Quantum Adiabatic Optimization

vs

Quantum Monte Carlo

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adiabatic algorithm

[Farhi, Goldstone, Gutmann, Sipser '00]

Problem: Given $f:\{0,1\}^n \rightarrow \mathbb{Z}$, minimize f(z).

Approach: apply $H(s) = (1-s)\, H_X + s\, H_f$

$$H_X = -\sum_{i=1}^{n} \sigma_x^{(i)} \qquad H_f = \sum_{z \in \{0,1\}^n} f(z)|z\rangle\langle z|$$

equiv: H(s) = (1-s) (hypercube Laplacian) + s diag(f)

Adiabatic theorem:
Running for time $\mathrm{poly}(1 / \min_s [\lambda_1(s) - \lambda_0(s)])$
guarantees that we will end in the ground state of H_1.

Not discussed in this talk:

- noisy dynamics
- non-stoquastic Hamiltonians

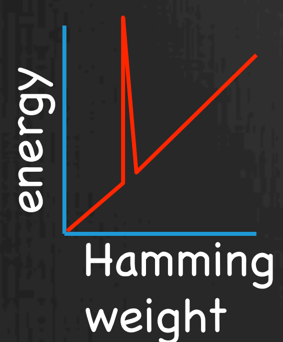
QAO vs simulated annealing (SA)

Simulated annealing:

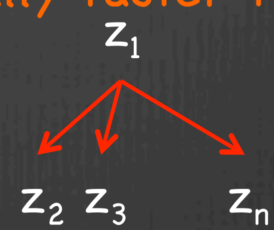
- Given state x repeatedly
  - Choose random neighbor y
  - With probability $\min(1, \exp((f(x)-f(y))/T))$ replace x with y. Otherwise do nothing.
- Gradually lower T

Farhi
Goldstone
Gutmann
q-ph/0201013

Problems where QAO is exponentially faster than SA



QMC succeeds



"bush of implications"

QMC succeeds (maybe)

Which problem features make QAO outperform classical?

possibilities for adiabatic optimization

pessimistic: There is a classical simulator that runs in time ≤ poly(time required by the adiabatic algorithm).

- Grover exhibits quadratic separation.
- evidence in favor: QMC (for stoquastic Hamiltonians).

optimistic: Stoquastic adiabatic evolution is universal for quantum computing.

- Would imply collapse of PH & "approx counting = exact counting". (Proof uses QMC + post-selection.)
- Nothing rules out fast adiabatic algorithms for factoring or 3SAT.

intermediate: Exponential speedups (i.e. no simulation) but weaker than general-purpose QC.

- Oracle speedup for mostly adiabatic evolution (NSK '12)
- evidence in favor: QMC sometimes takes exponential time

quantum Monte Carlo (QMC)

stoquastic Hamiltonians: $H_{xy} \leq 0$ for $x \neq y$.

- implies $\rho = \dfrac{e^{-\beta H}}{\operatorname{tr} e^{-\beta H}}$ is entrywise nonnegative
- $|\psi_0\rangle\langle\psi_0| = \lim_{\beta\to\infty} \rho$ is too.

aside: H gapped → $p(z)=\langle z|\psi_0\rangle^2$ has high conductance

$$Z = \sum_{z\in\{0,1\}^n} \langle z| \left(e^{\frac{-\beta H}{L}}\right)^L |z\rangle = \sum_{z_1,\ldots,z_L\in\{0,1\}^n} \prod_{i=1}^{L} \underbrace{\langle z_i|\, e^{-\frac{\beta H}{L}}\, |z_{i+1}\rangle}_{\geq 0}$$

