Spectral Gap Amplification: A technique to speed up MCMC

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Preparation of Eigenstates

$$H|\psi\rangle = \lambda|\psi\rangle$$

- In optimization, the lowest-energy state of H has large amplitude in a basis state that encodes the solution to the problem [E. Farhi, et.al., Nishimori, et.al., etc.]

- In physics simulations, the lowest-energy state is useful to compute a quantum-phase diagram and understand states of matter such as projected entangled pair states (PEPS) [Verstraete & Vidal]

- In quantum computing, the lowest-energy state has large amplitude in the quantum state output by a quantum circuit [D. Aharonov & D. Gottesman, et.al.] with additional results in quantum complexity

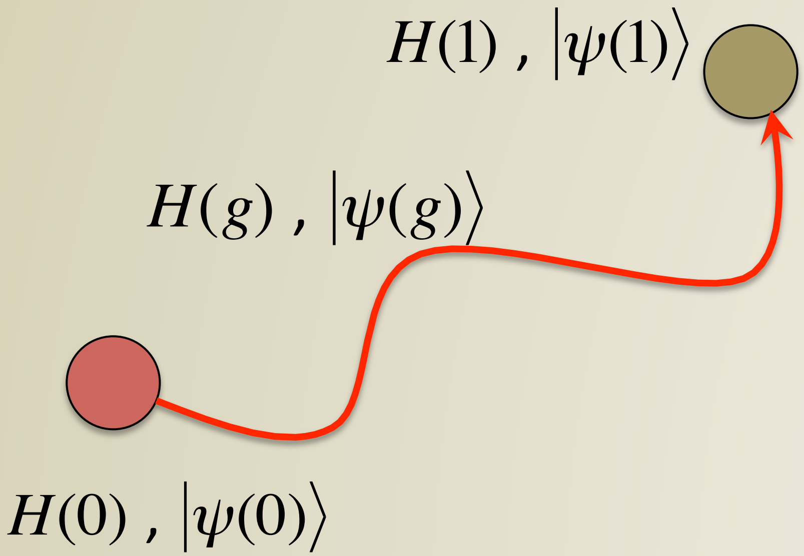
Fast quantum methods to compute expectation values of observables in eigenstates of H are desirable. Such methods usually result in speedups.

Adiabatic State Transformations

Goal : Transform $|\psi(0)\rangle$, the eigenstate of $H(0)$, into $|\psi(1)\rangle$, the eigenstate of $H(1)$.

- In classical computation, the AST problem may be solved by means of probabilistic methods such as quantum Monte-Carlo

- **In quantum computation, the AST problem may be solved by means of <u>quantum adiabatic evolutions</u>**



Prepare $|\psi(0)\rangle$

Evolve with $H(g)$ using an schedule $g(t)$

$g(0) = 0,\ g(T) = 1,\ \dot{g}(t) << 1$

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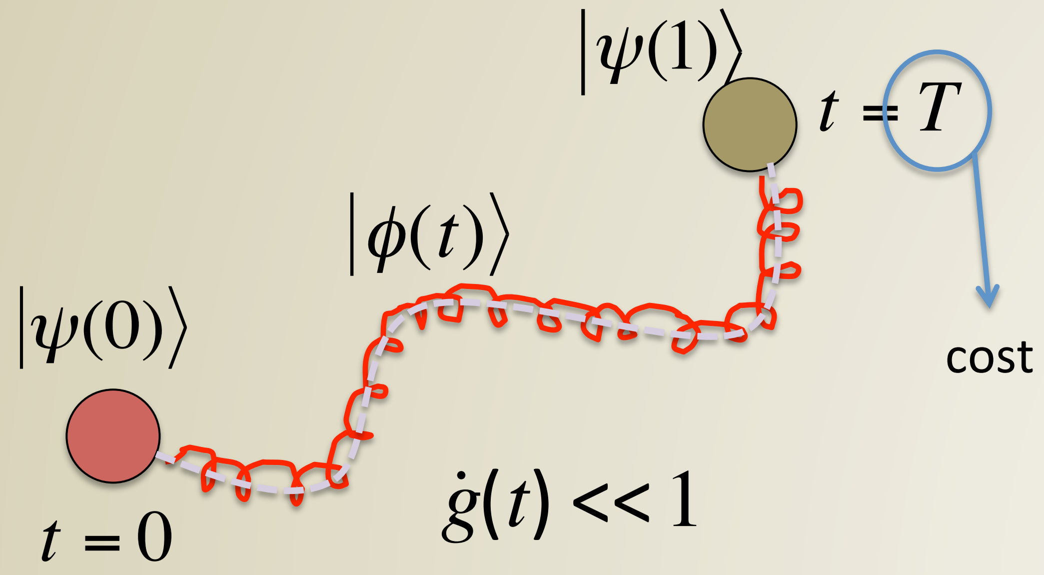
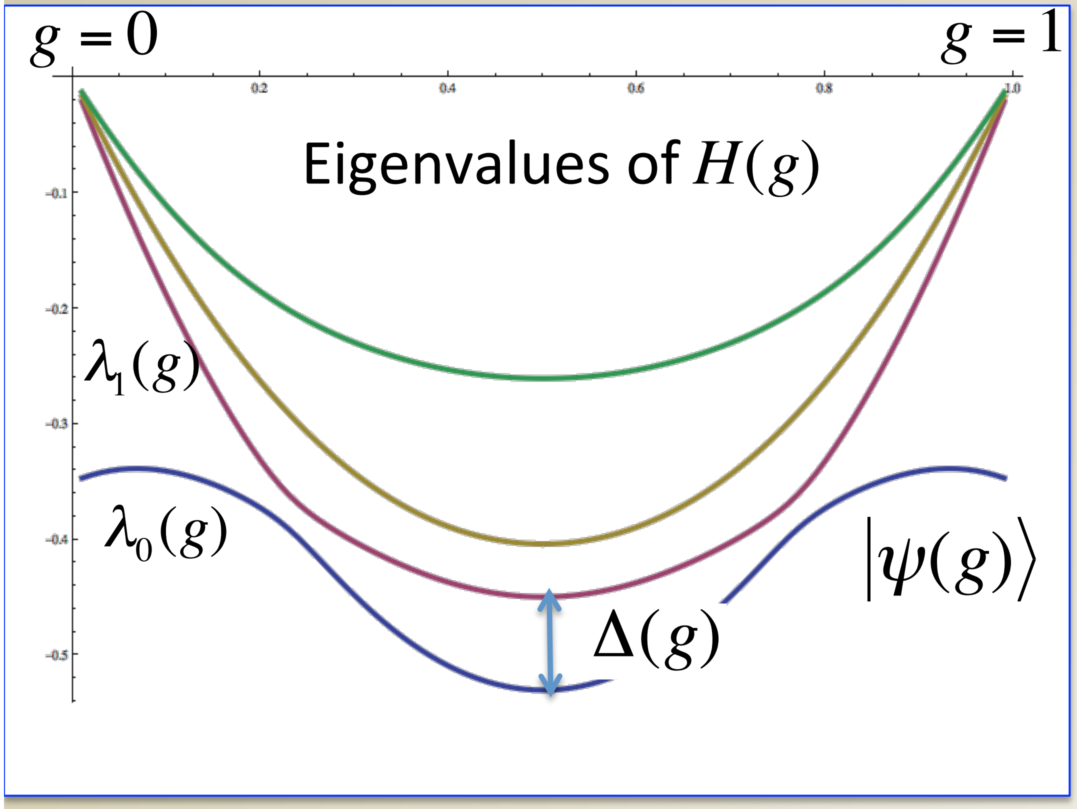


