Quantum Algorithms for Approximating Partition Functions

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(w/ Arjan Cornelissen)

Estimating partition functions

Given a classical Hamiltonian $H : \Omega \to \{0,1,\ldots,n\}$

and an inverse temperature β

approximate the partition function $Z(\beta) = \mathrm{Tr}\left(e^{-\beta H}\right)$

Energy basis = standard basis

Gibbs state: $|\pi_\beta\rangle \propto \sum_i e^{-\beta H(i)} |i\rangle$

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Gibbs state: $|\pi_\beta\rangle = \frac{1}{\sqrt{Z(\beta)}} \sum_i e^{-\beta H(i)} |i\rangle$

Quantum algorithms hold the promise of faster statistical estimation

- Heisenberg vs shot-noise limits, quantum metrology
- Quantum phase estimation
- Quantum counting, quantum mean estimation
- …

How far can we push this advantage?

- Generic methods to turn classical stat. algos into (faster) quantum algos?
- Quadratic speedups?
- Highly structured estimation tasks?

Estimating partition functions

- Partition functions are ubiquitous
  - statistical physics
  - combinatorics (counting matchings, independent sets…)
  - linear algebra (permanents)
  - convex geometry (volume of a body)
  - machine learning (graphical models)
  - …

Estimating partition functions

- Partition functions are ubiquitous
- Related to counting (generating functions) and phase transitions
- Exact computation is often #P-hard
- … but there exists efficient approximation methods (MCMC, Taylor's approximation, correlation decay, …)

Main Result

The classical Markov Chain Monte Carlo (MCMC) algorithms★ for estimating $Z(\beta)$ can be speed-up by quantum algorithms running in time

$$\approx \log^{1/4}|\Omega| \times \sqrt{\text{time of classical MCMC algo}}\,.$$

$\geq \log|\Omega|$

($\Omega =$ configuration space)

This class of methods includes the best known algorithms for:

- number of independent sets, colorings, matchings
- Ising, Potts, monomer-dimer,… models
- volume of convex bodies
- permanent of nonnegative matrices

★ Štefankovič, Vempala, Vigoda. "Adaptive Simulated Annealing: A Near-Optimal Connection between Sampling and Counting", 2009.

Main Result

$$\approx \log^{1/4}|\Omega| \times \sqrt{\text{time of classical MCMC algo}}\,.$$

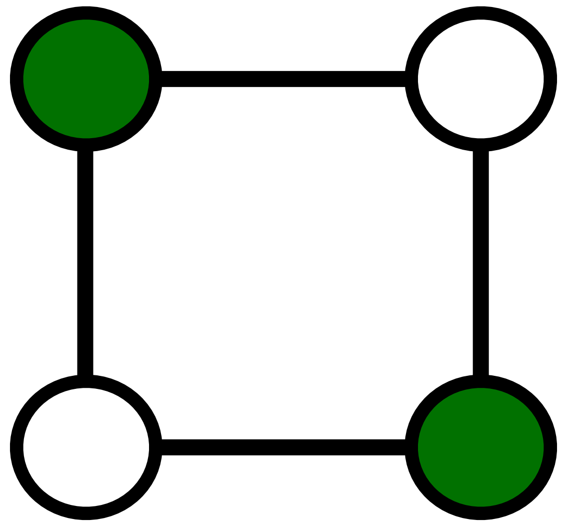
Aharonov, Ta-Shma 2003	Szegedy 2004	Wocjan, Abeyesinghe 2008	Montanaro 2015	Harrow, Wei 2020	Arunachalam, Havlicek, Nannicini, Temme, Wocjan 2022	H., Cornelissen 2023
1	2	1	3	4,5	5	3,4,6

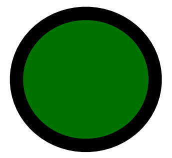
1. Quantum simulated annealing
2. Szegedy's quantum walk
3. Variance reduction
4. Non-destructive estimation
5. Cooling schedule computation
6. Unbiased estimation

The independent set partition function

Independent set

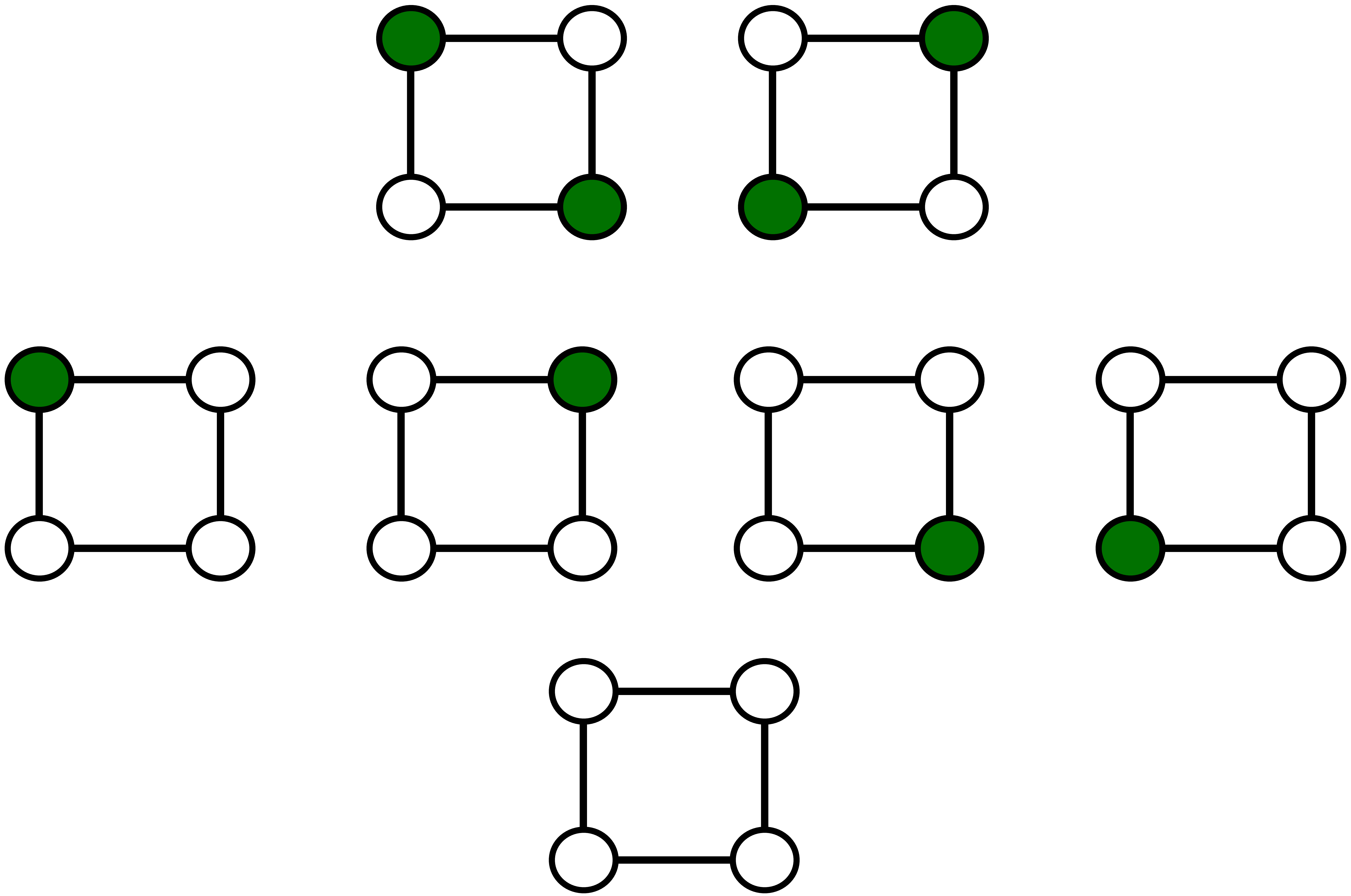
= subset of non-adjacent vertices



 = occupied

Hard-core gas model in statistical physics

independent sets = 7



Input: graph G
Output: # independent sets of G

#P-hard in many regimes

Bipartite graphs
[Provan,Ball’83]

3-regular graphs
[Dyer,Greenhill'00]

...