can estimate by sampling from

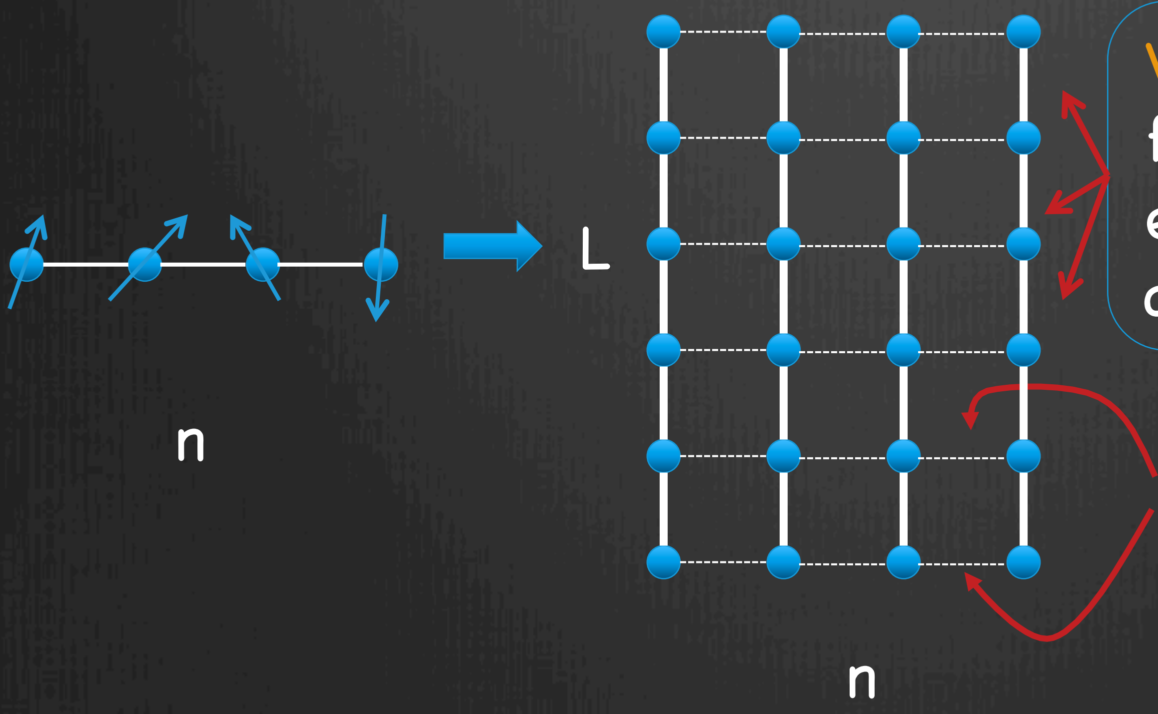
$$\pi(z_1,\ldots,z_L) = \frac{1}{Z}\prod_{i=1}^{L} \langle z_i|\, e^{-\frac{\beta H}{L}}\, |z_{i+1}\rangle =: \frac{1}{Z}\exp(-H_{\rm cl}(z_1,\ldots,z_L))$$

What is H_{cl}?

$$\langle z_i | e^{-\frac{\beta H}{L}} | z_{i+1} \rangle \approx e^{\frac{-\beta H_{\mathrm{diag}}(z_i)}{L}} \langle z_i | e^{-\frac{\beta H_{\mathrm{off}}}{L}} | z_{i+1} \rangle$$

e.g. 1-D transverse Ising model: $H = \sum_i Z_i Z_{i+1} - \Gamma \sum_i X_i$

→ 2-D classical ferromagnetic Ising model



Vertical bonds:
ferromagnetic
energy $\approx \ln(\beta L / \Gamma)$, i.e.
disagree prob $\approx \beta \Gamma / L$.