$$\boxed{|\dot{\phi}(t)\rangle = -iH(g(t))|\phi(t)\rangle}$$

Adiabatic Approximations in Quantum Mechanics



$$T \geq \frac{L}{\varepsilon . \min_g \Delta(g)}$$

The AST problem can be solved if [Boixo,Knill,RDS (2010)]

$$\dot{g}(t) \leq \varepsilon \frac{\min_g \Delta(g)}{L}$$

$$\Rightarrow \left\| |\varphi(T)\rangle - |\psi(1)\rangle \right\| \leq \varepsilon$$

Path length:

$$L = \int_{g=0}^{1} dg . \left\| \, |\dot{\psi}(g)\rangle \, \right\|$$

The evolution can be simulated by a quantum circuit of size (almost) linear in T using product formulas [DW Berry, Cleve, .. (2007)]

cost: $C(T) \propto T^{1+\gamma}$

Spectral Gap Amplification Problem (GAP)

The success of AQC is based on heuristics…

The spectral gap amplification problem is formulated so as to obtain ***provable*** quantum speedups.

Spectral Gap Amplification Problem (GAP)

The generic cost $C(T)$ of quantum algorithms that prepare the eigenstate depends on the inverse power of the spectral gap

Given H with eigenstate $|\psi\rangle$ and gap Δ

Can we construct H', with same eigenstate $|\psi\rangle$, but gap $\Delta' >> \Delta$?

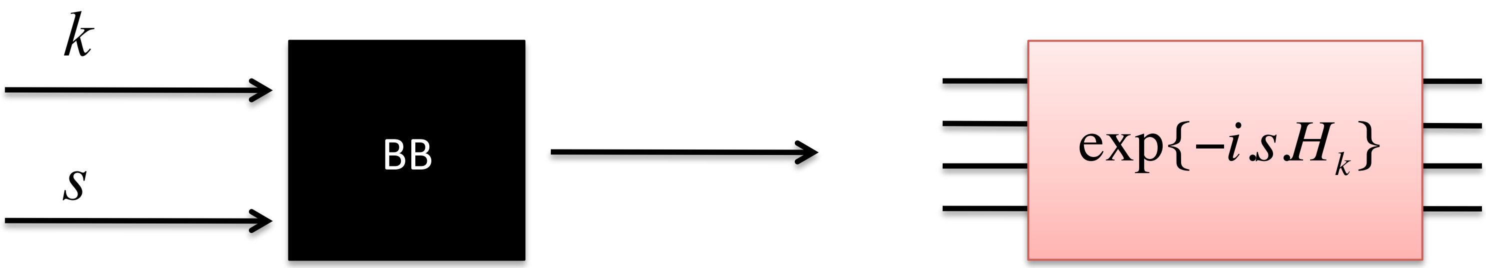
Yes & No

Quantum speedups that depend on the magnitude of the amplification

Spectral Gap Amplification Problem (GAP)

Some requirements....

We assume that H is $H = \sum_k H_k$ and that we have access to a black box



$Def.:$

The cost $C(t)$ of evolving with H for time t is the number of calls to the black box to approximate the evolution $\exp\{-i.t.H\} \rightarrow C(t) \leq c\ |t|^{1+\gamma}$ [DW Berry, et.al. (2007)]

Requirement : $C(t) \approx C'(t)$, the cost of evolving with H' for time t

$$\boxed{H' \cancel{=} \Lambda H\ ;\ \Lambda >> 1}$$

GAP: Frustration-free Hamiltonians

Thm. 1 (quadratic gap amplification):

If $H = \sum_{k=1}^{L} \Pi_k$ satisfies a frustration-free property, then $\Delta' \in \Omega\left(\sqrt{\Delta / L}\right)$

Def.: H is frustration free if

$(\Pi_k)^2 = \Pi_k \rightarrow$ Projector ; $H \geq 0$; $\Pi_k |\psi\rangle = 0 \; \forall \; k.$

Proof (sketched)

. Build the unitary $U = 1 - 2\sum_{k=1}^{L} \Pi_k \otimes |k\rangle\langle k|$

U can be implemented with unit cost!

. Define the ancillary state $|\mu\rangle = \frac{1}{\sqrt{L}} \sum_{k=1}^{L} |k\rangle$; $P = |\mu\rangle\langle\mu|$

$$\boxed{\Rightarrow \quad PUP = (1 - 2H / L) \otimes P}$$

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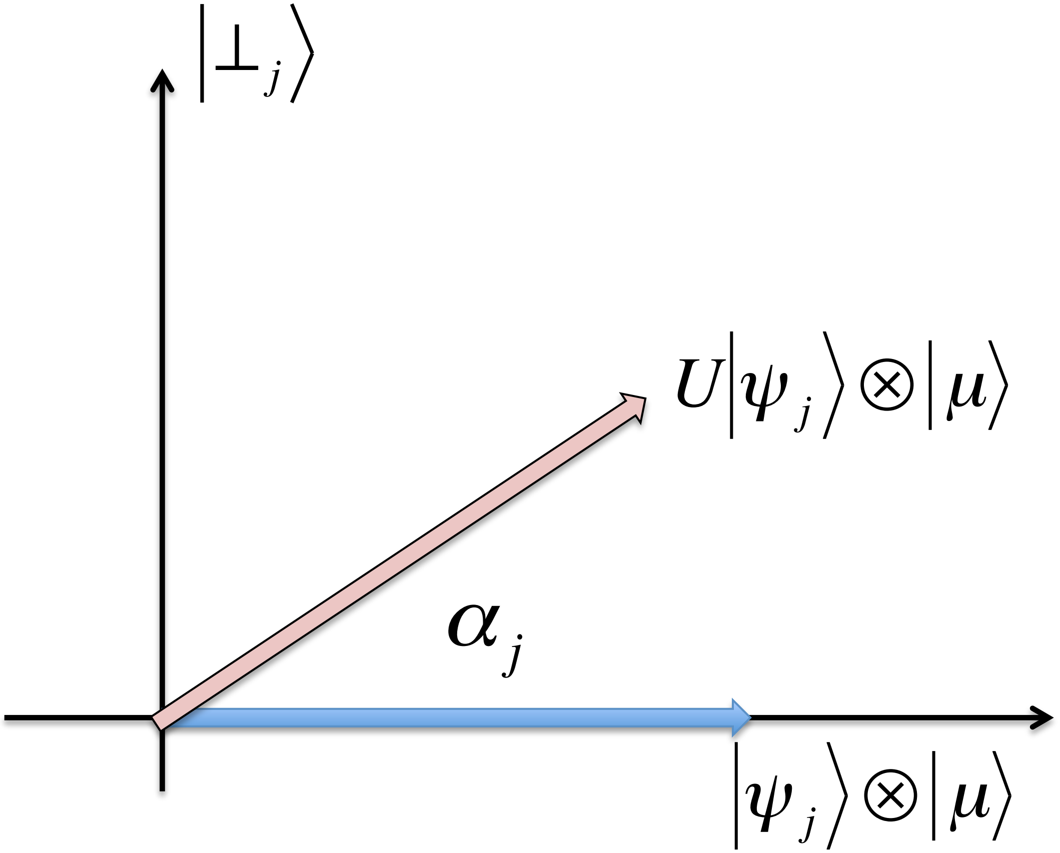
. If $H|\psi_j\rangle = \lambda_j|\psi_j\rangle \Rightarrow$ $1 - 2\,\lambda_j / L = \langle\psi_j| \otimes \langle\mu|U|\psi_j\rangle \otimes |\mu\rangle \equiv \cos(\alpha_j) \approx 1 - (\alpha_j)^2 / 2$