Exact counting → Approximate counting?

Input: graph G and $\epsilon \in (0,1)$
Output: S s.t. $(1-\epsilon)$ #ind $\leq S \leq (1+\epsilon)$ #ind

- Graphs with maximum vertex-degree ≤ 5: $(n = \#\text{vertices})$

Classical algorithms	Quantum algorithms
$\tilde{O}(n^2/\epsilon^2)$	$\tilde{O}(n^{5/4}/\epsilon)$
[Štefankovič,Vempala,Vigoda'09] [Chen,Liu,Vigoda'21]	[H. Cornelissen'23]

- Graphs with maximum vertex-degree > 5:

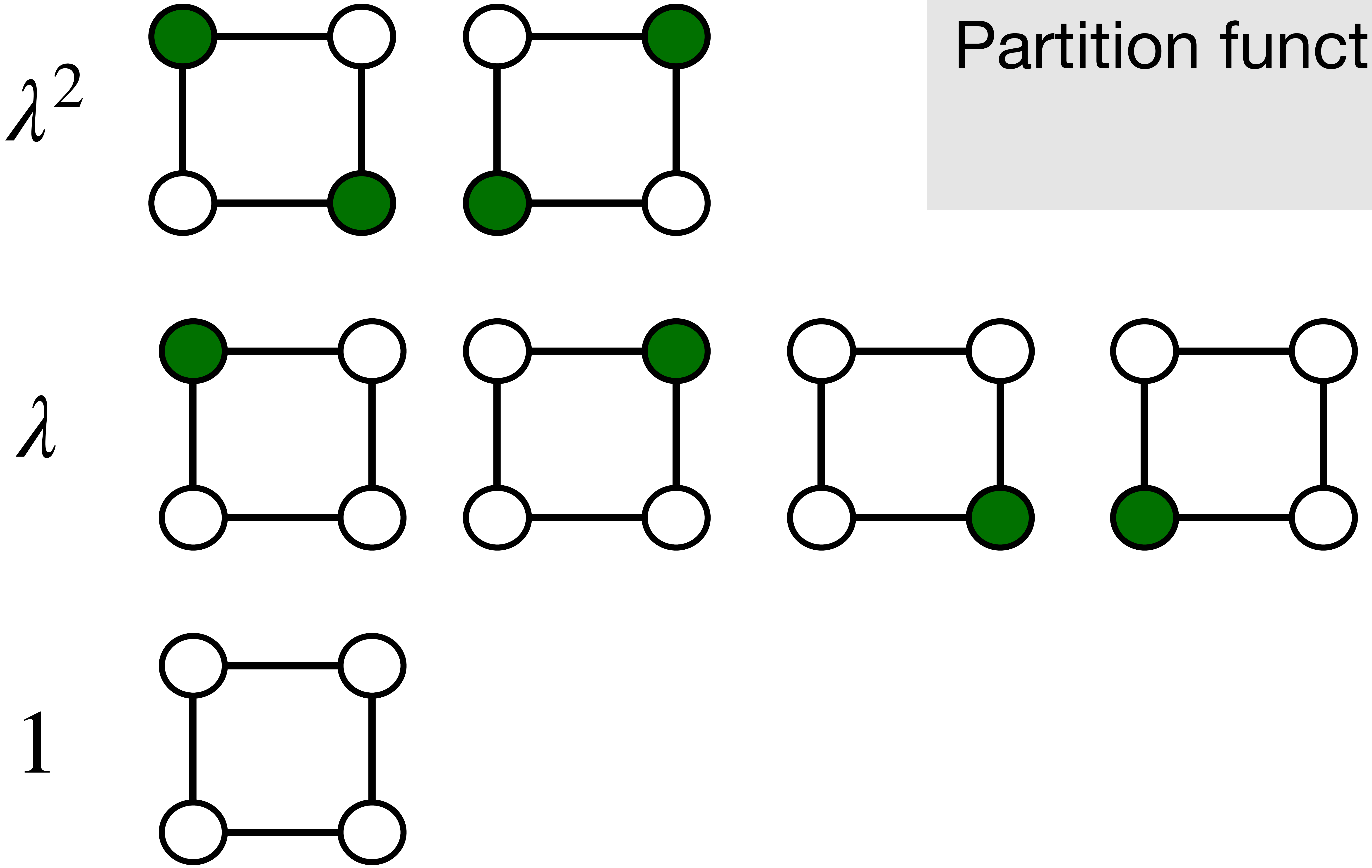
No FPRAS unless NP = RP [Sly'10]