Horizontal bonds:
$= \beta H_D / L$

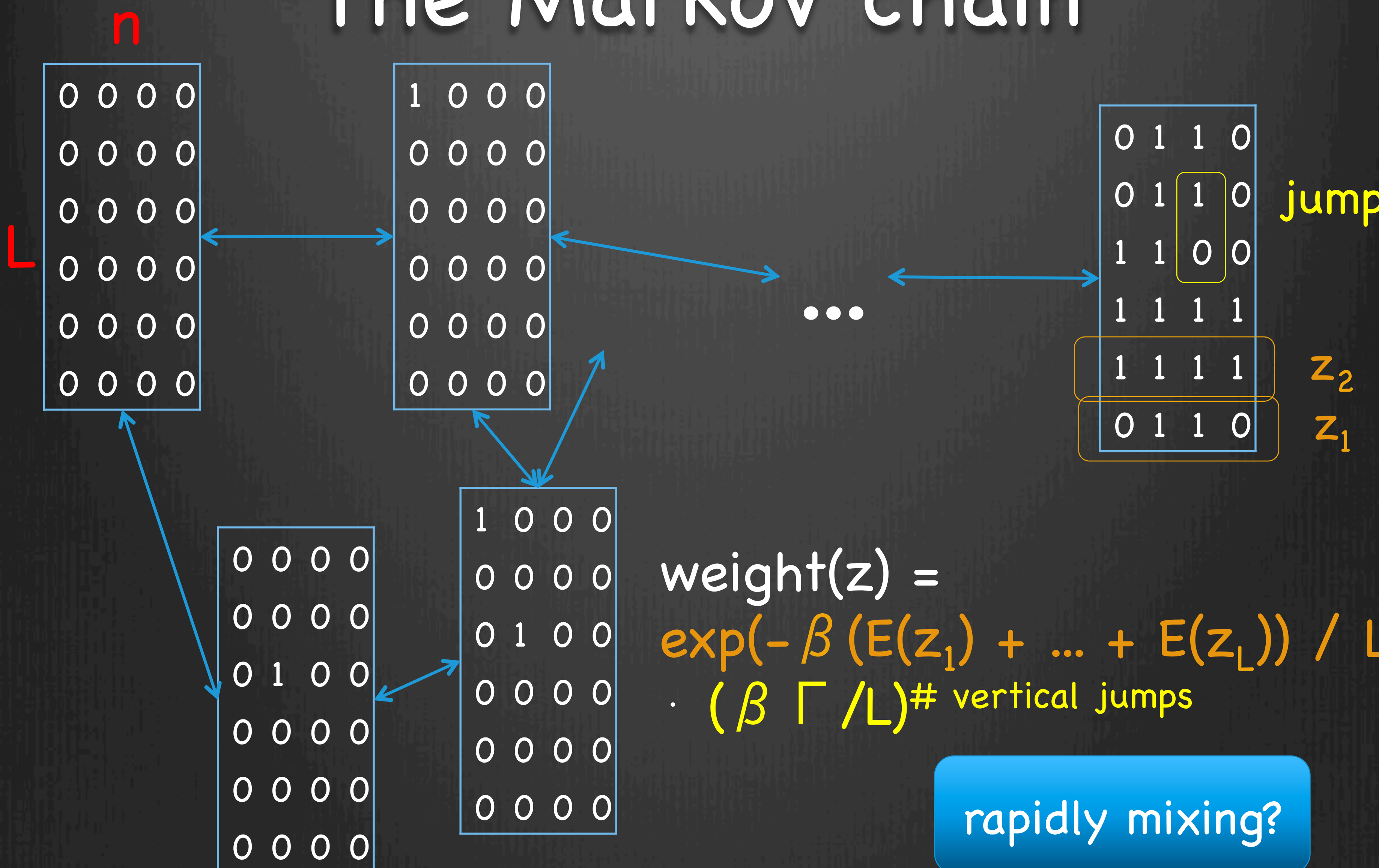
standard part of QMC

1. Use local moves (Glauber or Metropolis) to generate samples from $\pi(z_1, \ldots, z_L)$.
   Run-time/accuracy tradeoff unknown in general.

2. Use sampling-to-counting equivalence to estimate Z or $\langle O \rangle = \mathrm{tr}[O\, e^{-\beta H}]/Z$.

Problem reduces to bounding mixing time (equiv. gap) of a classical Markov chain.

The Markov chain



$$\text{weight}(z) = \exp(-\beta\,(E(z_1) + \ldots + E(z_L))\,/\,L) \cdot (\beta\,\Gamma\,/L)^{\#\text{ vertical jumps}}$$

rapidly mixing?

can QMC simulate adiabatic evolution?

- Only if gap ≥ 1/poly(n).
  since we need $\beta \gg 1/\text{gap}$ for $e^{-\beta H} \approx |gs\rangle\langle gs|$
  and $\beta \propto$ # of imaginary time steps
- Only if we follow the adiabatic path.
  - Otherwise would solve NP-complete problems.
  - Technically useful as a "warm start" and to avoid unphysical/unlikely configurations.
- Even then there may be topological obstructions [Hastings-Freedman '13]

the path measure

[see also JSIBMTN 1603.01293]

random walk $z_1,\ldots,z_L$ on hypercube $\{0,1\}^n$

- conditioned to return ($z_{L+1} = z_1$)
- alternatively can use open boundary conditions.
- typically $\approx \beta\ \Gamma\ n$ total jumps