Goal: Build H' so that its eigenvalues are the sines of the angles

GAP: Frustration-free Hamiltonians

$$H' = UPU - P$$

$$\left\{ \left|\psi_j\right\rangle \otimes |\mu\rangle, U\left|\psi_j\right\rangle \otimes |\mu\rangle \right\} \rightarrow \left\{ \left|\psi_j\right\rangle \otimes |\mu\rangle, U\left|\psi_j\right\rangle \otimes |\mu\rangle \right\}$$



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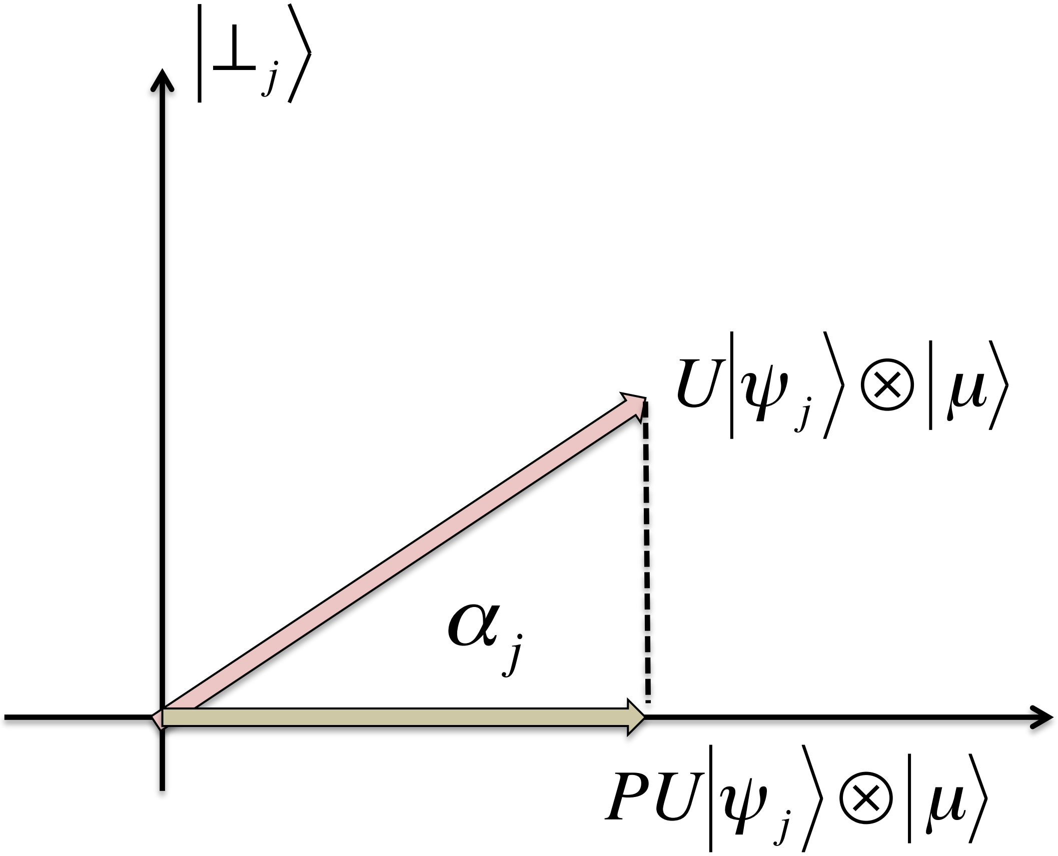

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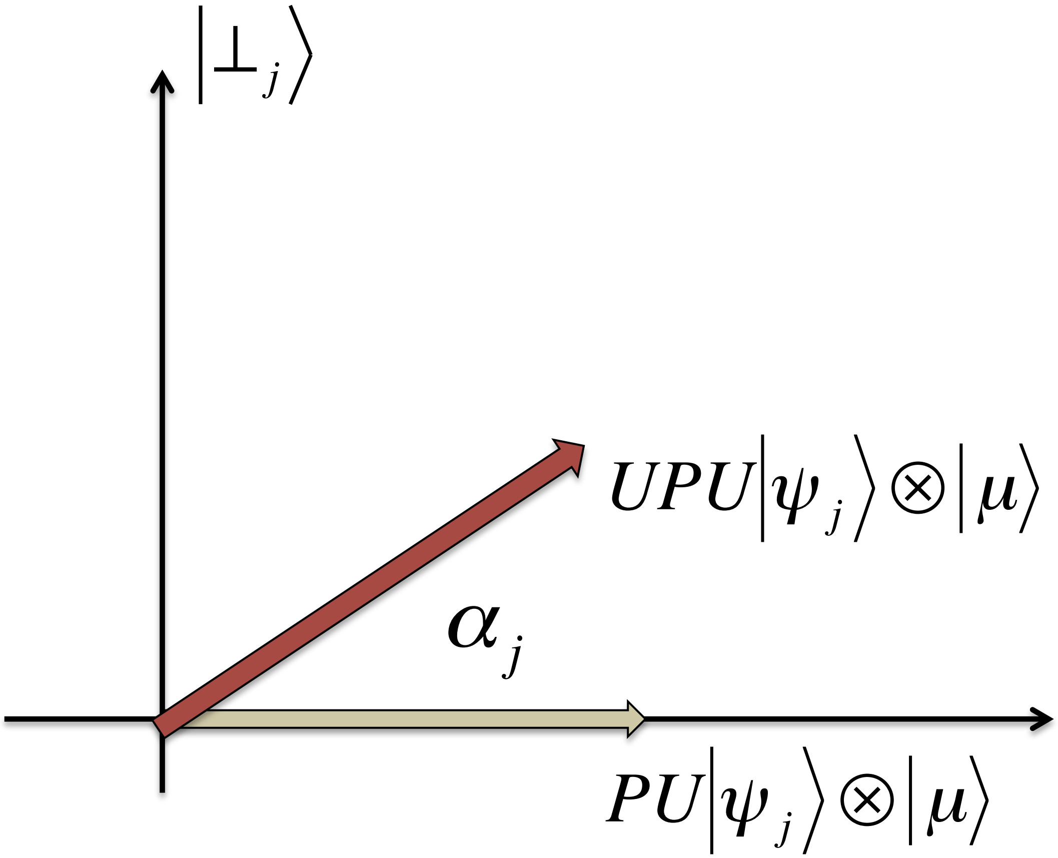