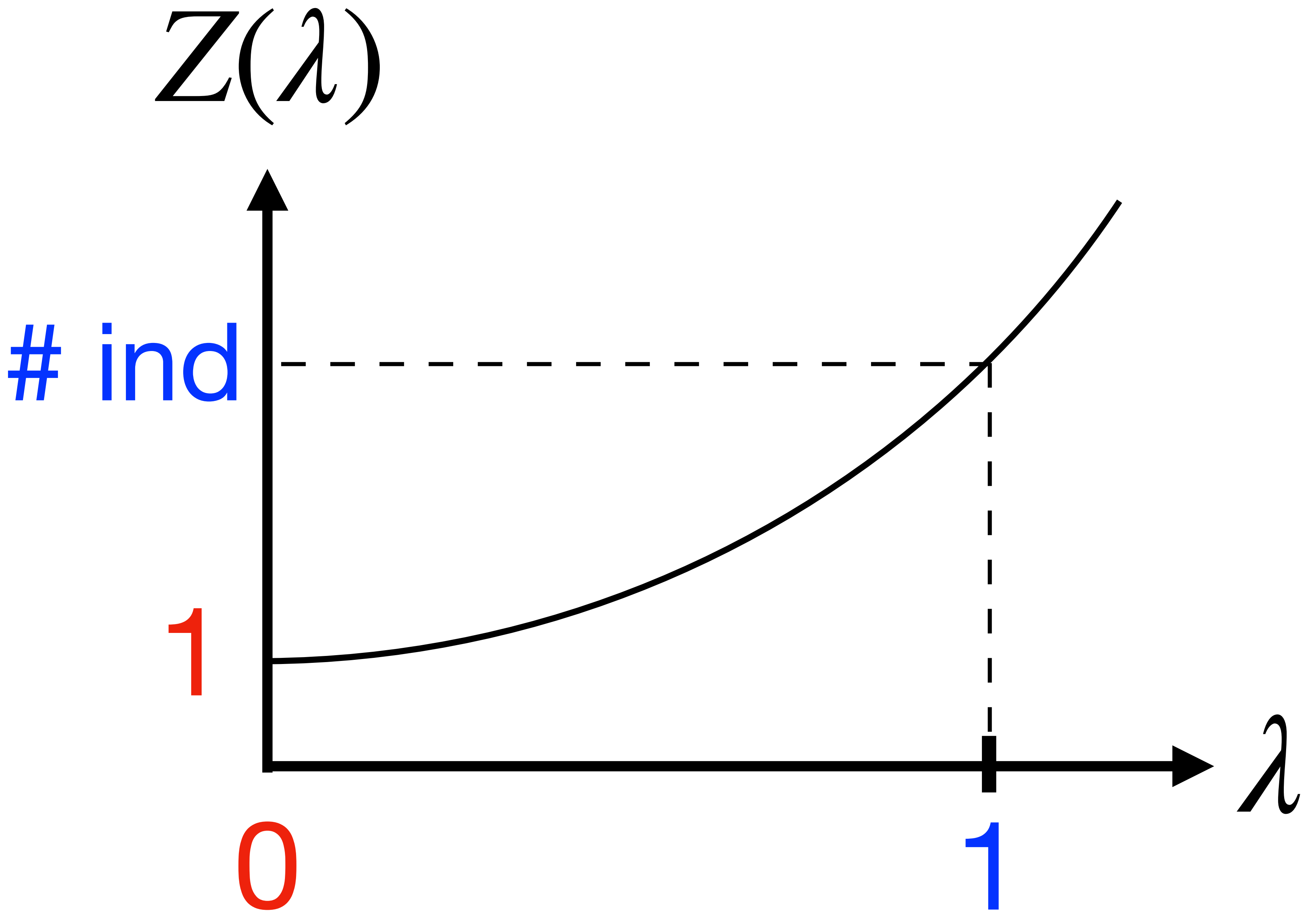
Classical MCMC method
for independent sets

Weighted independent sets

λ = fugacity

Partition function: $Z(\lambda) = \sum_{I \text{ ind. set}} \lambda^{|I|}$





Partition function: $Z(\lambda) = \sum_{I \text{ ind. set}} \lambda^{|I|}$

Sampling $\Rightarrow$ **Estimating**

Independent set I

with probability $\pi_\lambda(I) = \frac{\lambda^{|I|}}{Z(\lambda)}$

Gibbs sampling

Ratio estimation

$$\frac{Z(\lambda')}{Z(\lambda)} = \mathrm{E}_{I \sim \pi_\lambda}\left(\frac{\lambda'}{\lambda}\right)^{|I|}$$

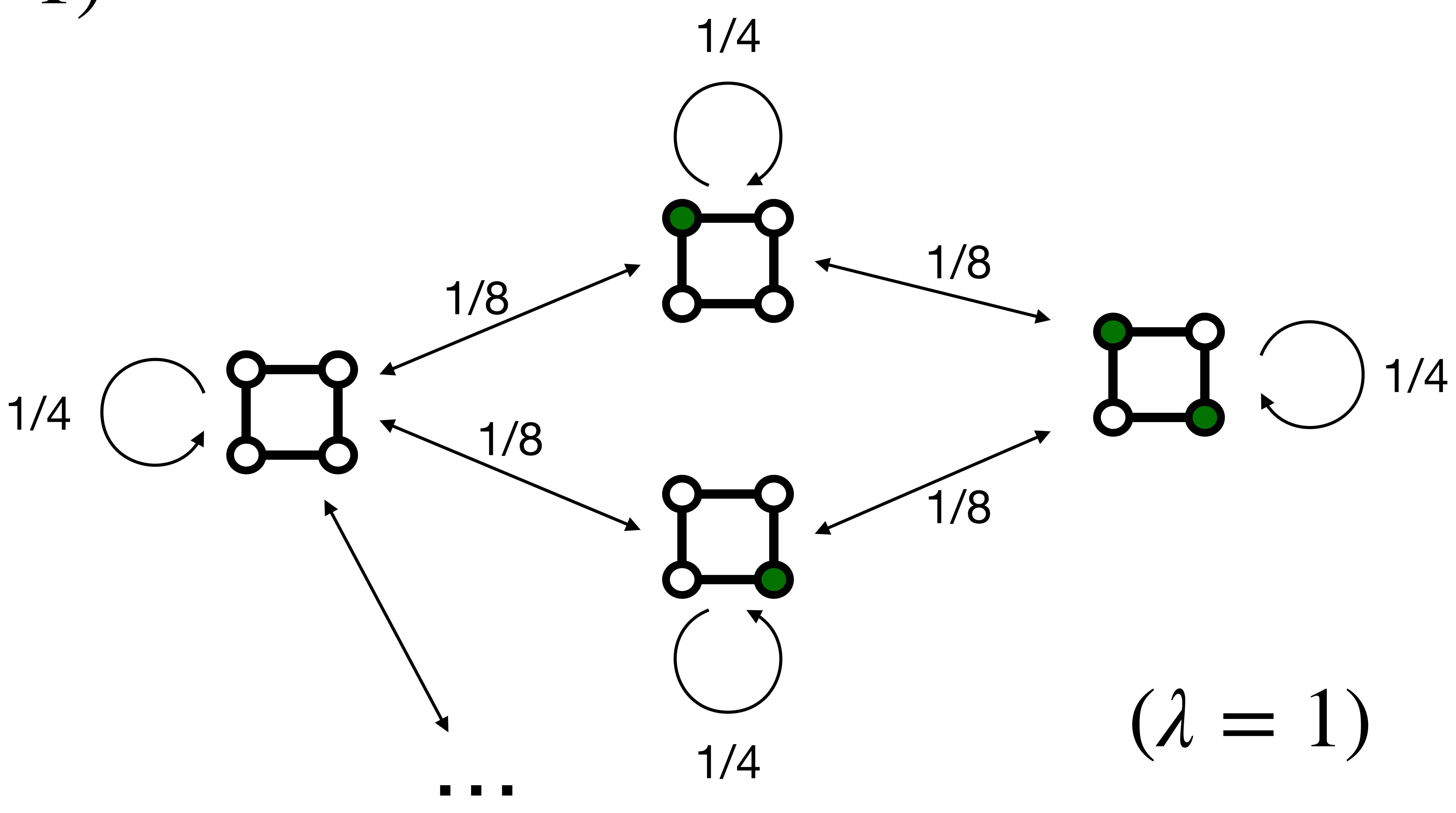
Unbiased estimator

Gibbs sampling

Run a Markov Chain with stationary distribution π_λ :

1. Choose a vertex uniformly at random
2. Make it occupied with proba $\lambda/(\lambda+1)$ if the set remains independent