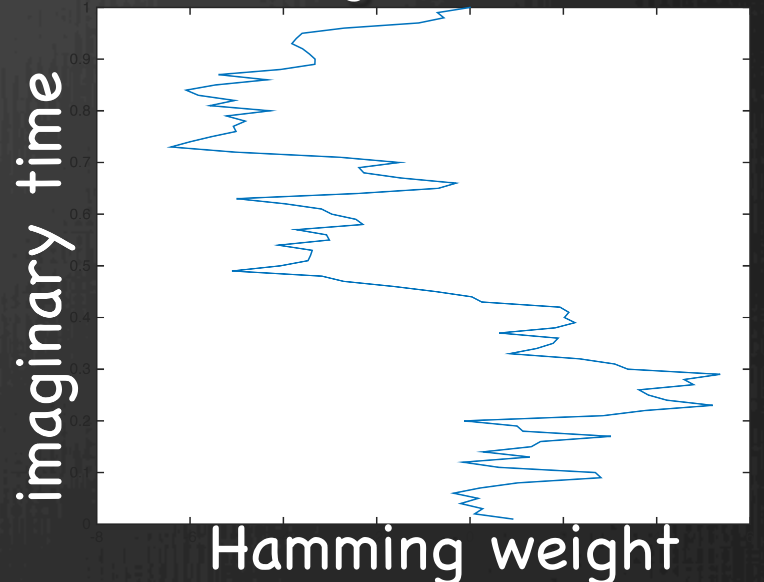
Suppose that f(z) depends only on Hamming weight |z|.

- look only at Hamming weight: $\{0,1\}^n \to \{0,1,\ldots,n\}$.
- take $n \to \infty$ and $\{0,1,\ldots,n\} \to [0,1]$.
- Brownian motion, or with closed B.C., "Brownian bridge"

with local Z fields ->
Brownian motion with drift
"Ornstein-Uhlenbeck bridge"

$dx(t) = \theta(\mu - x(t))\, dt + \sigma\ dB(t)$

θ = drift, μ = mean, σ = diffusion



local times of Brownian motion

Local time: $L^x(t)$ = amount of time Brownian motion $B(t)$ spends at point x.

Lévy's theorem: $\{L^0(t): t \geq 0\}$ and $\{S(t): t \geq 0\}$ have the same distribution, where $S(t) = \sup_{0 \leq s \leq t} B(s)$.

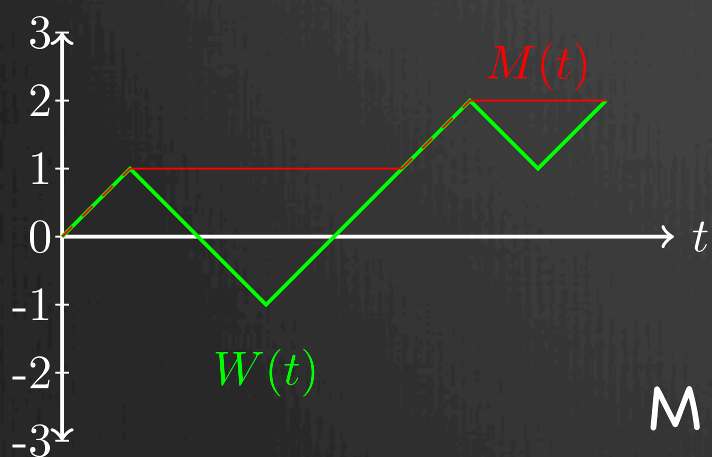
In fact, $(S-B, S) =^d (|B|, L^0)$
Additionally, $S =^d |B|$.

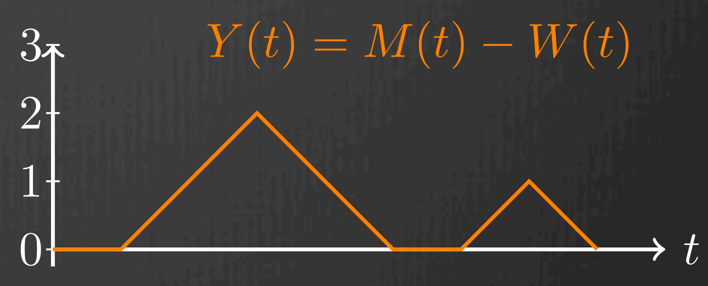
local times of Brownian motion

Local time: $L^x(t)$ = amount of time Brownian motion $B([0,t])$ spends at point x.

