Measurement based imaginary time evolution

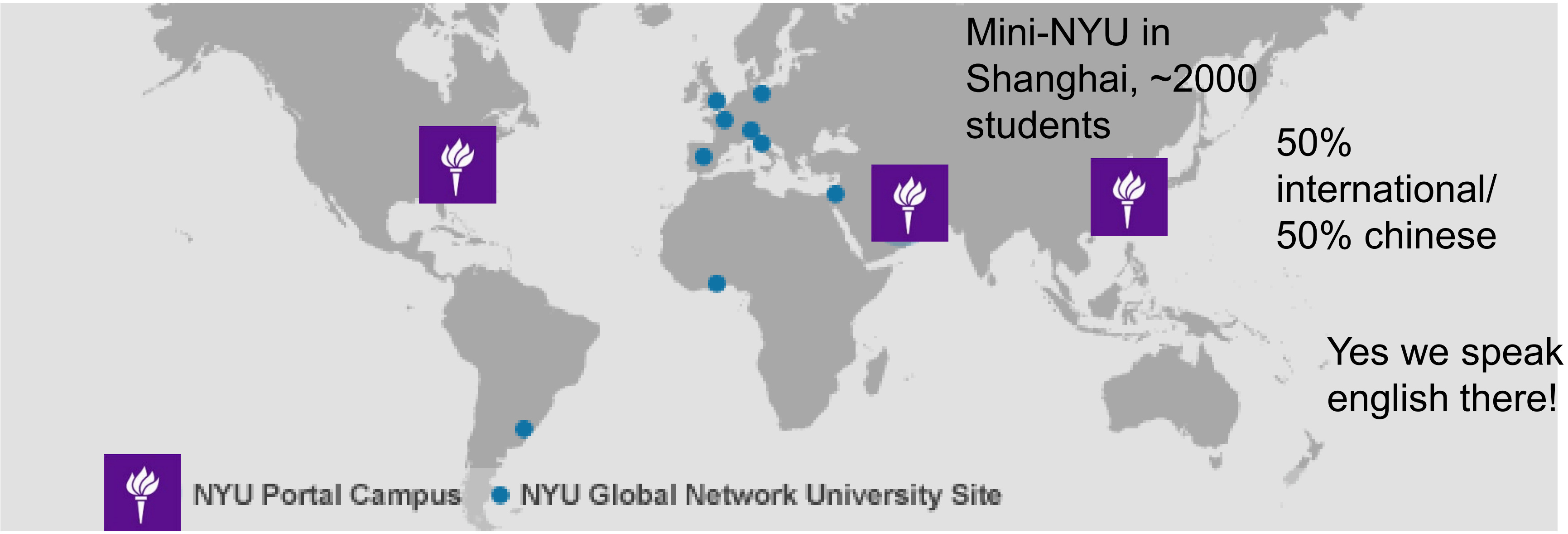
Tim Byrnes

New York University Shanghai

Center for Quantum and Topological Systems, NYUAD

State Key Laboratory of Precision Spectroscopy, ECNU

NYU Shanghai



Mini-NYU in Shanghai, ~2000 students

50% international/ 50% chinese

Yes we speak english there!

Quantum simulation

Feynman, Int. J. Theo. Phys. **21**, 467 (1982)

The aim of Quantum Simulation is to provide an alternative method to solving quantum many body problems to simulations on a classical computer.

Idea: Use quantum mechanics to simulate quantum mechanics!

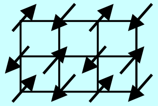
Why aren't classical computers very good at simulation?

N=50 S=1/2 spins need a Hilbert space dimension of $\dim(H) = 2^N \approx 10^{15}$ (~PB)

Applications

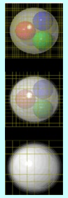
Solid state physics

Spin, electronic, bosonic models (e.g. Heisenberg, Hubbard, t-J, etc.),



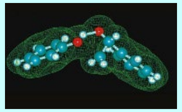
High energy physics

QCD lattice gauge theory



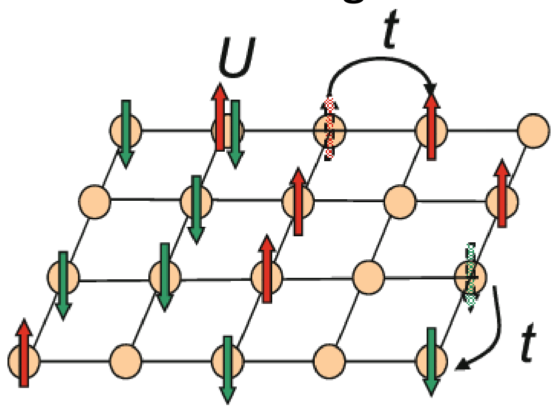
Quantum chemistry

Electronic structure of molecules

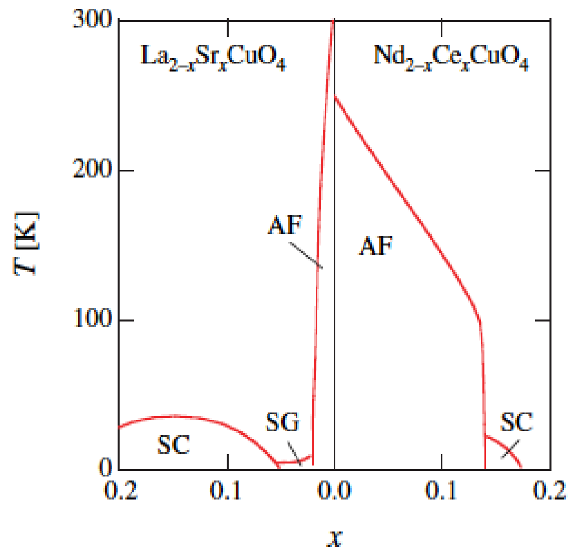


Aims of quantum simulation

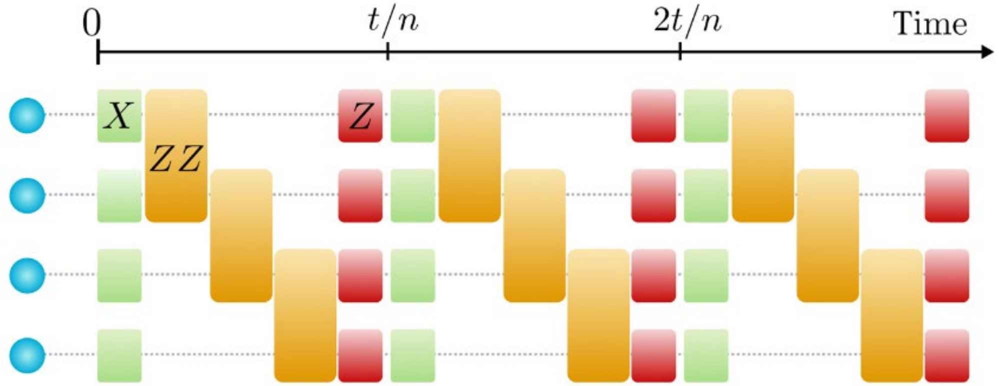
- Obtain the ground state (low energy state) of a Hamiltonian

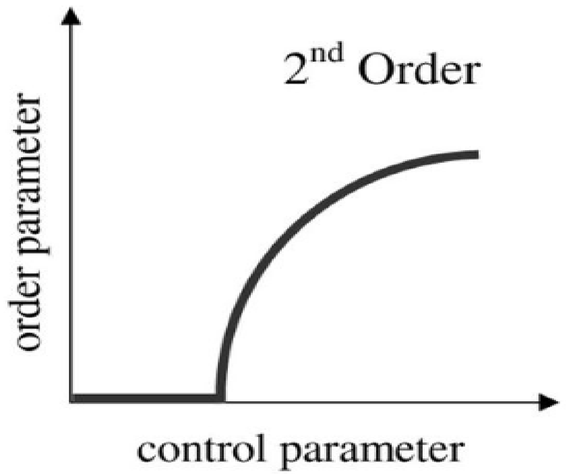


$$\hat{H} = -t \sum_{i,\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^{\dagger}_{i+1,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$



- Perform time evolution $e^{-iHt} = \left(e^{-iH_1 t/m} e^{-iH_2 t/m} \cdots e^{-iH_M t/m} \right)^m$





Lloyd, Science 273, 1073 (1996)

Computational problems as optimization

Many difficult computation problems (including NP-complete problems) can be formulated as an optimization problem