Glauber dynamics

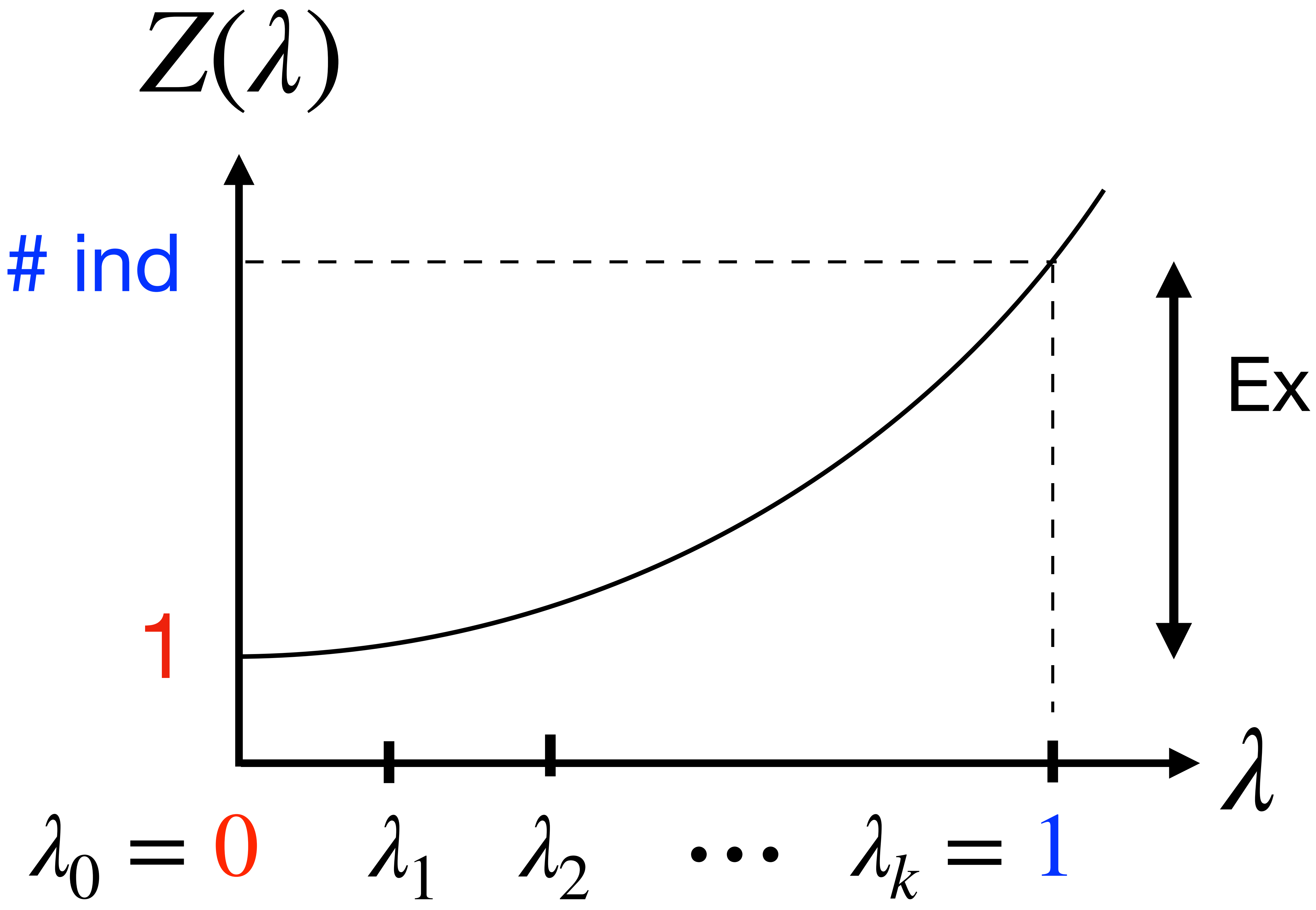


$(\lambda = 1)$

Mixing time = $O(n \log n)$

[Chen,Liu,Vigoda'21]

Partition function estimation



Slowly move from an estimate of $Z(0)$ to an estimate of $Z(1)$

$$Z(1) = \frac{Z(\lambda_1)}{Z(\lambda_0)} \cdot \frac{Z(\lambda_2)}{Z(\lambda_1)} \cdot \cdots \frac{Z(\lambda_k)}{Z(\lambda_{k-1})}$$

$$\uparrow \qquad \uparrow \qquad \uparrow$$

$$\mathrm{E}_{\pi_{\lambda_0}}\left(\frac{\lambda_1}{\lambda_0}\right)^{|I|} \quad \mathrm{E}_{\pi_{\lambda_1}}\left(\frac{\lambda_2}{\lambda_1}\right)^{|I|} \quad \mathrm{E}_{\pi_{\lambda_{k-1}}}\left(\frac{\lambda_k}{\lambda_{k-1}}\right)^{|I|}$$

Balance length of the sequence and variance of each estimator

Quantum MCMC method for independent sets

Two interlaced branches of work:

1

Converting classical reversible Markov chains into quantum walks

2

Estimating expectation values on the 1-eigenvector of a quantum walk

Glauber dynamics

Sample ind. set $I \sim \pi_\lambda$ in time $O(n \log n)$

No speedup for sampling? Diameter(Markov Chain) = n

We can simulate in time $\tilde{O}(\sqrt{n})$ the reflection through the state:

$$|\pi_\lambda\rangle = \sum_I \sqrt{\pi_\lambda(I)}\,|I\rangle$$

(quantum Gibbs sample)