Lévy's theorem: $(S-B, S) =^d (|B|, L^0)$

Proof: consider discrete r walk: $W(n) = X(1) + \ldots + X(n)$ with $X(t) = \pm 1$.
Let $M(n) = \max(W(0), \ldots, W(n))$.





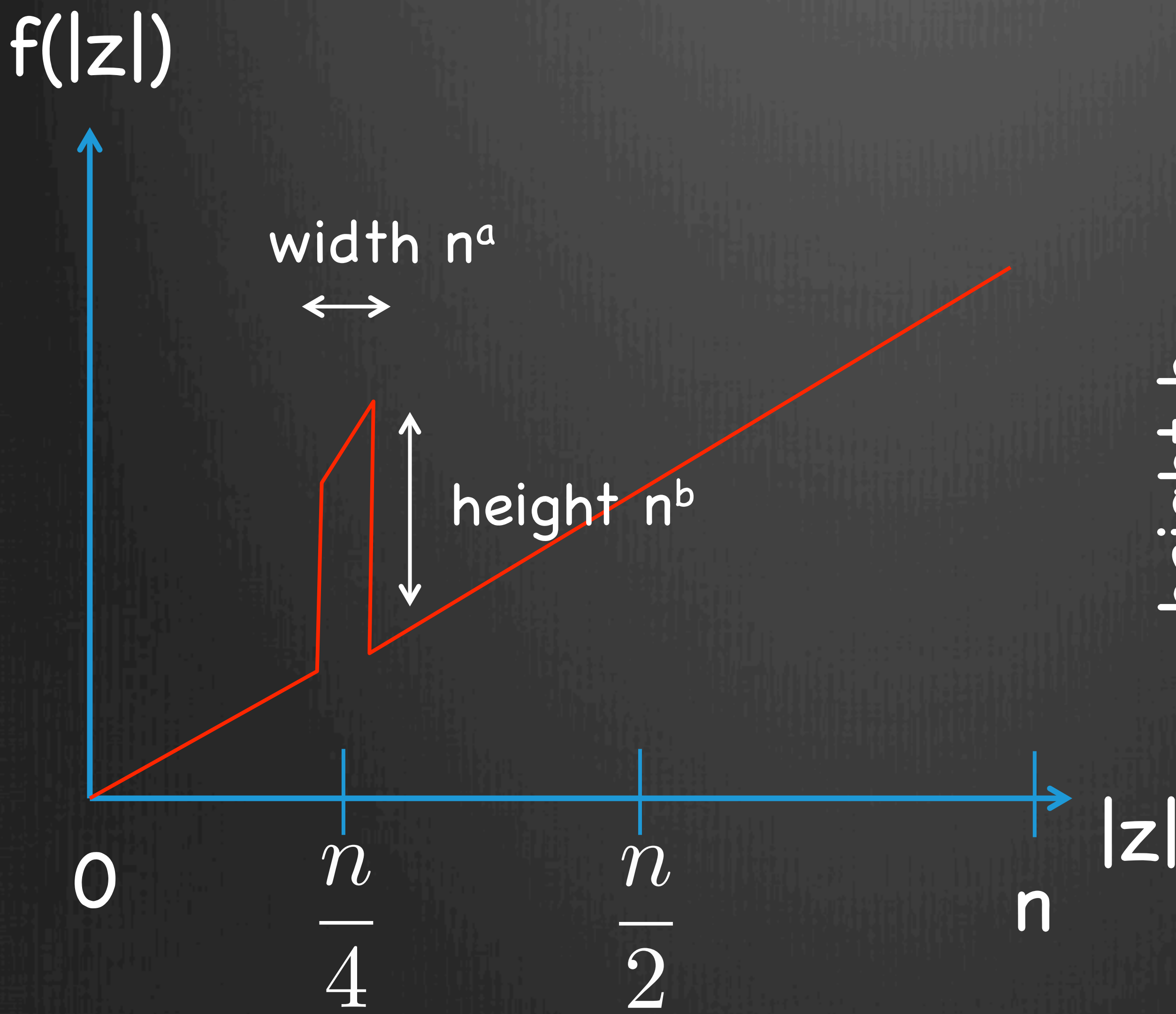
$Y(t) = M(t)-W(t) \approx^d |W(t)|$

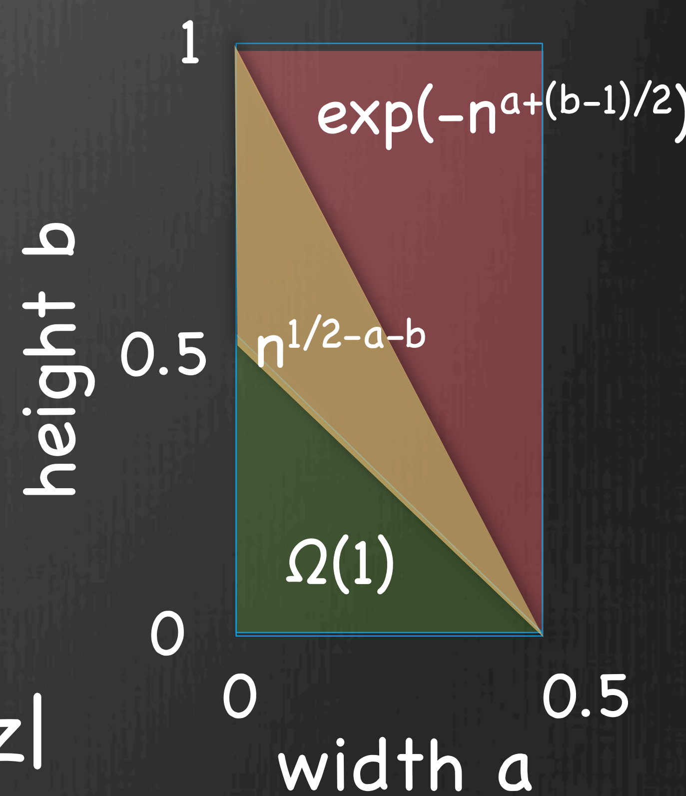
M = # of times M–W remains at 0 $\approx^d L^0$