Example

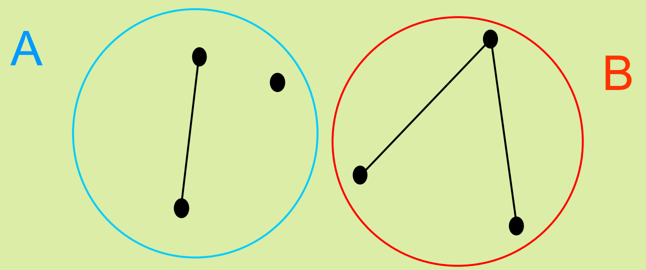
Consider the GPP, a known NP-complete problem. This may be equivalently formulated as a Hamiltonian

$$H_{GPP} = \sum_{i<j} J_{ij}\sigma_i^z \sigma_j^z$$

$$J_{ij} = \begin{cases} J & \text{if } i \text{ and } j \text{ connected} \\ 0 & \text{otherwise} \end{cases}$$

$$\sigma_i = \begin{cases} 1 & \text{if site } i \text{ in group A} \\ -1 & \text{if site } i \text{ in group B} \end{cases}$$

The graph partitioning problem (GPP)



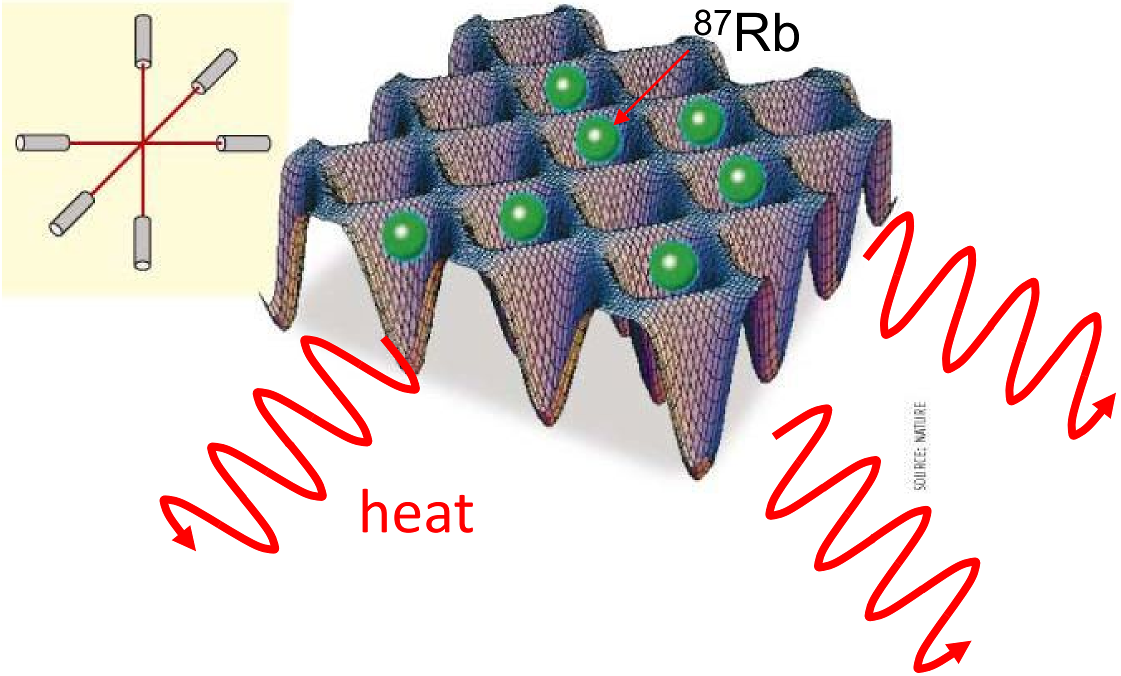
Given $2N$ points with arbitrary connections between them, the objective is to divide the points into two groups (A and B) of N points, minimizing the number of connections between them.

Analogue quantum simulation

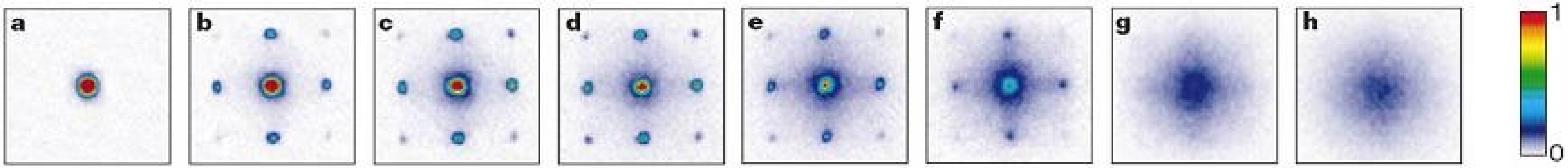
Application to quantum simulation:

Perform analogue of optical lattice superfluid to Mott insulator quantum phase transition experiment:

$$H_{BH} = -t\sum_{ij}\left(b_i^+ b_j + b_j^+ b_i\right) + \frac{U}{2}\sum_i n_i(n_i - 1)$$

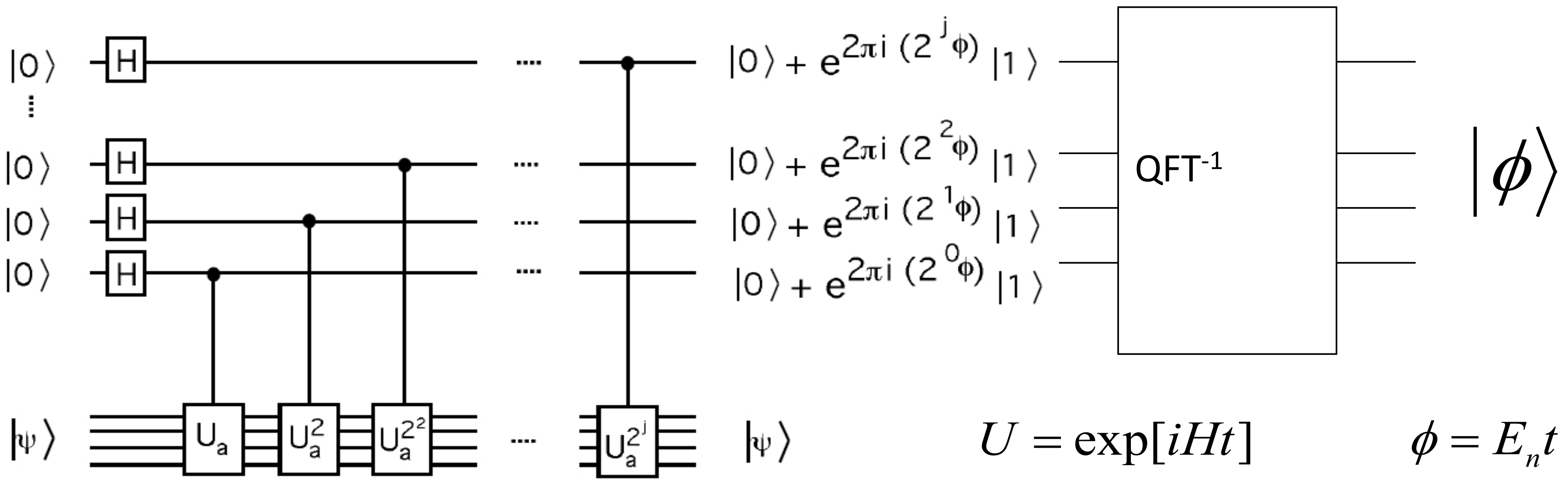


M. Greiner et al. Nature **415**, 39 (2002)



Quantum phase estimation

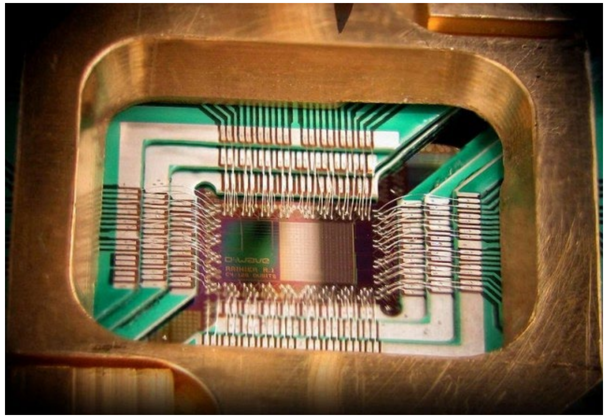
The eigenspectrum can be obtained using the quantum phase estimation circuit