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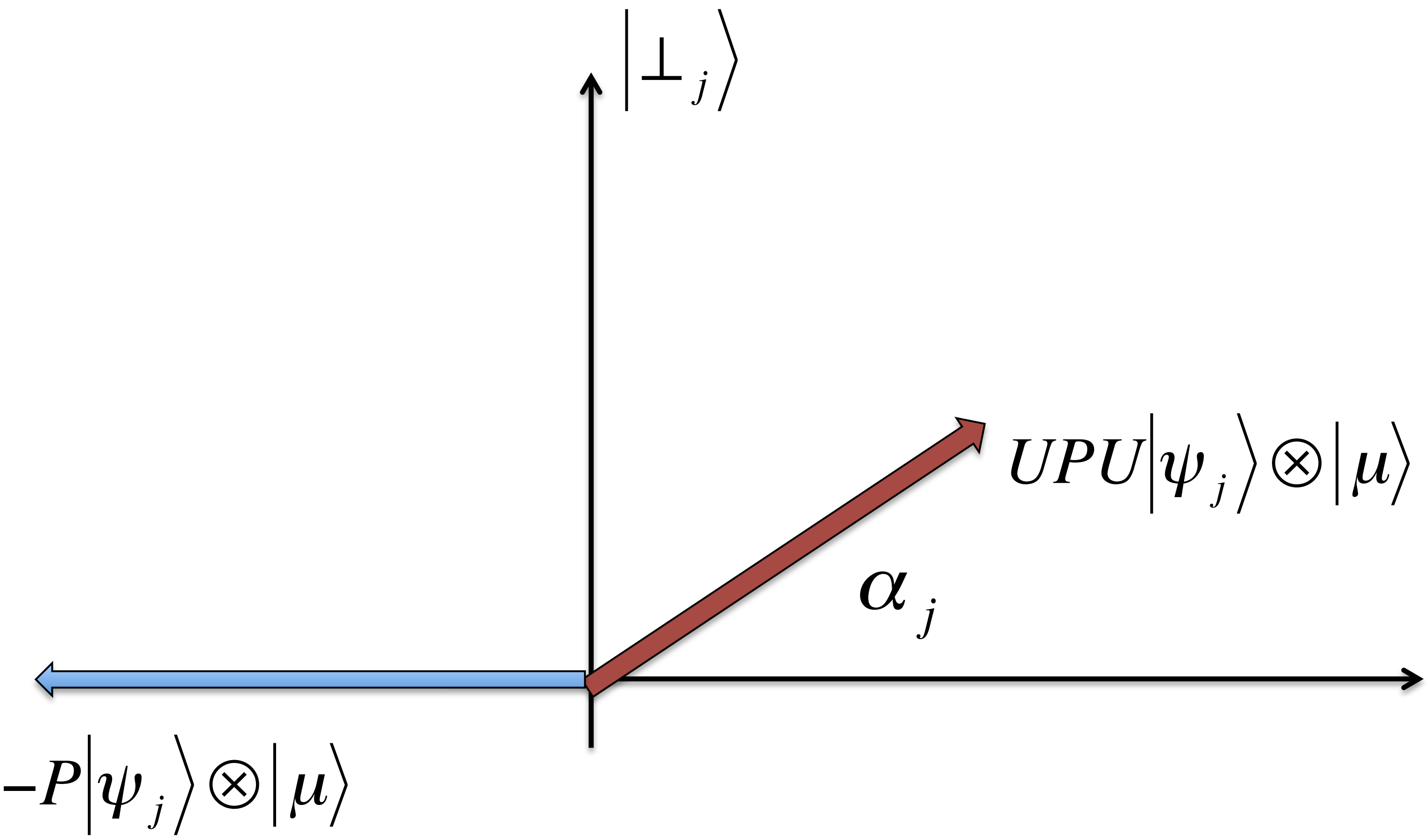

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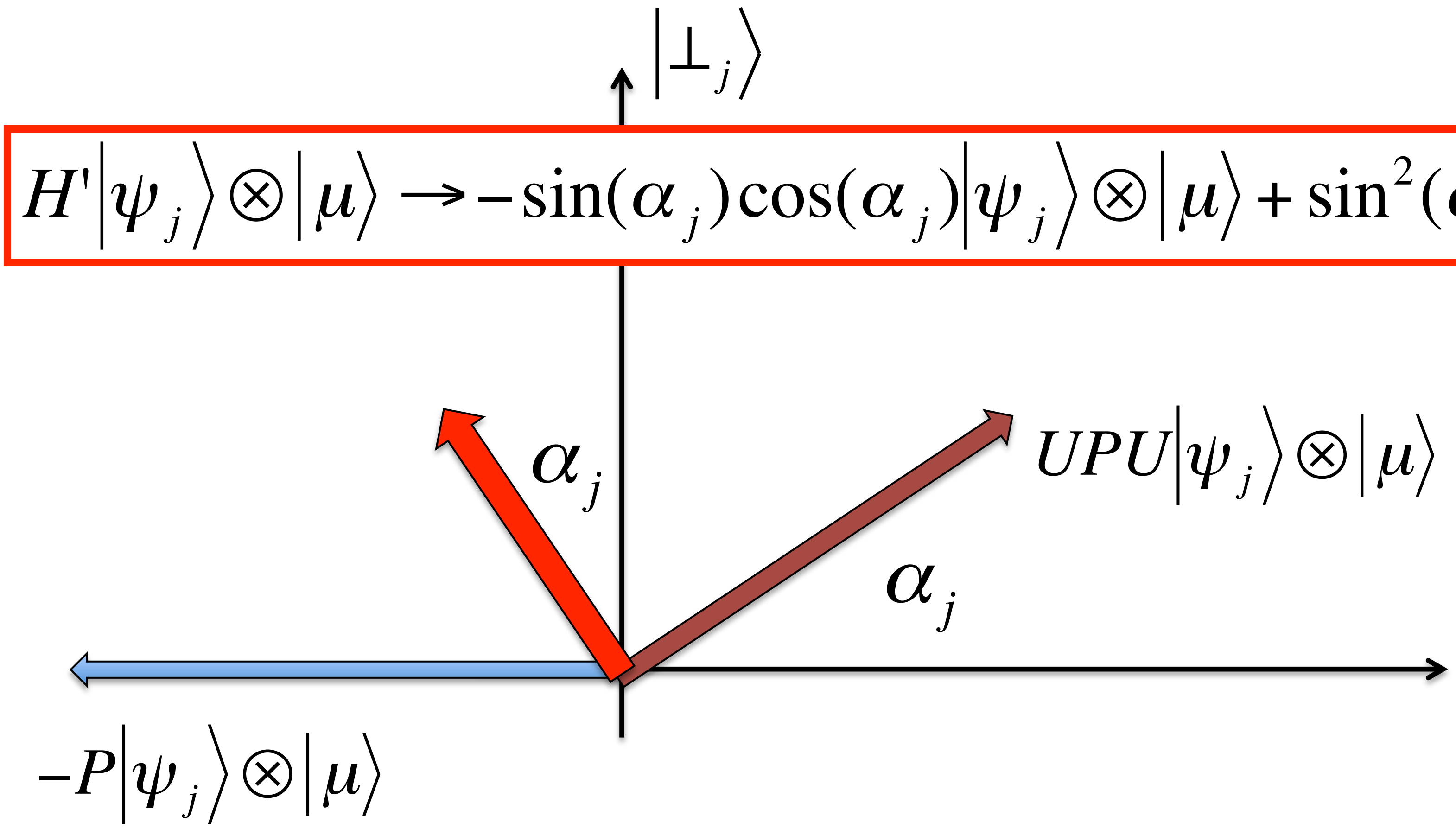