figure adapted from *Brownian Motion* by Mörters and Peres.

Hamming weight + spike

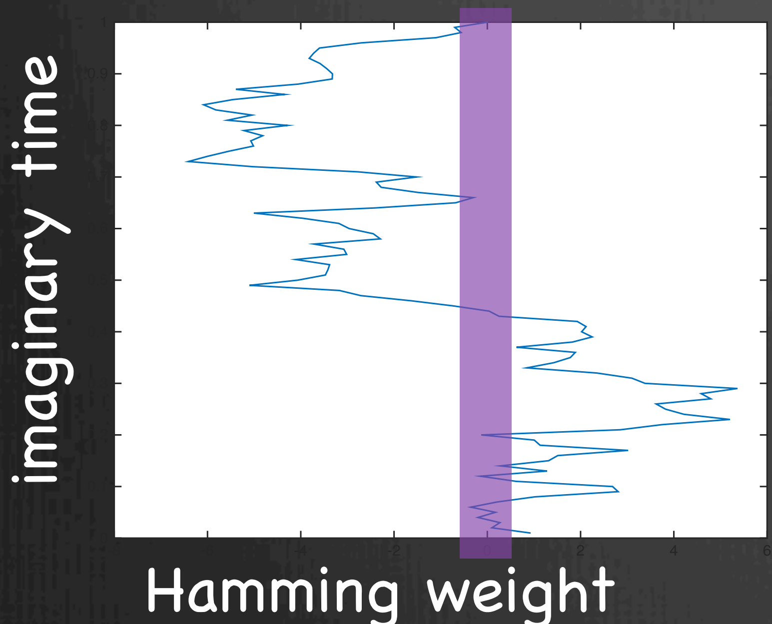
FGG '02
R '04
KC '15
BvD '16
JSIBMTN '16





QMC and tunnelling

spike
(width n^a, height n^b)



ST = normalized spike time
$\approx^d |N(0, n^{a-1/2})|$

proof using either Lévy's thm or quantum-classical correspondence.