1) Initialize qubits in a state of high overlap with states of interest. $|\Psi_{init}\rangle = \sum_n \Lambda_n |E_n\rangle$
2) Perform phase estimation of U(t) = exp[-iHt]
3) Obtain eigenvalue with probability $|\Lambda_n|^2$

➡ High probability only for a good initial guess

Quantum annealing

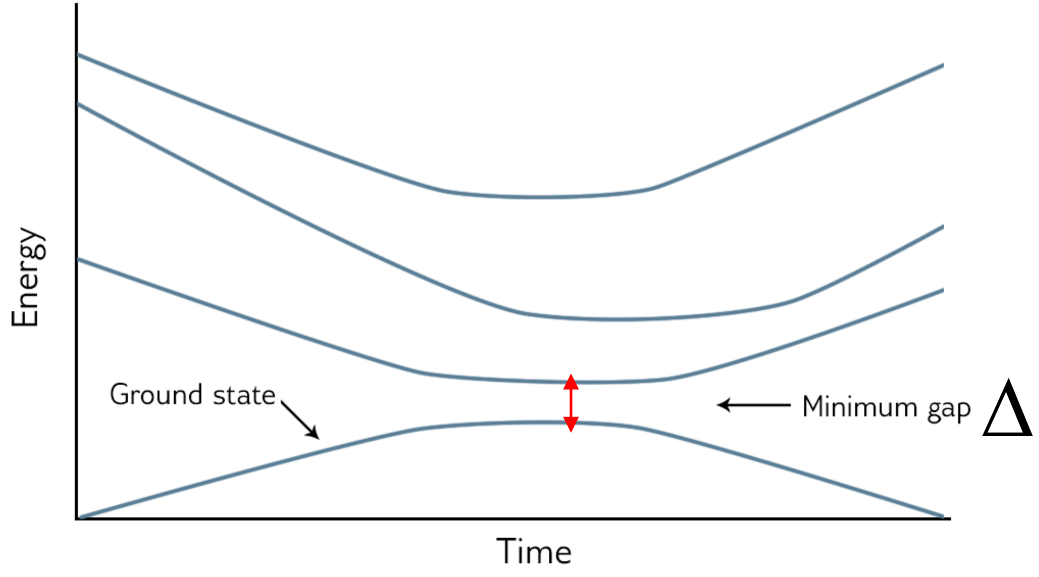


Another central technique in quantum computing is adiabatic quantum computing

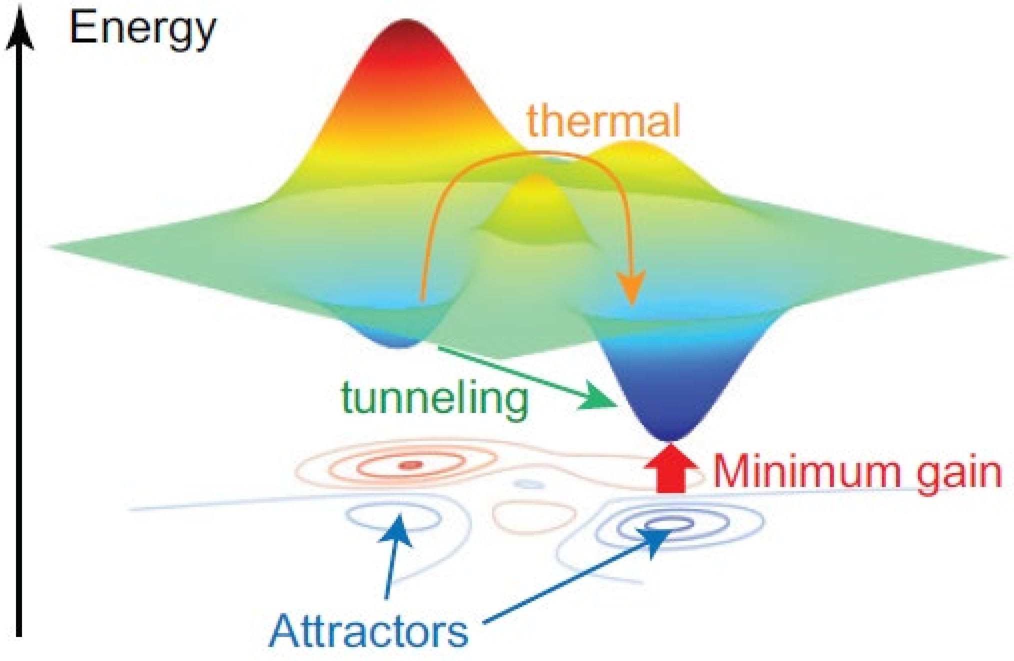
$$H = (1 - \lambda) H_X + \lambda H_Z$$

$$H_Z = \sum_{i=1}^{M} \sum_{j=1}^{M} J_{ij} \sigma_i^z \sigma_j^z + \sum_{i=1}^{M} K_i \sigma_i^z$$

$$H_X = - \sum_{i=1}^{M} \sigma_i^x$$



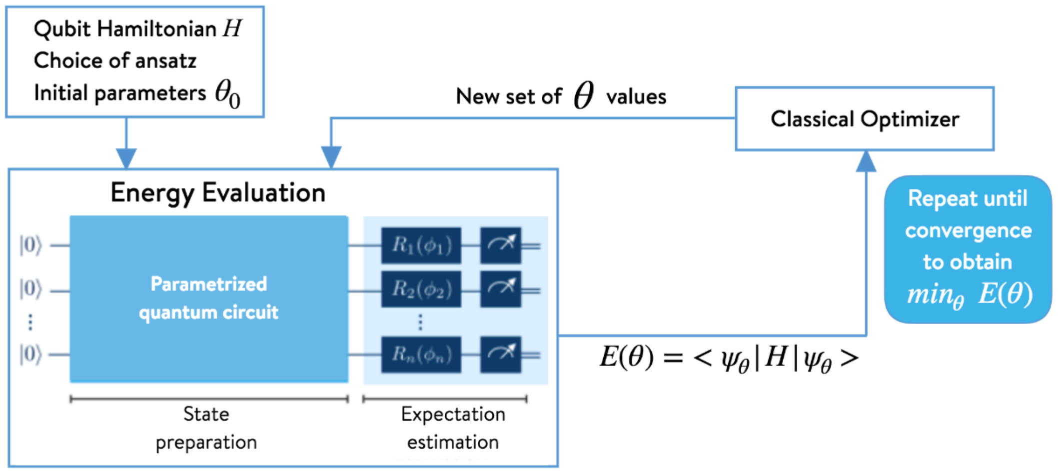
Time scaling $t \sim 1/\Delta^d$



Quantum-Classical hybrid approaches

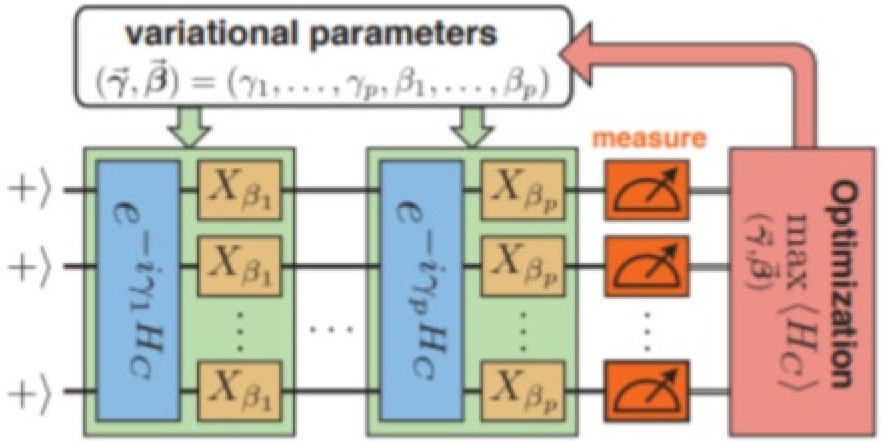
Basic idea: use quantum computer to estimate the energy of a ground state and use a classical feedback loop to optimize this

Variational Quantum Eigensolver



Perruzo et al. Nature Communications, 5, 4213 (2014)