$$\boxed{H' \left| \psi_j \right\rangle \otimes \left| \mu \right\rangle \rightarrow -\sin(\alpha_j)\cos(\alpha_j) \left| \psi_j \right\rangle \otimes \left| \mu \right\rangle + \sin^2(\alpha_j) \left| \perp_j \right\rangle}$$

GAP: Frustration-free Hamiltonians

$$H' = UPU - P$$

$$\begin{array}{cc} & \begin{array}{cc} |\psi_j\rangle \otimes |\mu\rangle & \qquad\qquad |\perp_j\rangle \end{array} \\ H' \to & \begin{pmatrix} -\sin^2(\alpha_j) & \sin(\alpha_j)\cos(\alpha_j) \\ \sin(\alpha_j)\cos(\alpha_j) & \sin^2(\alpha_j) \end{pmatrix} \end{array}$$

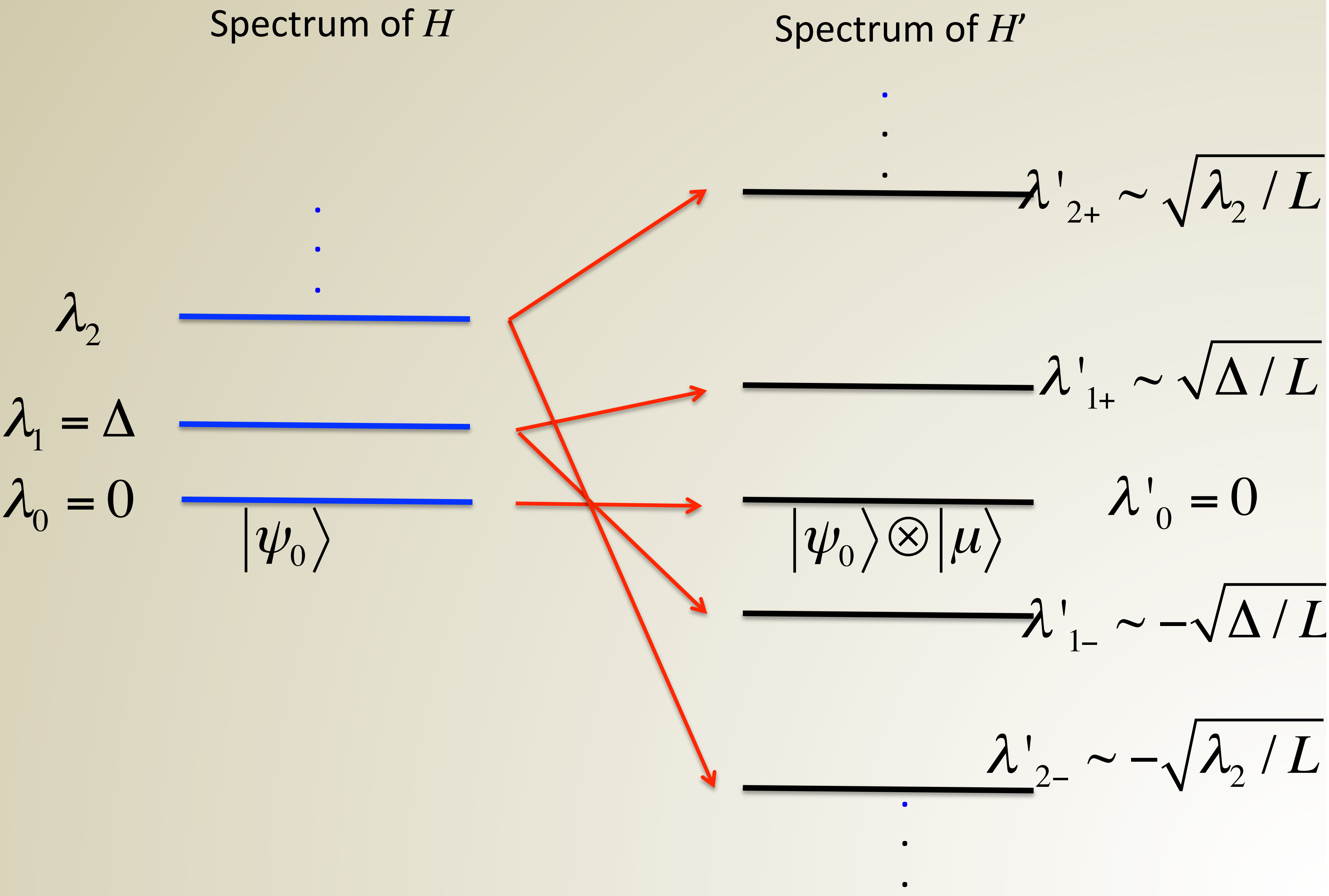
New eigenvalues: $\pm\sin(\alpha_j) \approx \pm\sqrt{\lambda_j / L}$

$$\boxed{H'|\psi_0\rangle \otimes |\mu\rangle = 0}$$

Gap amplification!!

[Szegedy, Ambainis,..]