Feynman-Kac thm:
Pr[path | spike] = $\exp(-\beta\ \mathrm{ST}\ n^b)$ Pr[path | no spike]

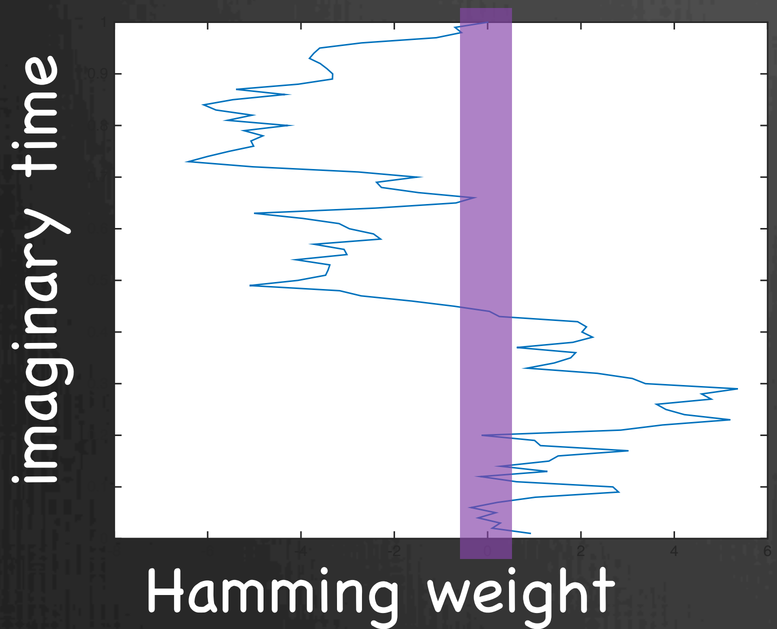
→ if $a+b<1/2$ then typical paths don't notice the spike.

instantons on the cheap

spike
(width n^a, height n^b)

$a<1/2$
$2a+b<1$

cf JSIBMTN'16



steps to traverse spike $\approx n^{2a}$

min ST $= n^{2a} / \beta \Gamma n$

Feynman-Kac →
prob reduced by $\approx \exp(-n^{2a+b-1})$

∴ $2a+b\leq 1$ is the theshold to cross the spike once.

canonical paths

Given Markov chain $P(x,y)$ with stationary distribution $\pi(x)$ and $Q(x,y) = P(x,y)\, \pi(y) = Q(y,x)$.
TFAE:

- P has a $\geq 1/\text{poly}(n)$ gap between the top two eigenvalues
- The conductance Φ is $\geq 1/\text{poly}(n)$.
  $\Phi = \min_S Q(S, S^c) / \pi(S)\, \pi(S^c)$
- For any x,y there exists a path γ_{xy} from x -> y routing $\pi(x)\, \pi(y)$ units of flow such that each edge e has load $\leq \text{poly}(n)\, Q(e)$.
  ("canonical paths/flows")

Heuristics analyze some plausible cut.
Proofs analyze all cuts or construct paths.