QAOA



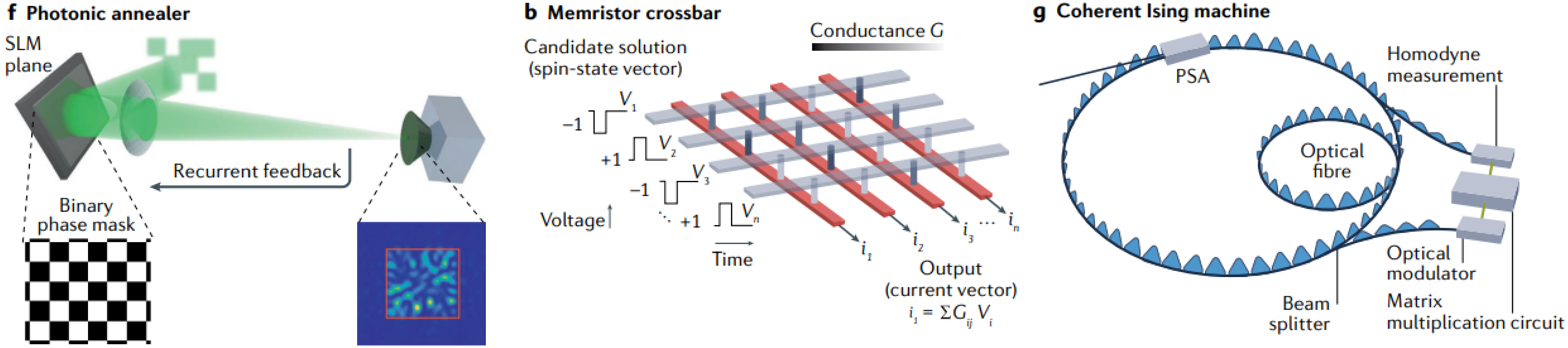
Farhi et al. *arXiv:1411.4028*

Ising machines

Ising machines are hardware devices that are specifically designed to solve the Ising model

$$H = \sum_{i<j} J_{ij} \sigma_i^z \sigma_j^z$$

1) Classical thermal annealing: Monte Carlo methods, physical stochastic systems
2) Dynamical system solvers: Oscillator based computing, Coherent Ising Machine, Chaotic dynamical systems
3) Quantum methods: Quantum annealing, Hybrid quantum-classical methods, Gibbs sampling
4) Other methods: Quantum inspired algorithms (simulated bifurcation), Machine learning



Ising machines as hardware solvers of combinatorial optimization problems

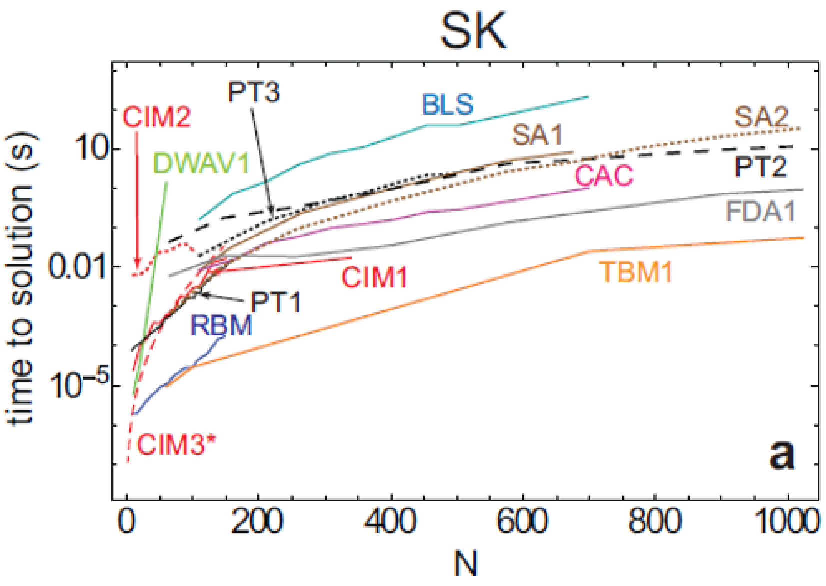
Mohseni, McMahon, TB, Nature Reviews Physics 4, 363 (2022)

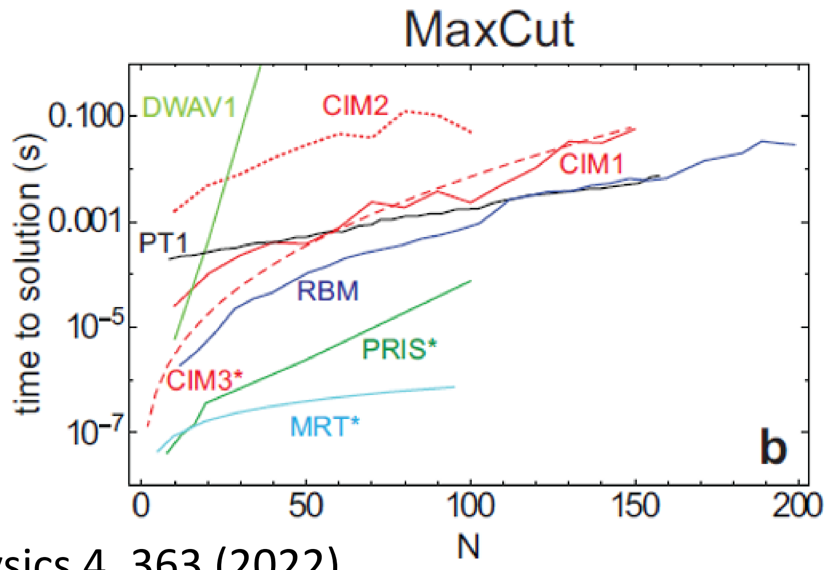
Performance of Ising machines

Ising machine/Algorithm	Acronym
Breakout local search	BLS
Chaotic amplitude control	CAC
Coherent Ising machine (NTT)	CIM1
Coherent Ising machine (Stanford)	CIM2
Coherent Ising machine	CIM3
D-Wave quantum annealer 2Q	DWAV1
D-Wave quantum annealer Advantage1.1	DWAV2
D-Wave quantum annealer 2KQ	DWAV3
D-Wave quantum annealer 2KQ	DWAV4
Fujitsu digital annealer	FDA1
Fujitsu digital annealer	FDA2
Hamze–de-Freitas–Selb	HFS
Memcomputing	MEM
Memristor annealing	MRT
Photonic recurrent Ising sampler	PRIS
Parallel tempering	PT1
Parallel tempering	PT2
Parallel tempering	PT3
Parallel tempering	PT4
Isoenergetic cluster moves+ parallel tempering	PT+ICM
Restricted Boltzmann machine	RBM
Simulated annealing	SA1
Simulated annealing	SA2
Simulated annealing	SA3
SATonGPU	SAT
Simulated quantum annealing	SQA1
Toshiba bifurcation machine	TBM1
Toshiba bifurcation machine	TBM2

Time to solution=Total time required to obtain the ground state with probability 99%, running the machine many times

$$T_{\mathrm{sol}} = \tau \frac{\ln 0.01}{\ln(1-p_{\mathrm{suc}})}$$





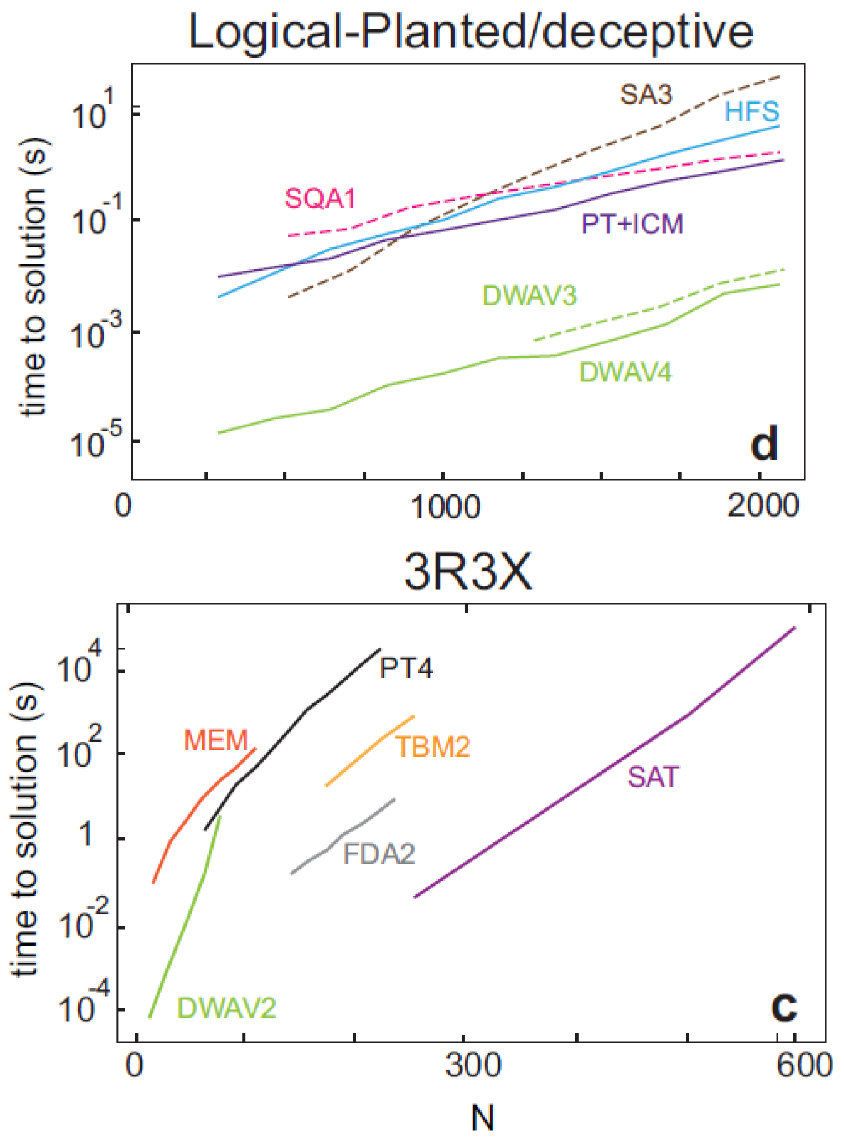
Mohseni, McMahon, TB, Nature Reviews Physics 4, 363 (2022)