GAP: Frustration-free Hamiltonians



Spectrum of H

λ_2

$\lambda_1 = \Delta$

$\lambda_0 = 0$

$|\psi_0\rangle$

Spectrum of H'

$\lambda'_{2+} \sim \sqrt{\lambda_2 / L}$

$\lambda'_{1+} \sim \sqrt{\Delta / L}$

$\lambda'_0 = 0$

$|\psi_0\rangle \otimes |\mu\rangle$

$\lambda'_{1-} \sim -\sqrt{\Delta / L}$

$\lambda'_{2-} \sim -\sqrt{\lambda_2 / L}$

GAP: Frustration-free Hamiltonians

Implementation cost

$$H' = UPU - P = H_0 + H_1$$

$$\rightarrow \exp\{-iH't\} \approx \exp\{-iH_0 s_1\}\exp\{-iH_1 s_2\}\ldots\exp\{-iH_0 s_m\}\exp\{-iH_1 s_m\}$$

$$= \underbrace{U\exp\{-iPs_1\}U\exp\{iPs_2\}\ldots U\exp\{-iPs_m\}U\exp\{iPs_m\}}$$

$m \in O(|\cancel{t}|^{1+\gamma})$ [DW Berry, et.al.]

$$m \in O[|t|.\log(|t|)]$$

[R Cleve, S Gharibian, and **RS**, in preparation]

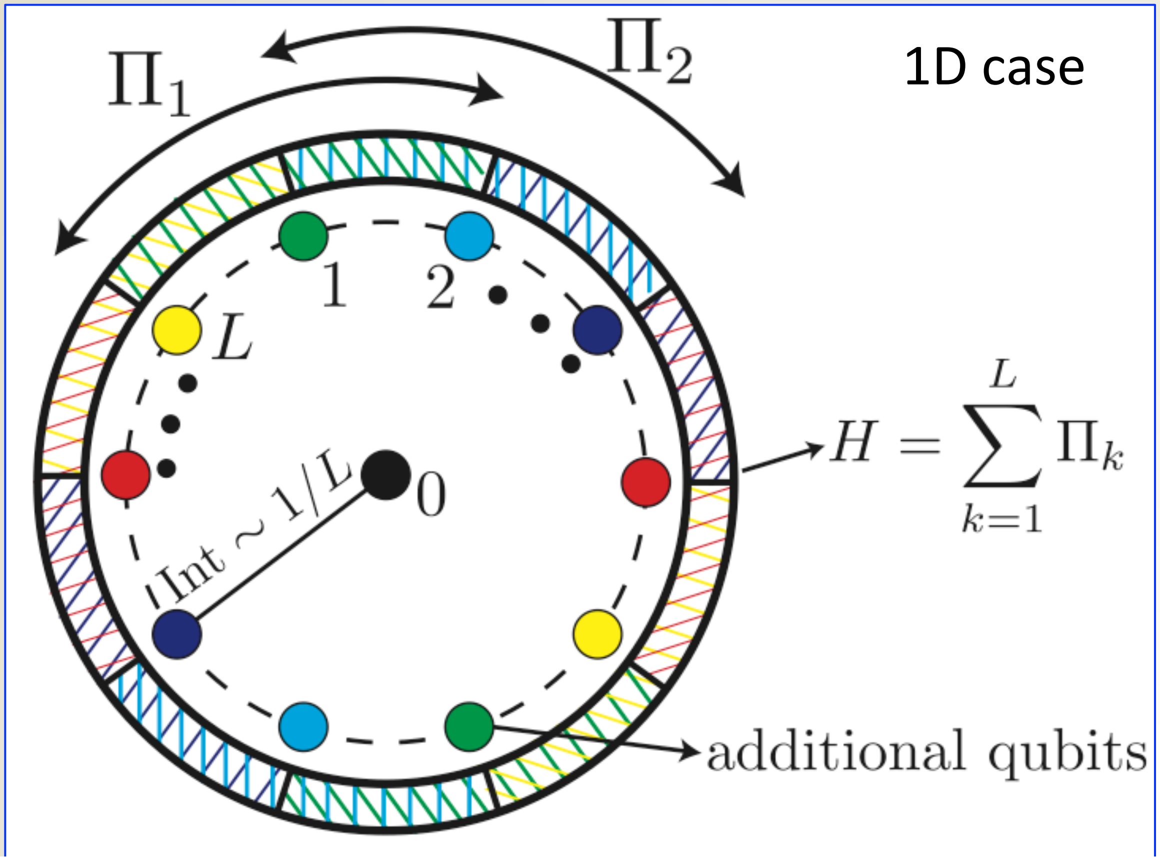
The evolution for time *t* can be simulated with (almost) a linear number of calls to the black box ✓

GAP: Other Constructions

$$H' = UPU - P$$
$$H' = i(UP - PU)$$
$$\vdots$$
$$H' = \frac{1}{L}\sum_{k=1}^{L}\Pi_k \otimes \left[|k\rangle\langle 0| + |0\rangle\langle k|\right]$$

Improved constructions for the quantum adiabatic simulation of quantum circuits:

$\Delta \rightarrow O(1/L^{3/2})$ [S. Boixo]



GAP: Optimal amplification for frustration-Free Hamiltonians

Thm. 2 (optimal amplification) : $\Delta' \in \Theta\left(\sqrt{\Delta}\right)$

Proof (main idea):

Reduce instances of SEARCH to GAP

Prove that if a better-than-quadratic amplification for FF Hamiltonians were possible, then SEARCH could be solved faster than known possible.

$$H_X = \sum_{k=1}^{L} \Pi_k \in C^{NXN}$$

$$\left\langle s \middle| \psi_X \right\rangle \in O(1) \ ; \ |s\rangle = \frac{1}{\sqrt{N}} \sum_{Y=0}^{N-1} |Y\rangle$$

$$\left\langle X \middle| \psi_X \right\rangle \in O(1)$$

Prepare (efficiently) $|s\rangle$

↓

Measure $|\psi_X\rangle$

↓

Measure in $\{|Y\rangle\}$

↓

Obtain $|X\rangle$ with large Pr.

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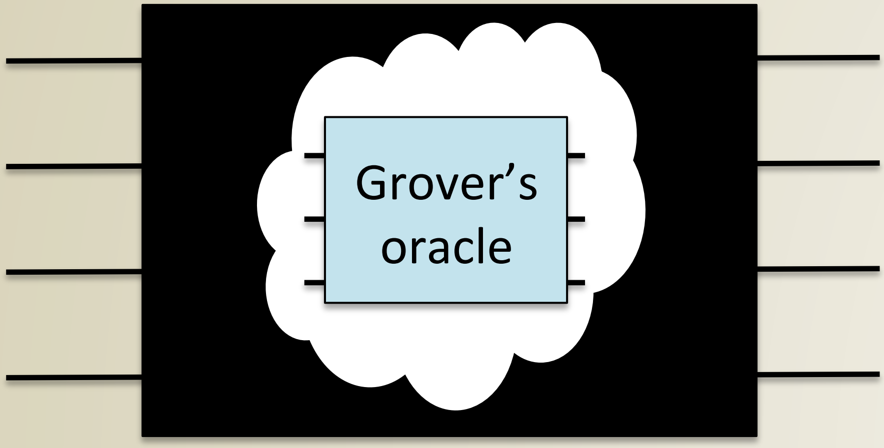

SEARCH can be solved with

$O(1/\sqrt{\Delta})$ oracles

Find H so that $\Delta \in O(1/N)$

Solves SEARCH in optimal time $O(\sqrt{N})$

Limits the gap amplification!