Classical sampling resource

$$I \sim \pi_\lambda$$

Time $\tilde{O}(n)$

Quantum sampling resource

$$2|\pi_\lambda\rangle\langle\pi_\lambda| - I$$

Time $\tilde{O}(\sqrt{n})$

Szegedy Quantum Walk

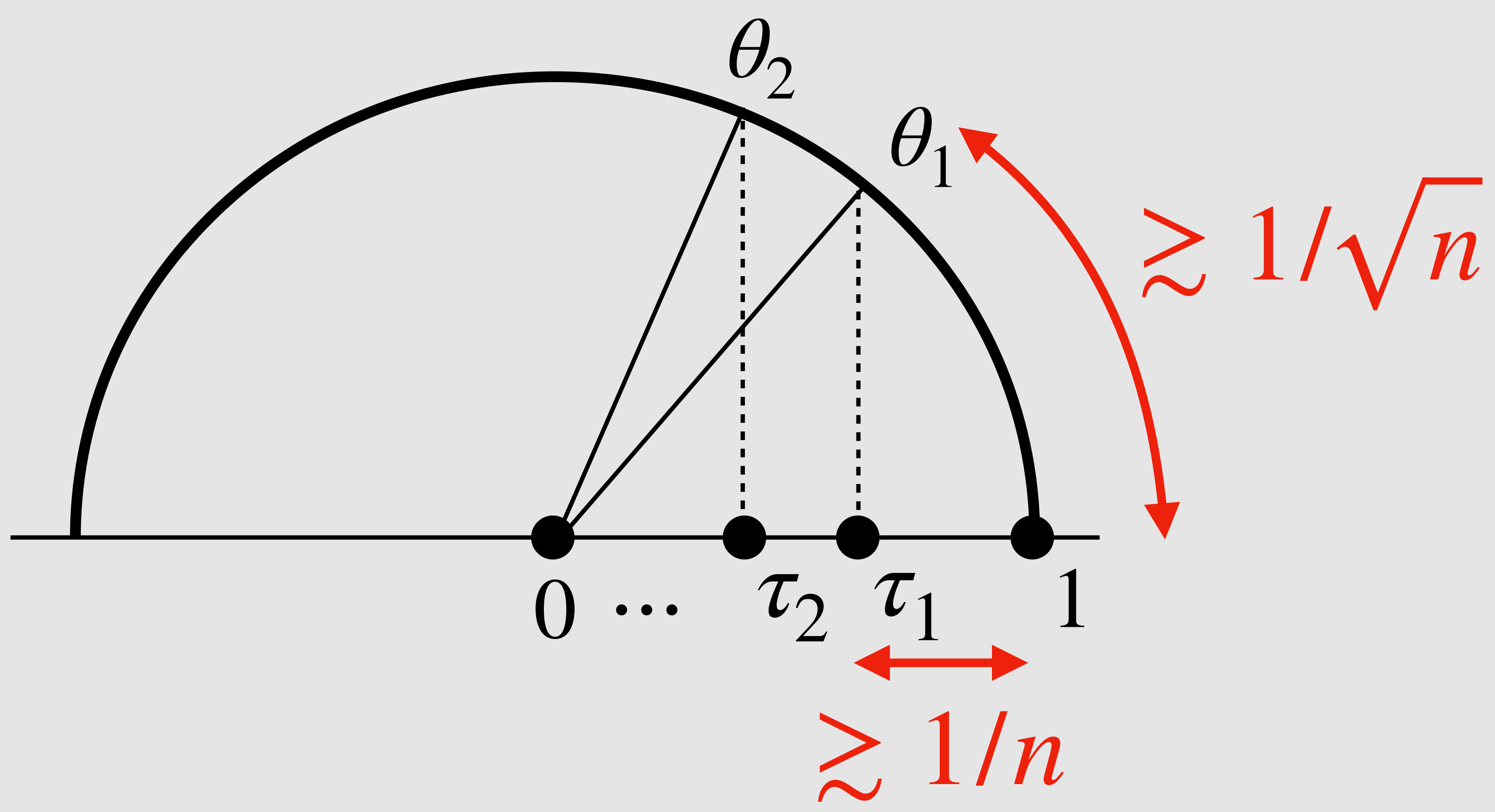
Markov chain (ergodic reversible) with stationary distribution π_λ $\Rightarrow$ Quantum walk with 1-eigenvector $|\pi_\lambda\rangle$

Transition matrix P

Unitary $W(P)$

$$\mathrm{Spec}(P) = \{1,\ \tau_1,\ \tau_2,\ \ldots\}$$

$$\mathrm{Spec}(W(P)) = \{1,\ e^{\pm 2i\theta_1},\ e^{\pm 2i\theta_2},\ \ldots\}$$



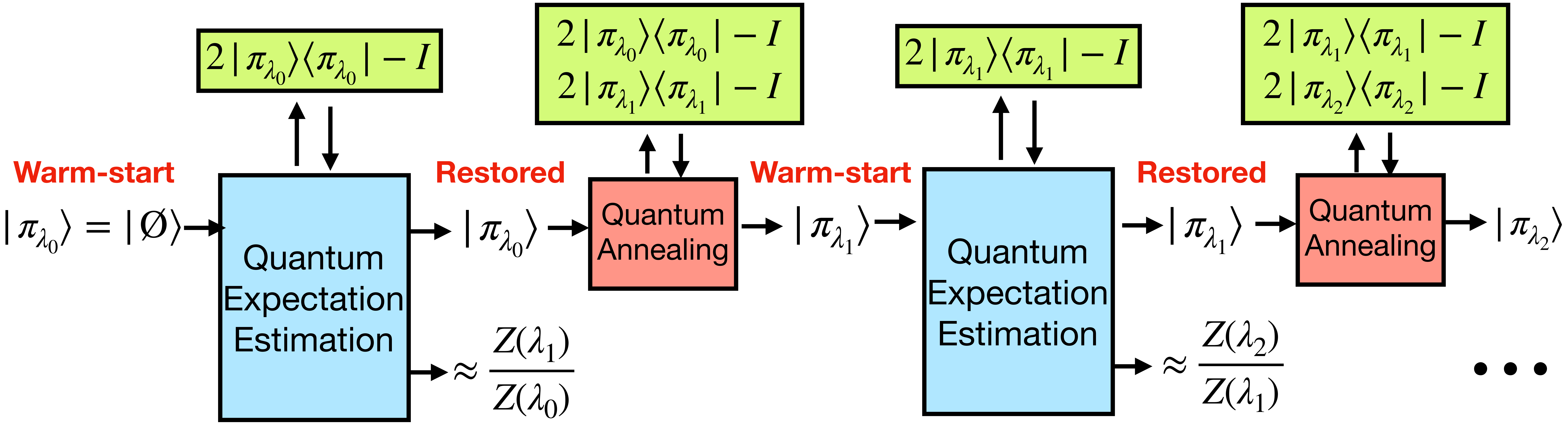
Run $\tilde{O}(\sqrt{n})$ steps of quantum phase estimation on the quantum walk operator $W(P)$ to simulate the reflection

$$2|\pi_\lambda\rangle\langle\pi_\lambda| - I$$

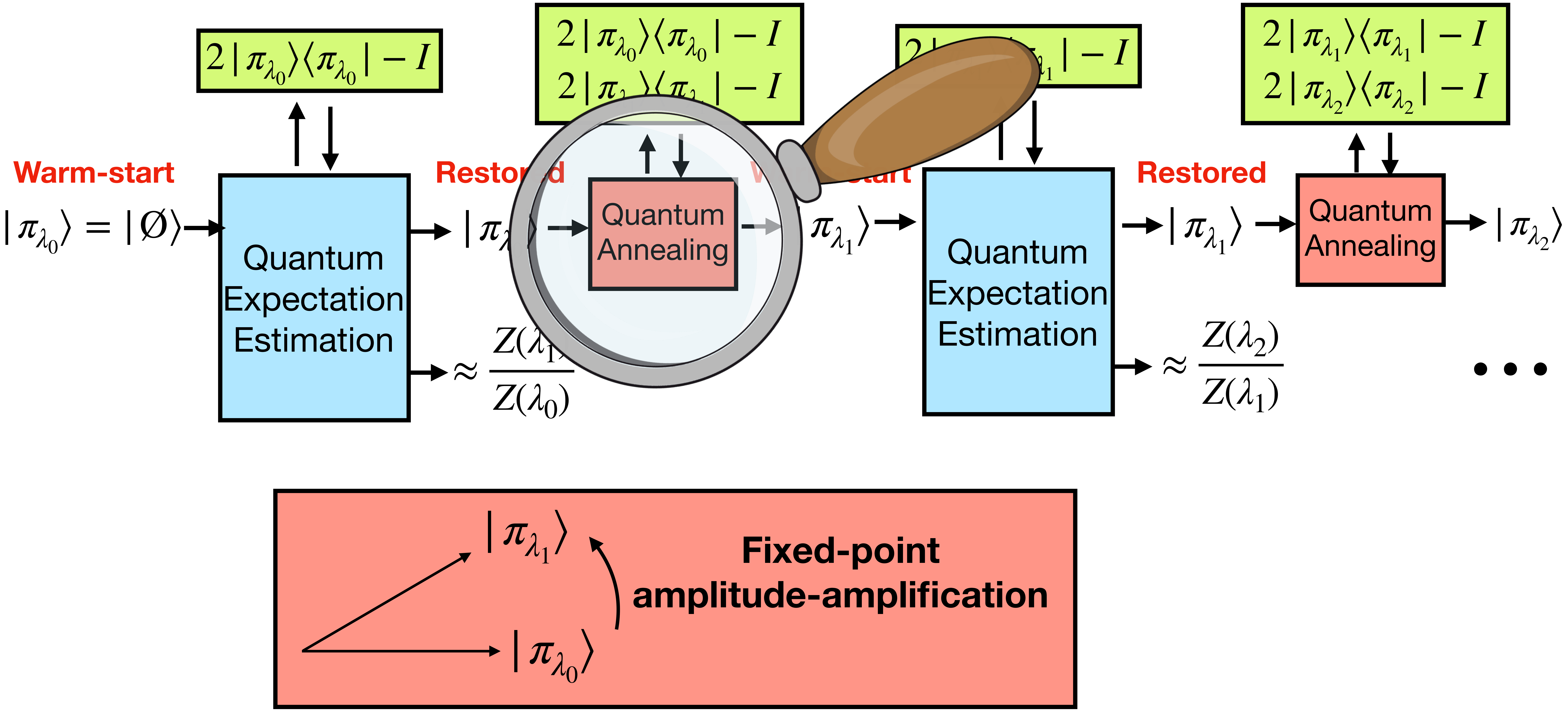
How to use this reflection to estimate expectation values on $|\pi_\lambda\rangle$?