Performance of Ising machines

Ising machine/Algorithm	Acronym
Breakout local search	BLS
Chaotic amplitude control	CAC
Coherent Ising machine (NTT)	CIM1
Coherent Ising machine (Stanford)	CIM2
Coherent Ising machine	CIM3
D-Wave quantum annealer 2Q	DWAV1
D-Wave quantum annealer Advantage1.1	DWAV2
D-Wave quantum annealer 2KQ	DWAV3
D-Wave quantum annealer 2KQ	DWAV4
Fujitsu digital annealer	FDA1
Fujitsu digital annealer	FDA2
Hamze–de-Freitas–Selb	HFS
Memcomputing	MEM
Memristor annealing	MRT
Photonic recurrent Ising sampler	PRIS
Parallel tempering	PT1
Parallel tempering	PT2
Parallel tempering	PT3
Parallel tempering	PT4
Isoenergetic cluster moves+ parallel tempering	PT+ICM
Restricted Boltzmann machine	RBM
Simulated annealing	SA1
Simulated annealing	SA2
Simulated annealing	SA3
SATonGPU	SAT
Simulated quantum annealing	SQA1
Toshiba bifurcation machine	TBM1
Toshiba bifurcation machine	TBM2

Time to solution=Total time required to obtain the ground state with probability 99%, running the machine many times

$$T_{\rm sol} = \tau \frac{\ln 0.01}{\ln(1-p_{\rm suc})}$$



Mohseni, McMahon, TB, Nature Reviews Physics 4, 363 (2022)

Deterministic Measurement-based Imaginary Time Evolution

Yuping Mao

Manikandan Kondappan

Manish Chaudhary

Ebubechukwu Ilo-Okeke

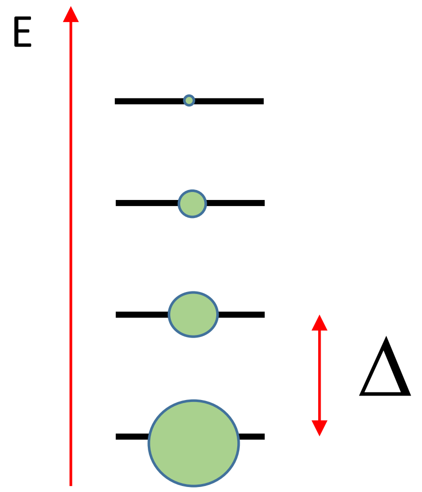
Y. Mao, M. Chaudhary, M. Kondappan, J. Shi, E. O. Ilo-Okeke, V. Ivannikov, TB, arxiv 2202.09100
M. Kondappan, M. Chaudhary, E. O. Ilo-Okeke, V. Ivannikov, TB, Phys. Rev. A 107, 042616 (2023)
E. O. Ilo-Okeke, Y. Ji, P. Chen, Y. Mao, M. Kondappan, V. Ivannikov, Y. Xiao, TB Phys. Rev. A **106**, 033314 (2022)

Imaginary time evolution

Imaginary time evolution obtain the ground state, exponentially converging in time

$$e^{-Ht}\left|\Psi_{init}\right\rangle = \sum_n e^{-E_n t}\Lambda_n \left|E_n\right\rangle$$

$$t \sim 1/\Delta$$



IF this was directly applicable it would be efficient in the number of gates

$$e^{-Ht} = \left(e^{-H_1 t/m} e^{-H_2 t/m} \cdots e^{-H_M t/m}\right)^m$$

$$H = \sum_i H_i$$

In the same way that real time evolution can be performed efficiently in a quantum computer

$$e^{-iHt} = \left(e^{-iH_1 t/m} e^{-iH_2 t/m} \cdots e^{-iH_M t/m}\right)^m$$

Unfortunately this doesn’t really help in terms of getting the ground state

$$e^{-iHt}\left|\Psi_{init}\right\rangle = \sum_n e^{-iE_n t}\Lambda_n \left|E_n\right\rangle$$

Previous algorithms

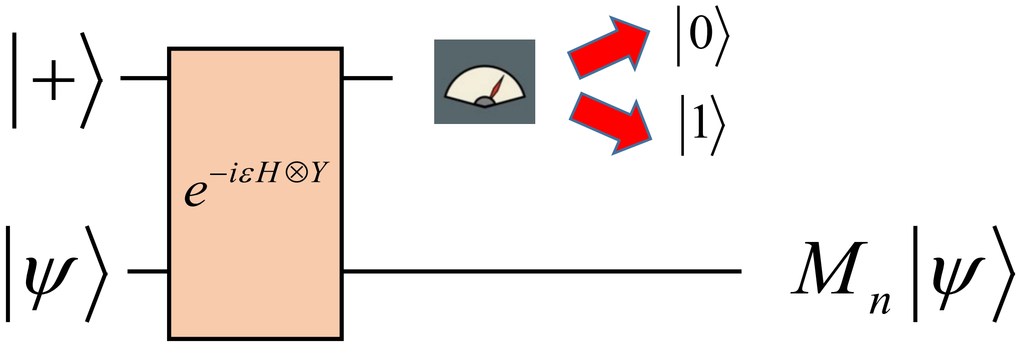
S. McArdle,.., X. Yuan, npj Quantum Information 5, 1 (2019).
M. Motta, … G. K.-L. Chan, Nature Physics 16, 205 (2020).
Colin P. Williams, Proc. SPIE 5436 (2004)

Measurement operators

Consider a measurement of the form

$$M_0 = \langle 0|_a e^{-i\epsilon H\otimes Y}|+\rangle_a = \frac{1}{\sqrt{2}}(\cos\epsilon H - \sin\epsilon H) \quad = \frac{1}{\sqrt{2}}\sum_n(\cos\epsilon E_n - \sin\epsilon E_n)|E_n\rangle\langle E_n| \approx \frac{e^{-\epsilon H}}{\sqrt{2}}$$

$$M_1 = \langle 1|_a e^{-i\epsilon H\otimes Y}|+\rangle_a = \frac{1}{\sqrt{2}}(\cos\epsilon H + \sin\epsilon H) \quad = \frac{1}{\sqrt{2}}\sum_n(\cos\epsilon E_n + \sin\epsilon E_n)|E_n\rangle\langle E_n| \approx \frac{e^{\epsilon H}}{\sqrt{2}}$$



Performing this measurement can be efficiently Performed:

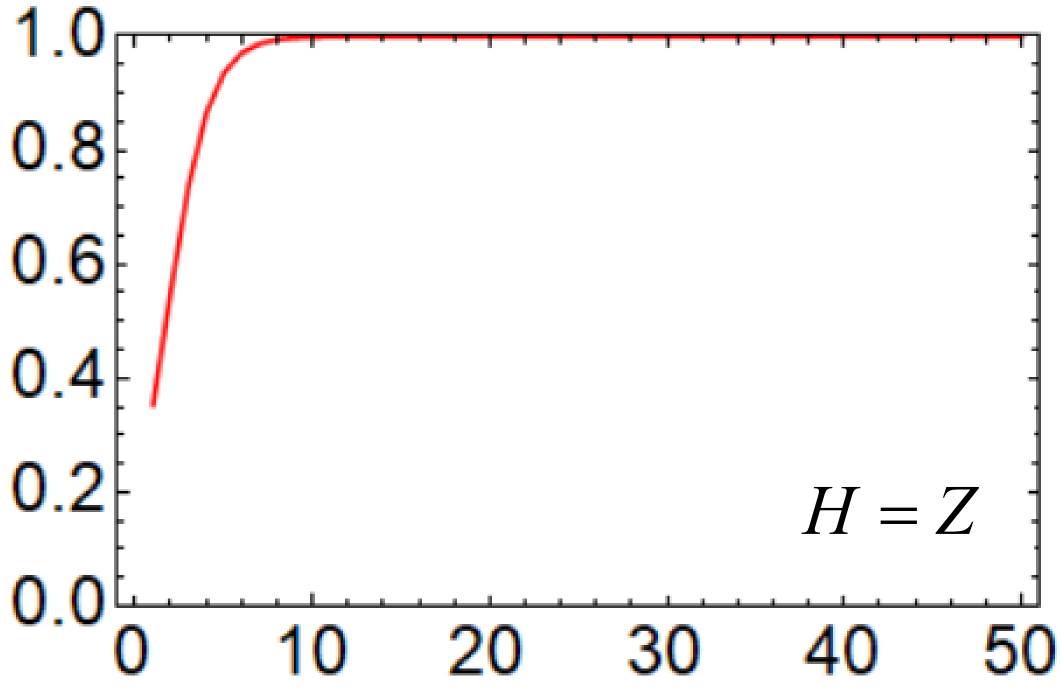
$$e^{-HYt} = \left(e^{-H_1Yt/m}e^{-H_2Yt/m}\cdots e^{-H_MYt/m}\right)^m$$

The lucky outcome

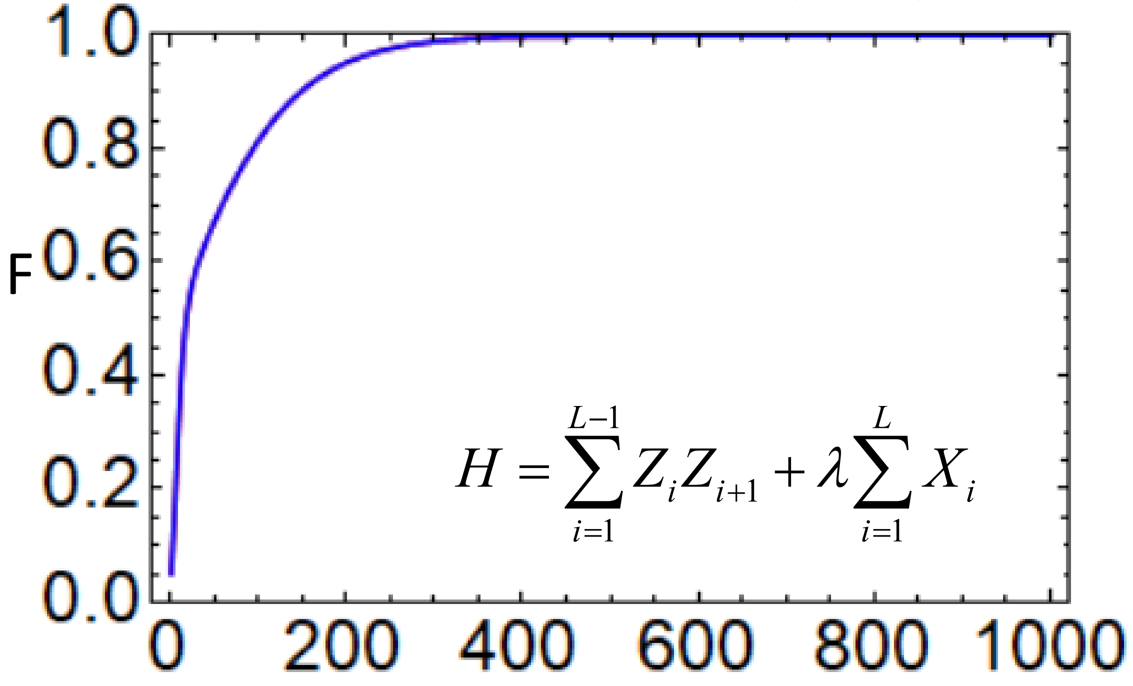
Suppose we obtained the outcome M0 a total of t times:

$$|\psi_t\rangle = \frac{(M_0)^t |\psi_0\rangle}{\sqrt{p_0}} \approx \frac{e^{-\varepsilon t H}|\psi_0\rangle}{\sqrt{p_0}}$$

$\varepsilon = 0.2$



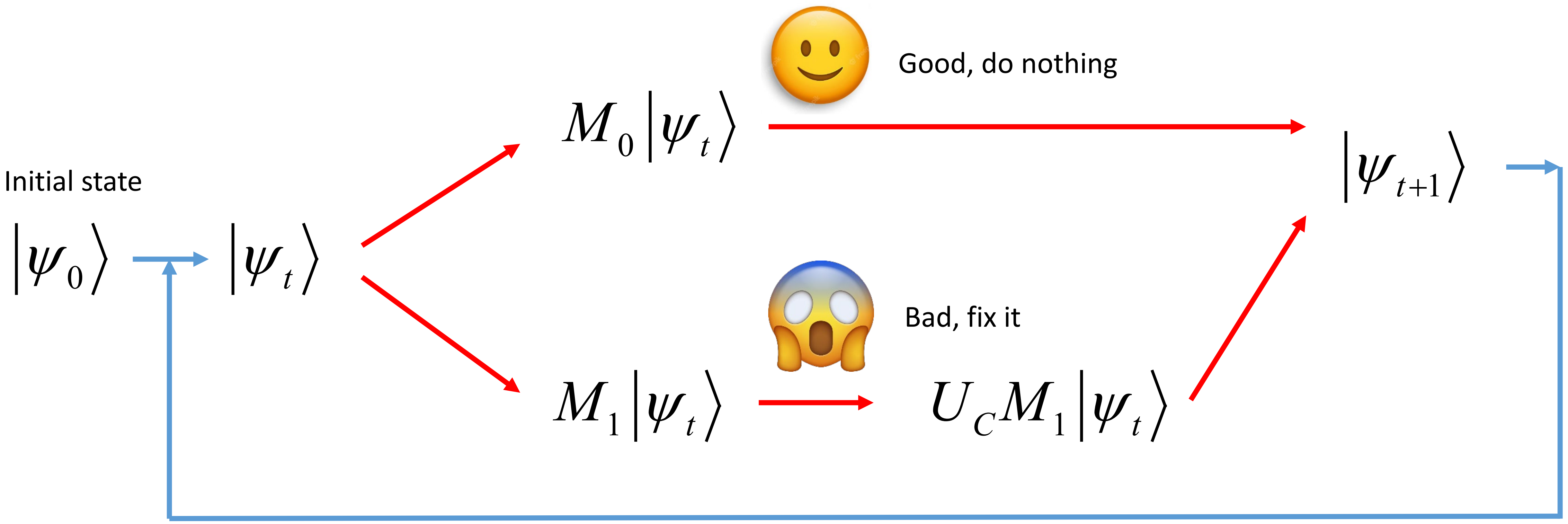
$\varepsilon = 0.12, \lambda = 1, L = 5$



$$p_0 = \langle\psi_0|(M_0^\dagger)^t (M_0)^t|\psi_0\rangle \sim 1/2^L$$

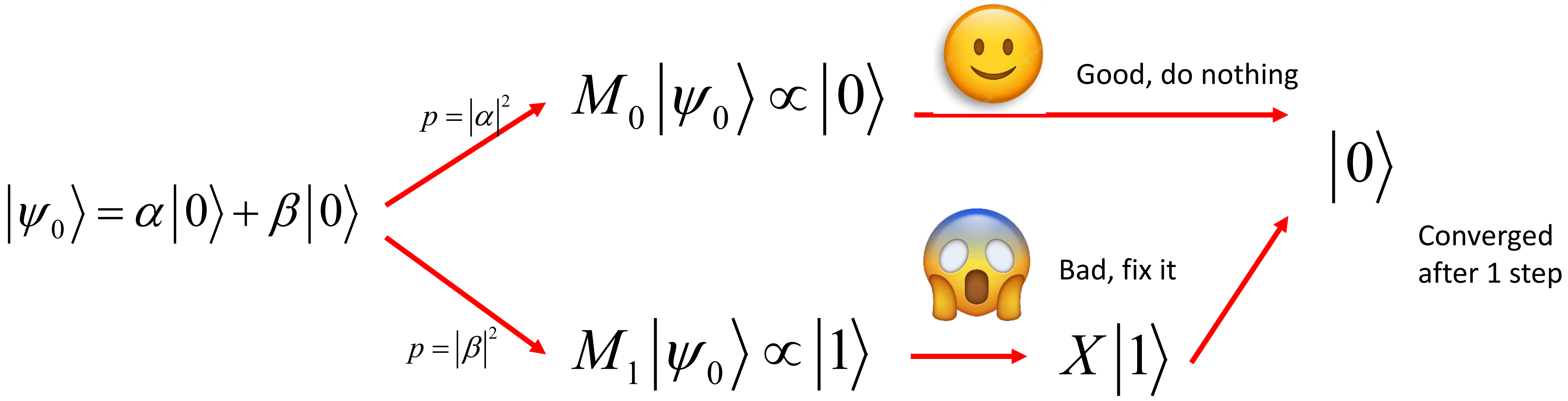
Very unlikely outcome… how to make this deterministic?