GAP: No Amplification in General

Thm. 3 (no general amplification) : In general, $\Delta' \in O(\Delta)$

Proof (main idea):

Reduce instances of SEARCH to GAP

Find $H = \sum_{k=1}^{L} \Lambda_k$ so that $\Delta \in O(1/\sqrt{N})$

Solves SEARCH in optimal time $O(\sqrt{N})$

Limits the gap amplification!

Applications of GAP: Quantum speedups of Monte Carlo for COPs

MC: A quick review

$i.$ Sample from the initial distribution Π_0

$ii.$ Construct and apply a stochastic process $S \rightarrow \Pr(\sigma | \sigma')$

$iii.$ Sample from $\Pi_f = S^n \Pi_0$

A convergence Lemma : Let Π be the fixed point of S, i.e. $S\Pi = \Pi$. Then, if $n \in O(1/\Delta_S)$ is the mixing time, $|\Pi_f - \Pi| \leq 1/e$.

Applications of GAP: Quantum speedups of Monte Carlo for COPs

From a stochastic matrix to a frustration-free Hamiltonian:

$$H \rightarrow \langle \sigma | H | \sigma' \rangle = \delta_{\sigma\sigma'} - \sqrt{\Pr(\sigma | \sigma').\Pr(\sigma' | \sigma)}$$

$$|\psi_0\rangle = \sum \sqrt{\Pi_\sigma} |\sigma\rangle$$

$$H = \sum_k \alpha_k \Pi_k$$

$H|\psi_0\rangle = 0$ [frustration free]

$$\Delta_H = \Delta_S$$

Using H', we can sample from Π_f' by preparing a state close to $|\psi_0\rangle$ and measuring in the computational basis.

Methods to evolve ‘adiabatically’ at cost that depends on the inverse gap only (not higher powers) exist [**RS**, et.al., PRL’08]

$$Cost: \quad C \in O(1/\sqrt{\Delta_S}) << n$$

GAP: Summary

- We introduced the GAP problem that resulted in (quadratic) quantum speed ups: gap amplification of FF yields quantum speedups of classical Monte Carlo Methods [RS,et.al.,PRL'08]

[1]

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- We introduced the GAP problem that resulted in (quadratic) quantum speed ups: gap amplification of FF yields quantum speedups of classical Monte Carlo Methods [RS,et.al.,PRL'08]

- We proved that the quadratic amplification is optimal for FF

[2]

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[4]

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Other interesting results in arXiv: 1110.2494

[>4]

GAP: Some Interesting Questions

- Other implications in quantum complexity? Speedups?

- Can we amplify the gap even further by allowing increases in the number of systems?

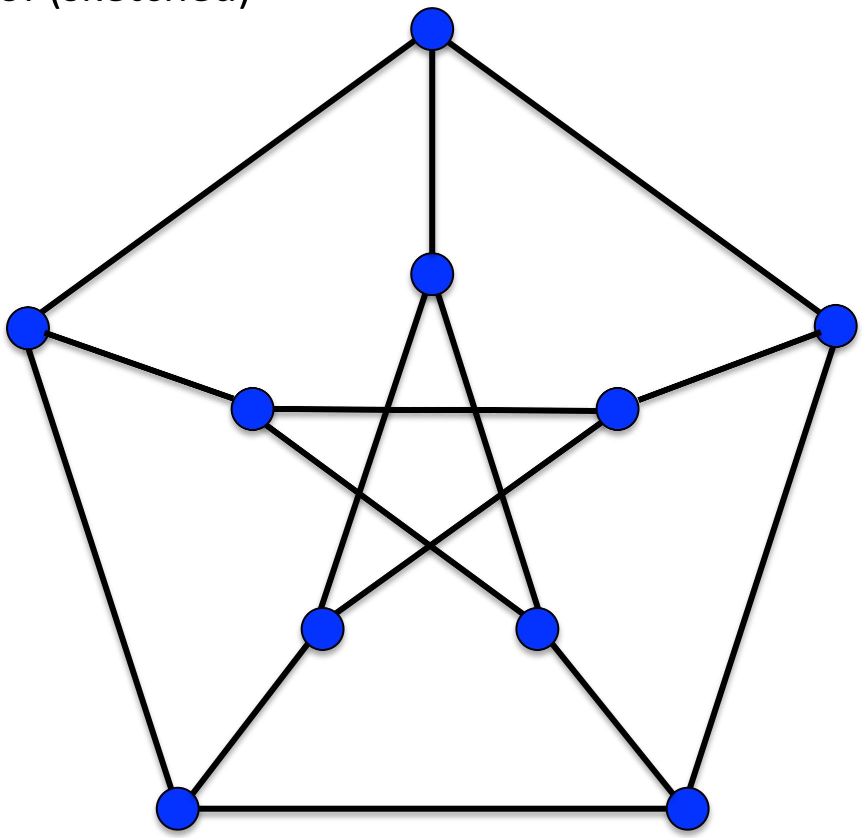
THANK YOU!

GAP: Optimal amplification for frustration-Free Hamiltonians

Thm. 3 (optimal amplification):

$$\Delta' \in \Theta\left(\sqrt{\Delta}\right)$$

Proof (sketched)



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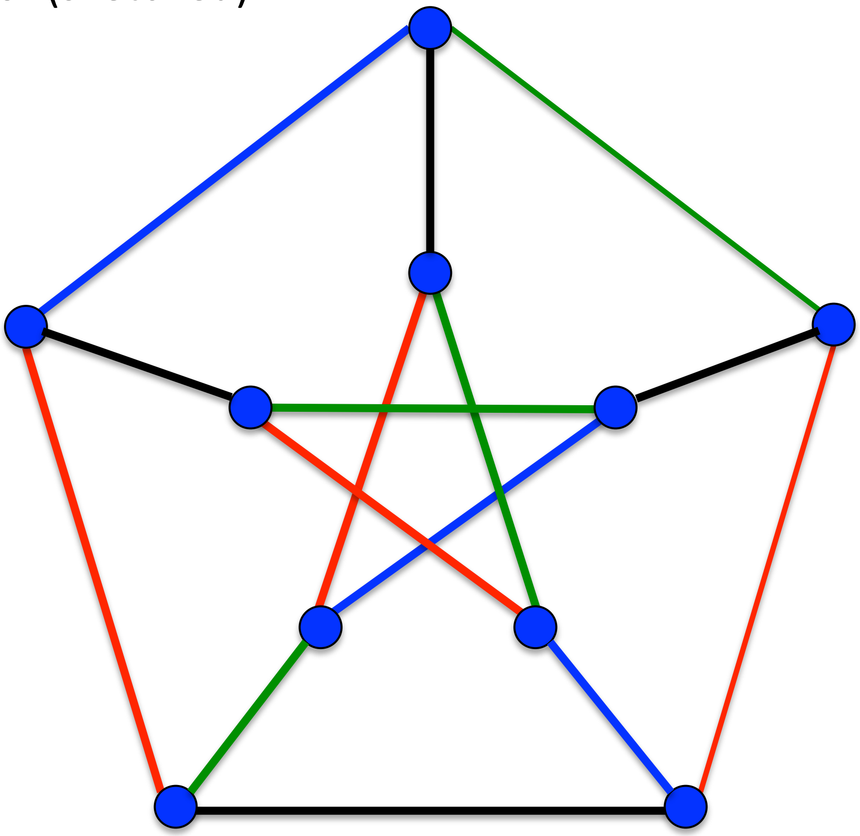