Example: $\dfrac{Z(\lambda')}{Z(\lambda)} = \langle\pi_\lambda|e^{-(\lambda'-\lambda)H}|\pi_\lambda\rangle$

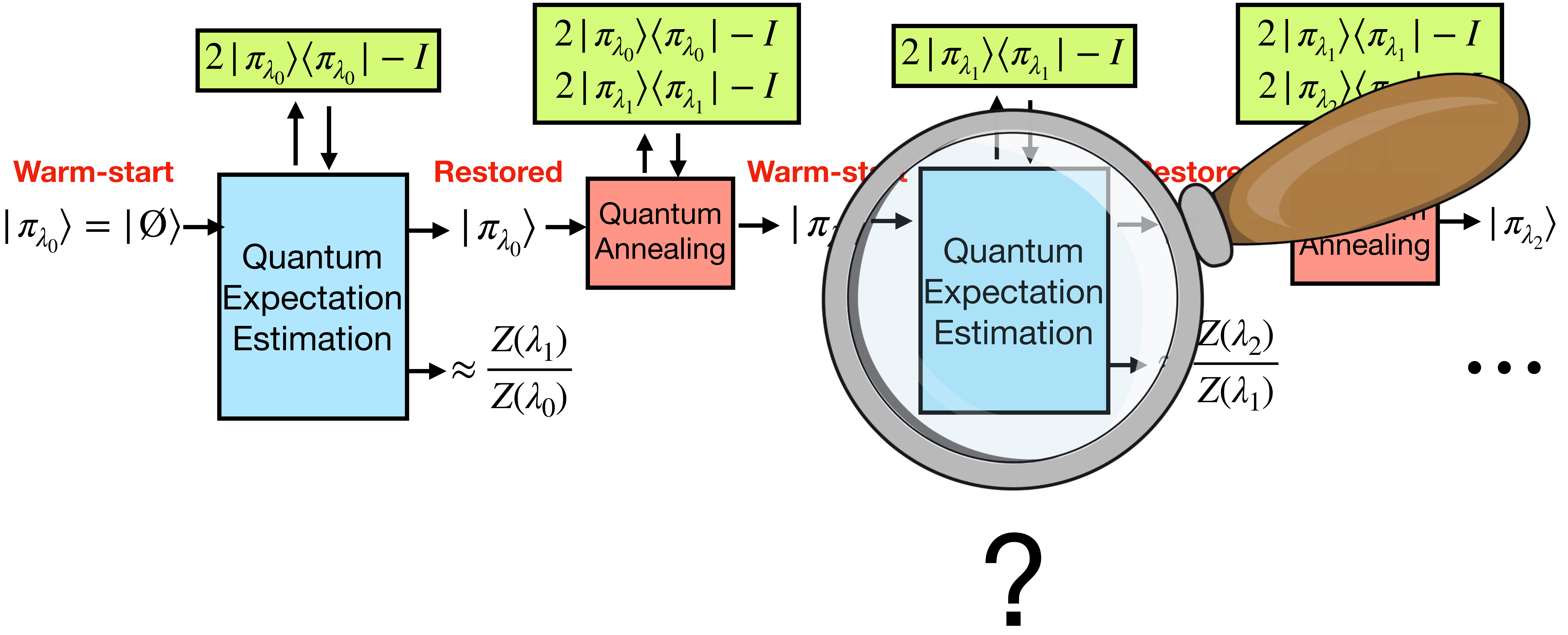
Quantum partition estimation framework



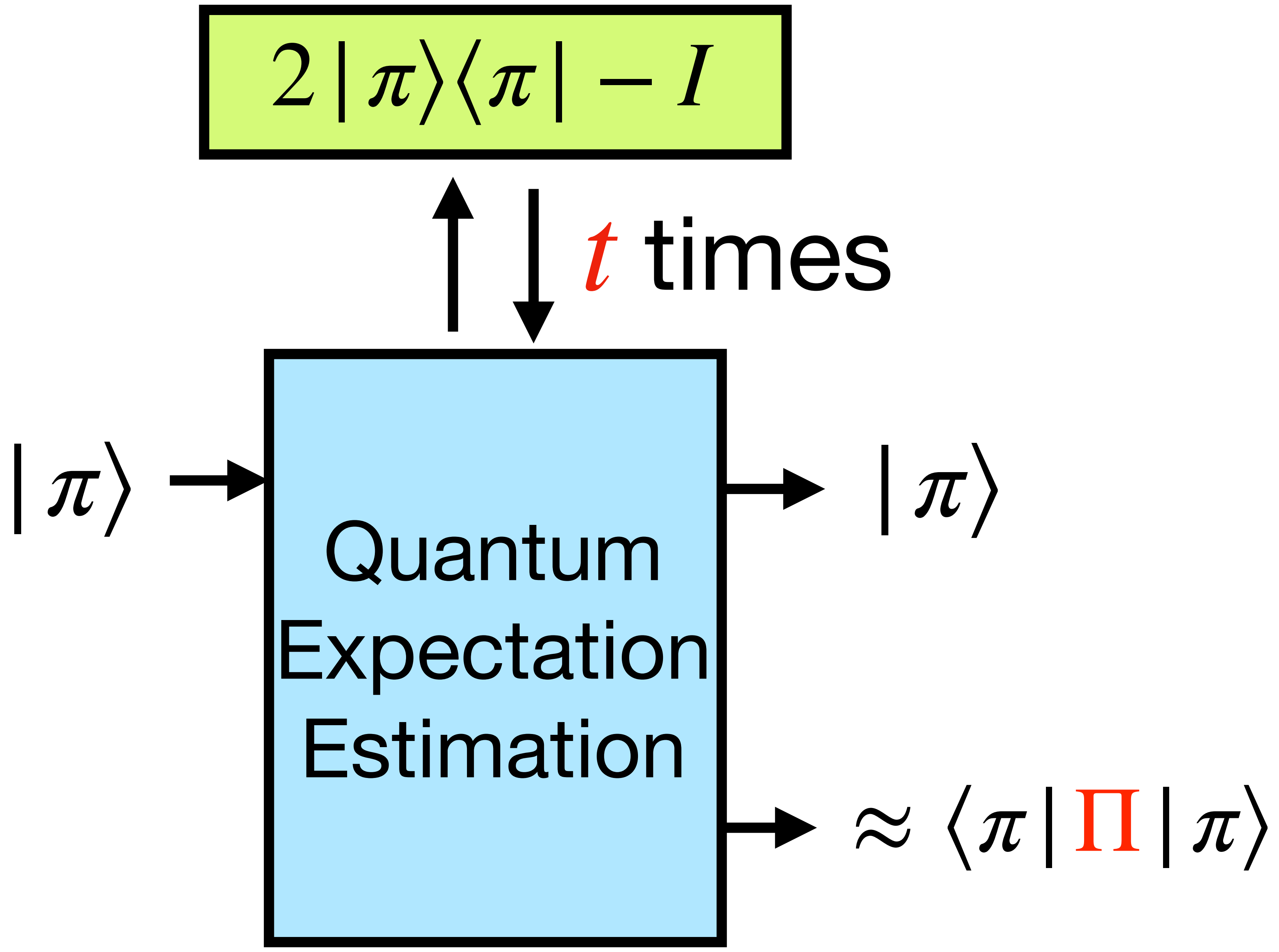
Quantum partition estimation framework



Quantum partition estimation framework



Base case: projection observables



Input:
- description of projector Π
- 1 copy of $|\pi\rangle$
- t access to $2|\pi\rangle\langle\pi| - I$

  (morally, t = sample complexity)

Output:
- 1 new copy of $|\pi\rangle$
- estimate of $\langle\pi|\Pi|\pi\rangle$

  (unbiased + low variance)