The basic idea



Strong measurement example

$H = -Z$ $\qquad M_0 = |0\rangle\langle 0| \qquad M_1 = |1\rangle\langle 1|$



How to choose $U_C = X$? Basically need off-diagonal in energy basis: $|\langle E_n|U_C|E_m\rangle| > 0$

Repeated weak measurement case

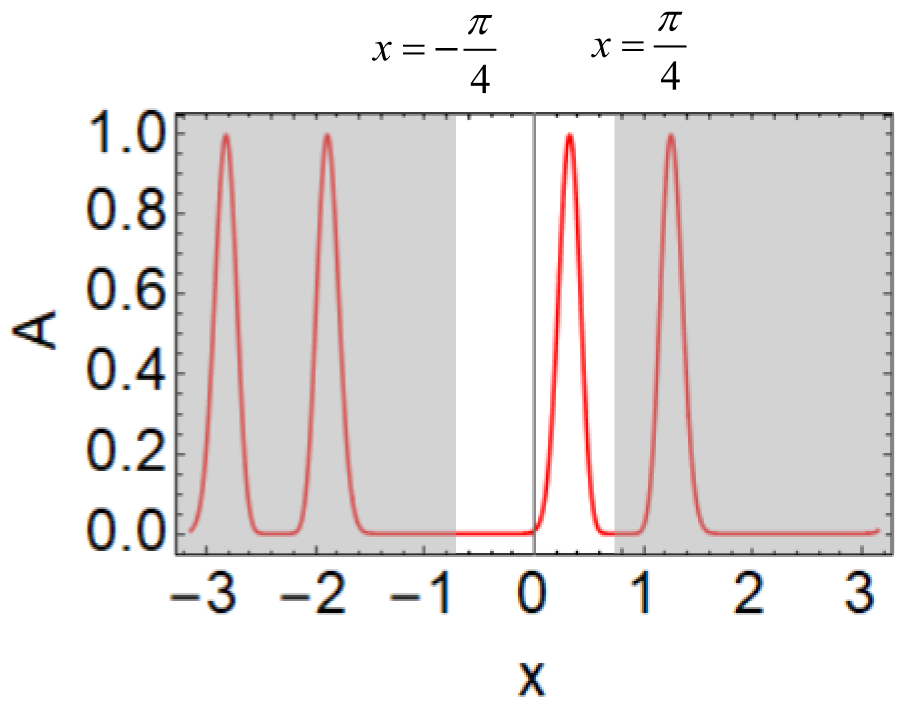
$$M_0 M_1 M_0 M_1 \dots M_1 M_0 M_0 \left|\psi_0\right\rangle =$$

$$M_0^{k_0} M_1^{k_1} |\psi_0\rangle = \sum_n A_{k_0 k_1}(\epsilon E_n) \langle E_n|\psi_0\rangle |E_n\rangle$$

$$M_0 = \frac{1}{\sqrt{2}} \sum_n (\cos \epsilon E_n - \sin \epsilon E_n) |E_n\rangle\langle E_n|$$

$$M_1 = \frac{1}{\sqrt{2}} \sum_n (\cos \epsilon E_n + \sin \epsilon E_n) |E_n\rangle\langle E_n|$$

$$\begin{aligned} A_{k_0 k_1}(x) &= \frac{1}{\sqrt{2^{k_0+k_1}}} (\cos x - \sin x)^{k_0} (\cos x + \sin x)^{k_1} \\ &= \cos^{k_0}(x + \pi/4) \sin^{k_1}(x + \pi/4). \end{aligned}$$



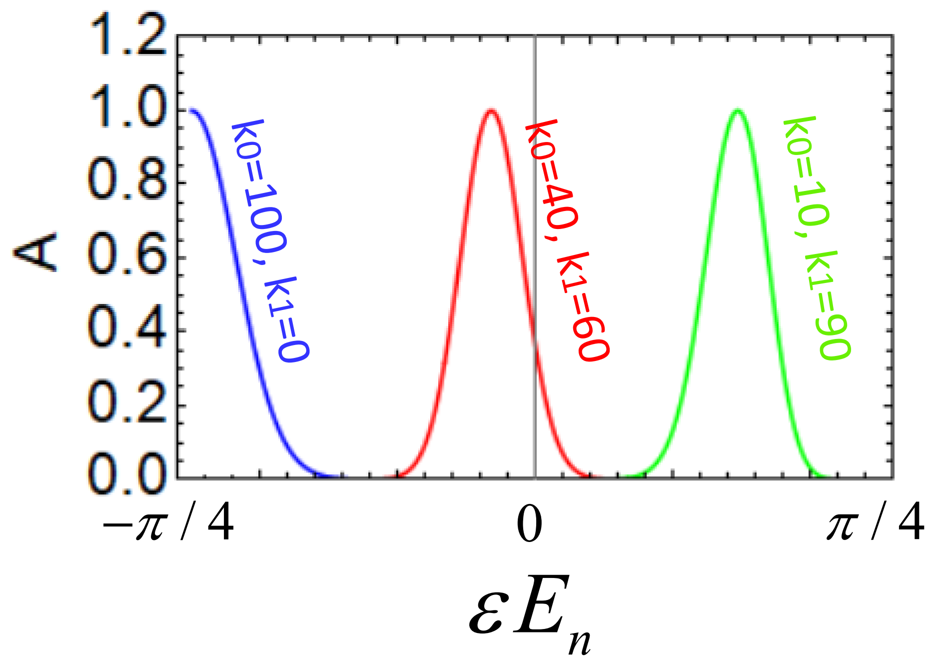
In the range $-\frac{\pi}{4} < x < \frac{\pi}{4}$, is a Gaussian

Gaussian measurements

$$M_0^{k_0} M_1^{k_1} |\psi_0\rangle = \sum_n A_{k_0 k_1}(\epsilon E_n) \langle E_n | \psi_0 \rangle | E_n \rangle$$

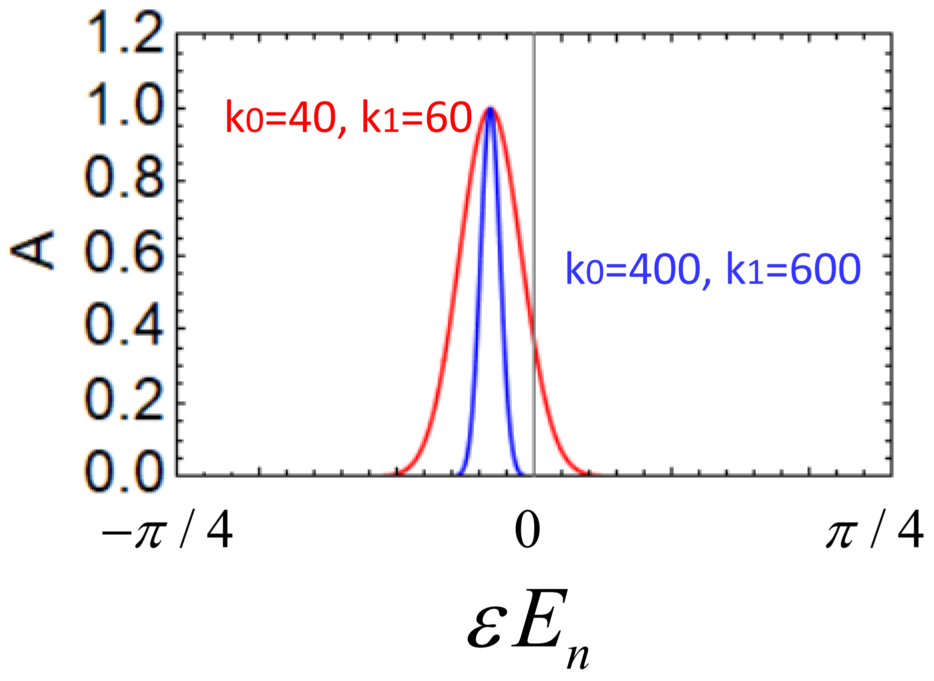
$$A_{k_0 k_1}(x) \propto \exp\left(-\frac{(x - x_{k_0 k_1}^{\max})^2}{2\sigma^2}\right)$$