conductance

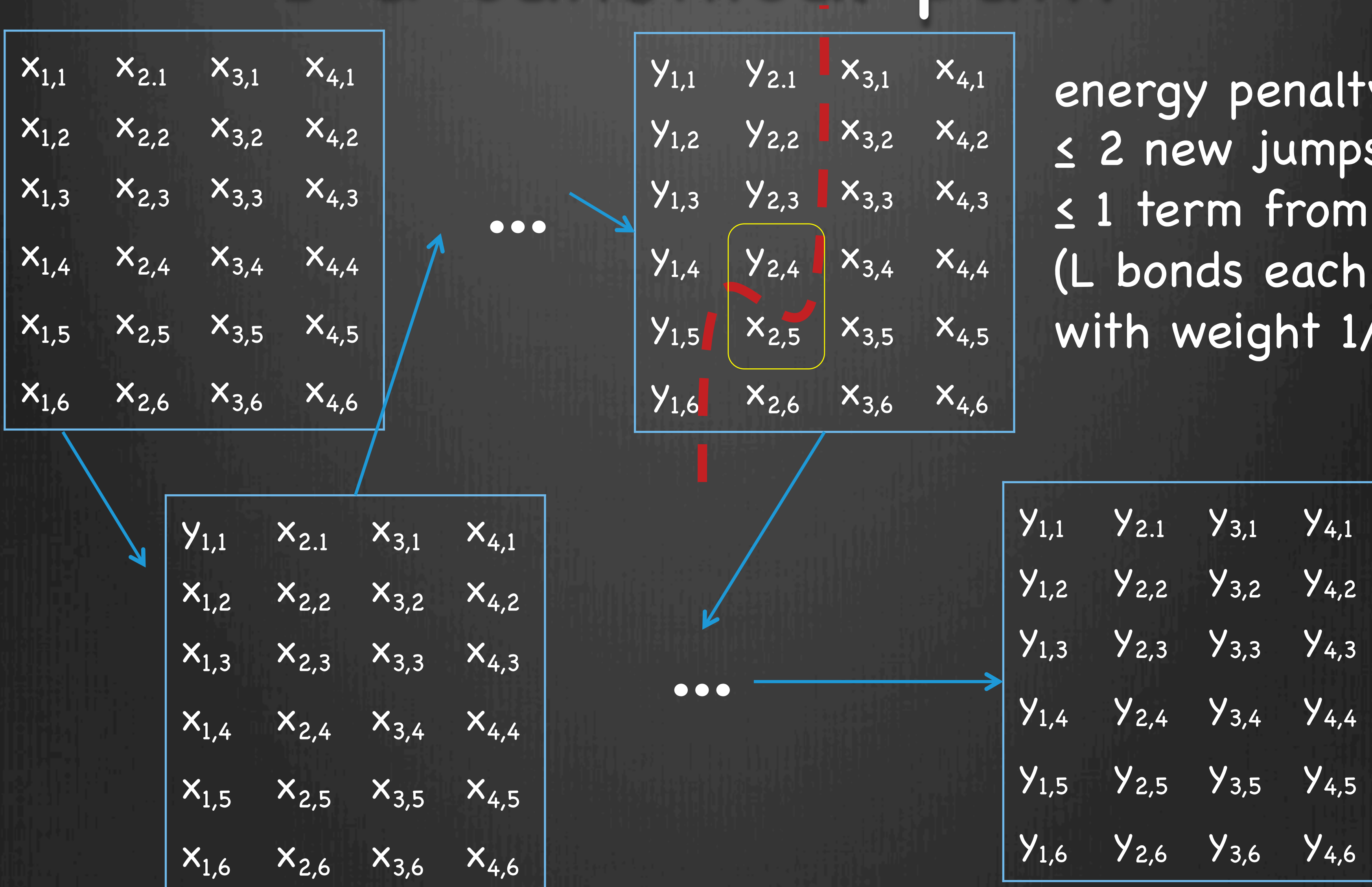
canonical paths

open questions

- multidimensional / non-bit-symmetric tunneling.
  The $a+b<1/2$ approach generalizes to whenever
  - The unperturbed problem has good canonical paths.
  - The perturbation is small relative to the gap.

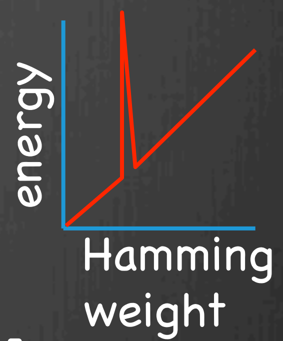
  What about the $2a+b < 1$ scenario?
- Quantum state geometry vs QMC geometry.
  - Ground states of gapped Hamiltonian have high conductance.
  - When does this imply that paths in QMC do too?
- Poly-time simulation of AQC or exponential separation?

1-d canonical path



energy penalty:
≤ 2 new jumps
≤ 1 term from H_D
(L bonds each
with weight 1/L.)

QMC on the spike



$$E'(z) = |z| + n^{\alpha} \, 1_{|z|=n/4}$$

Quantum gap $\propto 1 - n^{\alpha - 1/2}$ for $\alpha < 1/2$ [Reichardt]
or $n^{\alpha - 1/2}$ for $\alpha > 1/2$.
We show QMC works when $\alpha < 1/2$.

relate to spikeless Hamiltonian

$$E(z) = |z|$$

$$\pi(z_{1,1}, \ldots, z_{n,L}) = \pi_0(z_{1,1}, \ldots, z_{1,L}) \cdot \ldots \cdot \pi_0(z_{n,1}, \ldots, z_{n,L})$$

n decoupled 1-D Ising models.

$$\pi'(z) = C \, \pi(z) \exp(-n^{\alpha} \, [\# \, |z_i| = n/4] \, / \, L)$$