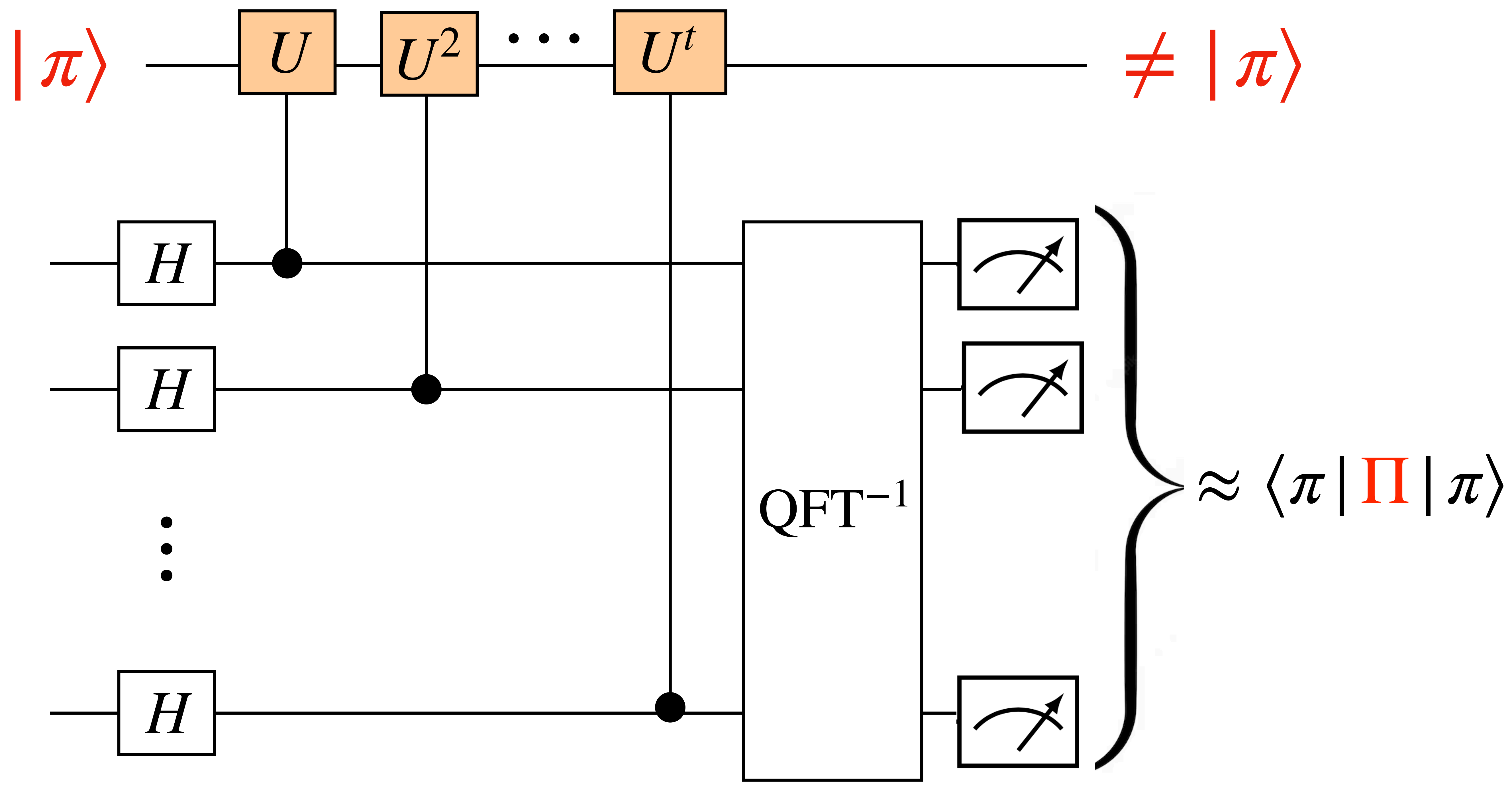
Base case: projection observables

Grover operator

$$U = (2|\pi\rangle\langle\pi| - I)(2\Pi - I)$$

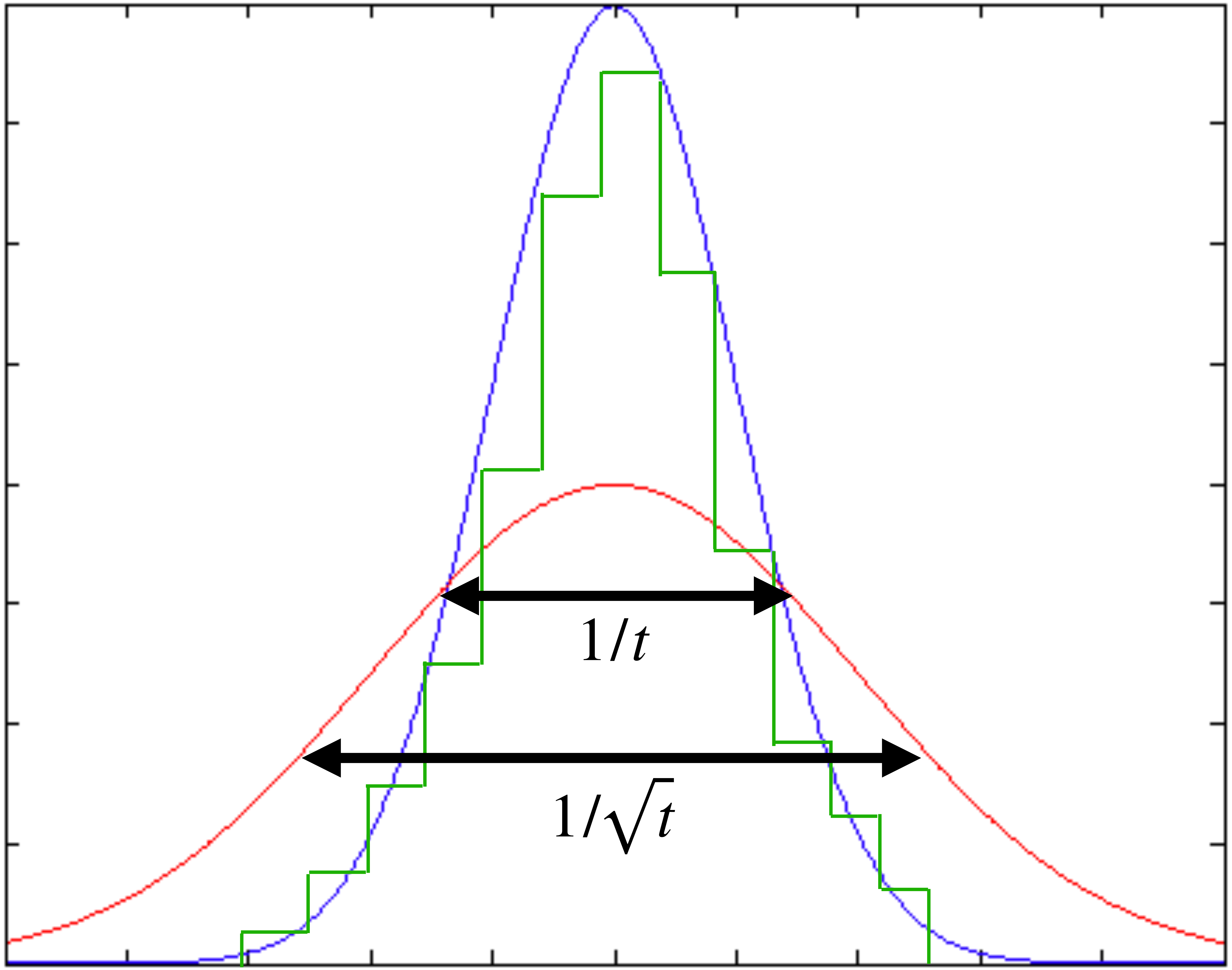
$|\pi\rangle$ is a superposition over the $(\pm 2\sin^{-1}\sqrt{\langle\pi|\Pi|\pi\rangle})$-eigenvectors of U

Quantum Phase estimation



New phase estimation primitive

New phase estimation primitive



Outcome distributions after **t steps** of:

- Empirical mean (classical)
- Standard phase estimation
- Enhanced phase estimation

Open questions

Classical partition functions

The partition function $Z(\beta)$ of classical Hamiltonians can be estimated in

$$\approx \log^{1/4}|\Omega| \times \sqrt{\text{time of classical MCMC algo}}\,.$$