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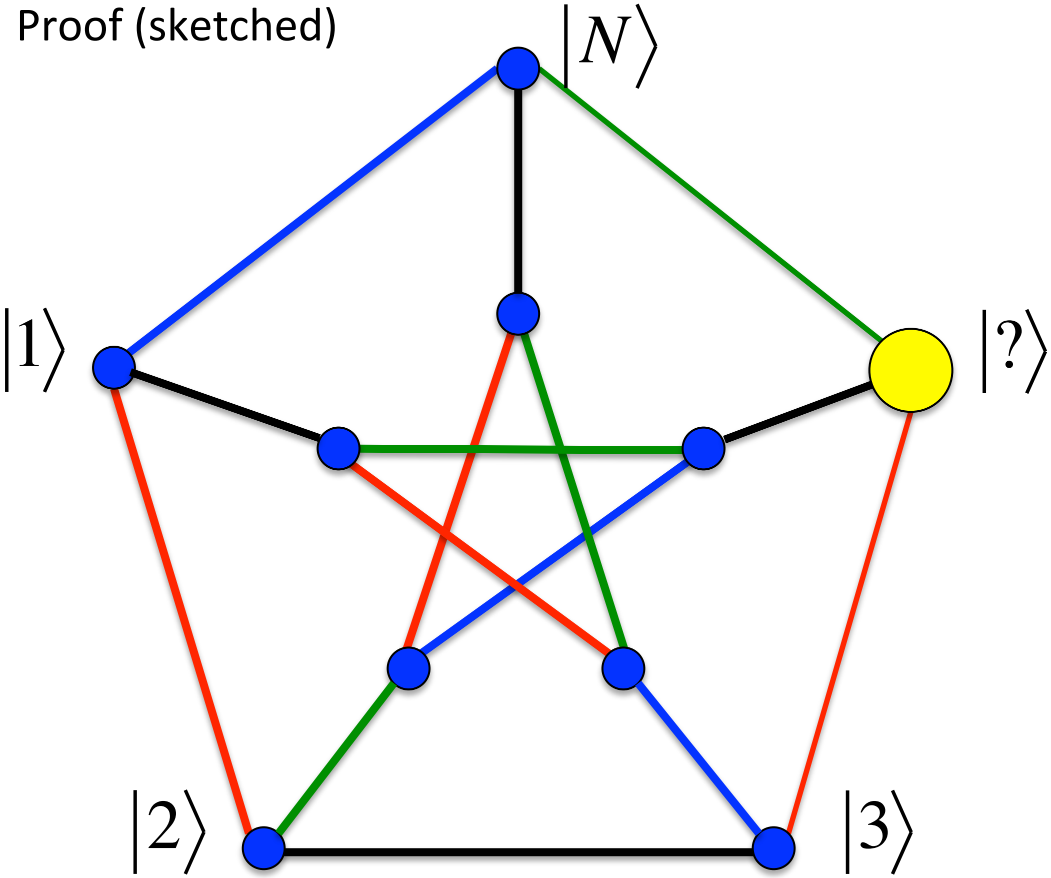

Goal:
Build a frustration-free Hamiltonian whose lowest-eigenvalue eigenstate has large amplitude in the marked vertex and in the uniform superposition state.

The search problem can be solved by first preparing the uniform superposition state, then measuring the lowest-eigenvalue state, and then measuring in the computational basis

cost: $T \sim \dfrac{1}{\Delta}$

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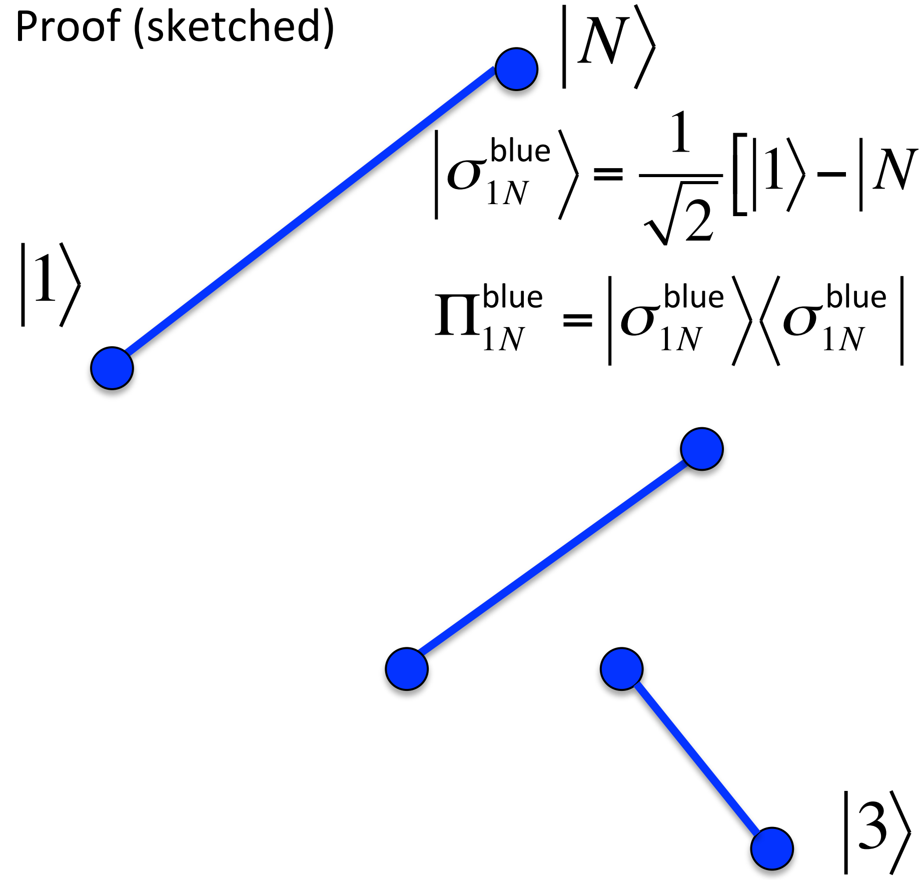

$$\left|\sigma_{1N}^{\text{blue}}\right\rangle = \frac{1}{\sqrt{2}}\left[|1\rangle - |N\rangle\right]$$

$$\Pi_{1N}^{\text{blue}} = \left|\sigma_{1N}^{\text{blue}}\right\rangle\left\langle\sigma_{1N}^{\text{blue}}\right|$$