exponential complexity



$\alpha \approx 0.15 \Rightarrow N_c \sim 1000$



Cf. Sherrington-Kirkpatrick model:

- Classical gap scales as $1/\sqrt{N}$
- Barrier heights scale as $N^{1/3}$
- Stronger disorder fluctuations, $J_{ik} \sim 1/\sqrt{N}$