- Can we remove the $\log^{1/4}|\Omega|$ factor to get a full-quadratic speedup?

  ⇒ counting independent sets in time $\tilde{O}(n/\epsilon)$?

  ⇒ quantum sampling π_β and estimating $Z(\beta)$ would have ≈ complexity!

- … or show a polynomial separation $T_{\text{estim.}} \geq T^{c}_{\text{sampl.}}$ for some Hamiltonian

Quantum partition functions

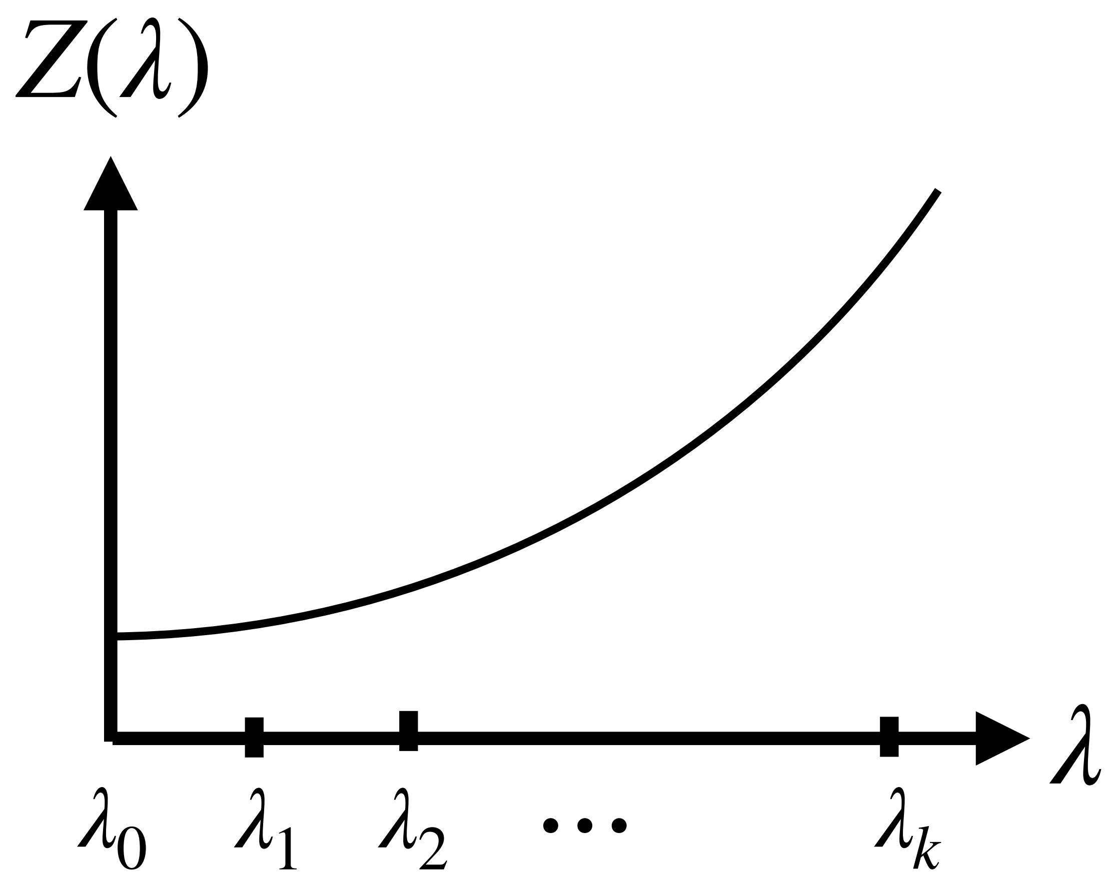
Estimate $Z(\beta) = \mathrm{Tr}\left(e^{-\beta H}\right)$

when H is a quantum Hamiltonian

Efficient reduction from quantum partition function estimation to quantum Gibbs sampling?

$$\frac{Z(\lambda')}{Z(\lambda)} = \mathrm{Tr}\left(e^{-(\lambda'-\lambda)H}\pi_\lambda\right)$$

Ratio estimation?



Cooling schedule?