The k0,k1 readouts estimate the energy



$$x_{k_0 k_1}^{\max} = \frac{1}{2} \arcsin\left(\frac{k_1 - k_0}{k_1 + k_0}\right)$$

More measurements collapse the state:

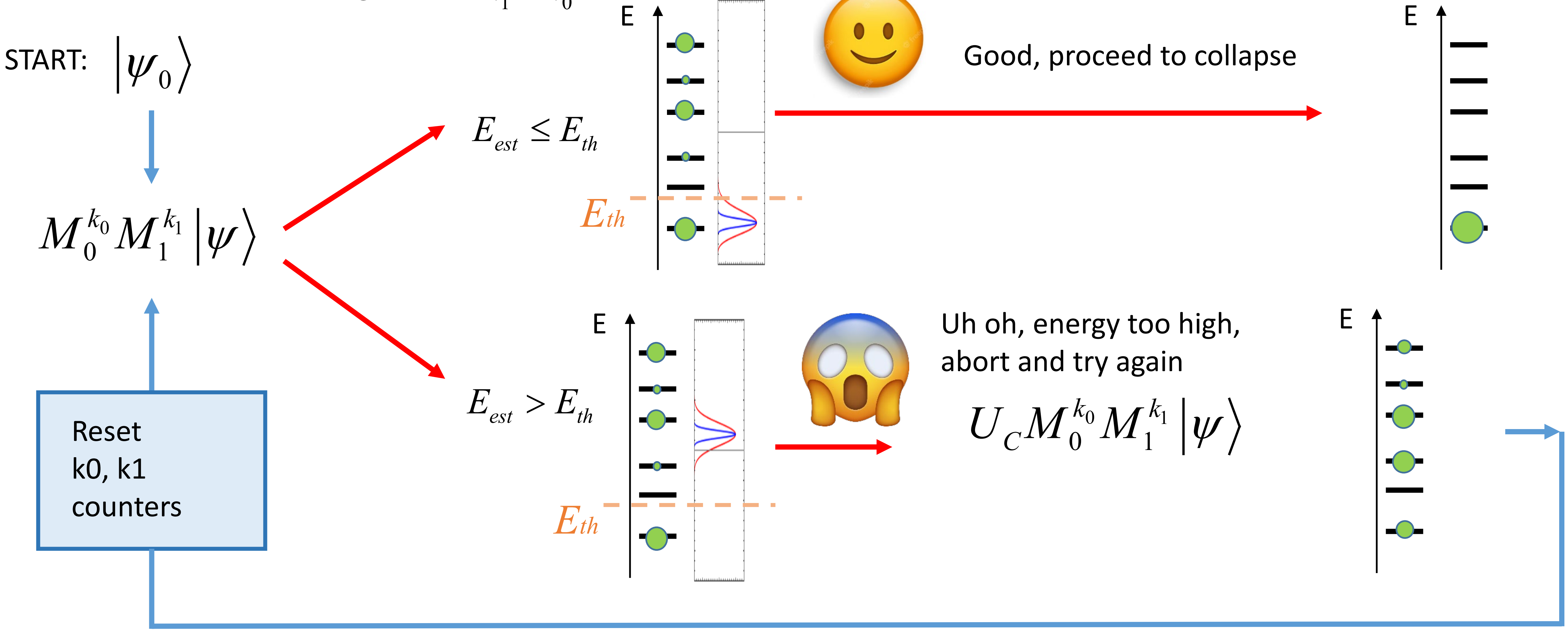


$$\sigma \approx \frac{1}{\sqrt{2(k_0 + k_1)}}$$

The MITE routine

Since the measurement operators only cause a partial collapse we modify the procedure as

$$E_{est} = \frac{1}{2\varepsilon}\arcsin\left(\frac{k_1 - k_0}{k_1 + k_0}\right)$$



The unitary correction operator

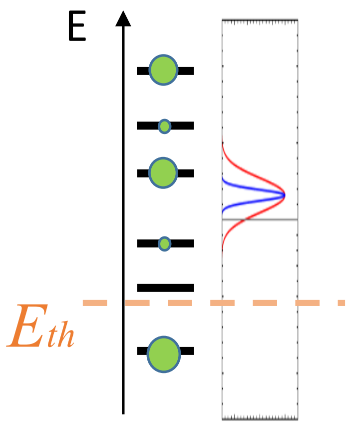
How to choose U_C ?

This is applied after a partial collapse on a high energy state.

Ideally we redistribute the population back to the ground state.

A simpler strategy is simply to choose U_C such that

$$|\langle E_n|U_C|E_m\rangle| > 0, \forall n, m$$



This ensures that eventually convergence occurs on a state with $E_{est} \leq E_{th}$

This is typically not very hard to satisfy since the energy eigenstates are some complex superposition.

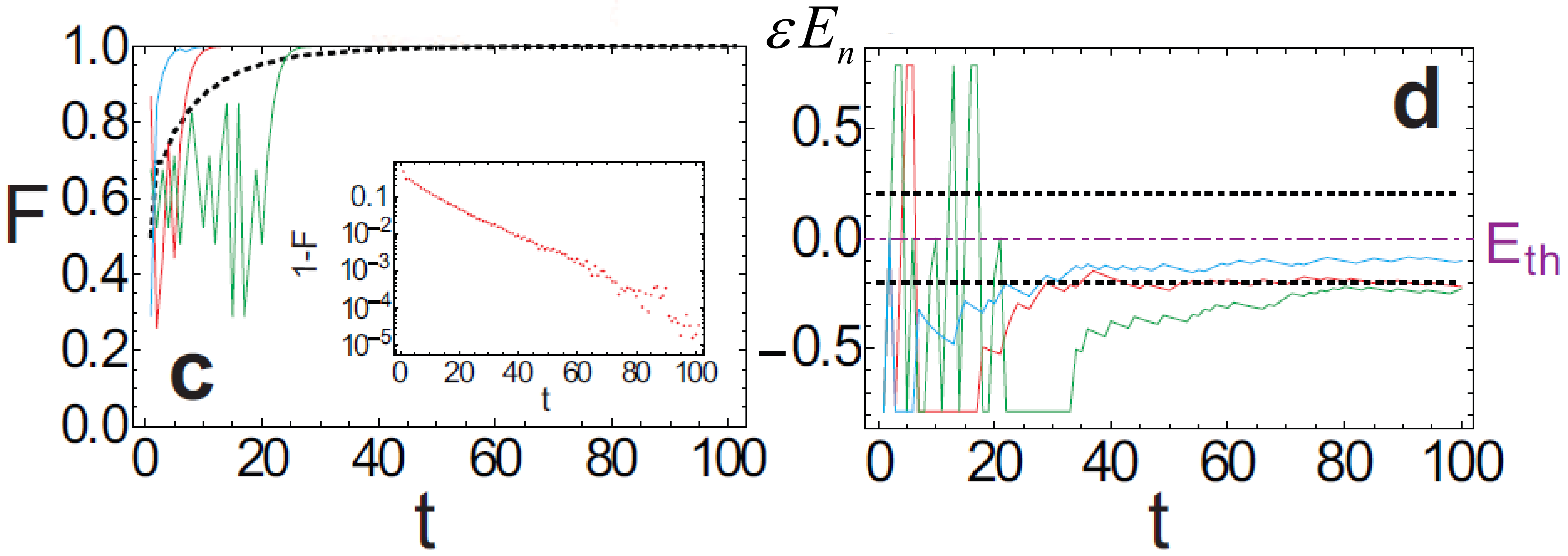
e.g. for transverse Ising model choose random local unitaries

$$U_C = \otimes_{n=1}^{L} e^{2\pi i(\phi_n^x X_n + \phi_n^y Y_n + \phi_n^z Z_n)}$$

Qubit Hamiltonian

$H = Z$

$U_C = X \qquad \epsilon = 0.2$



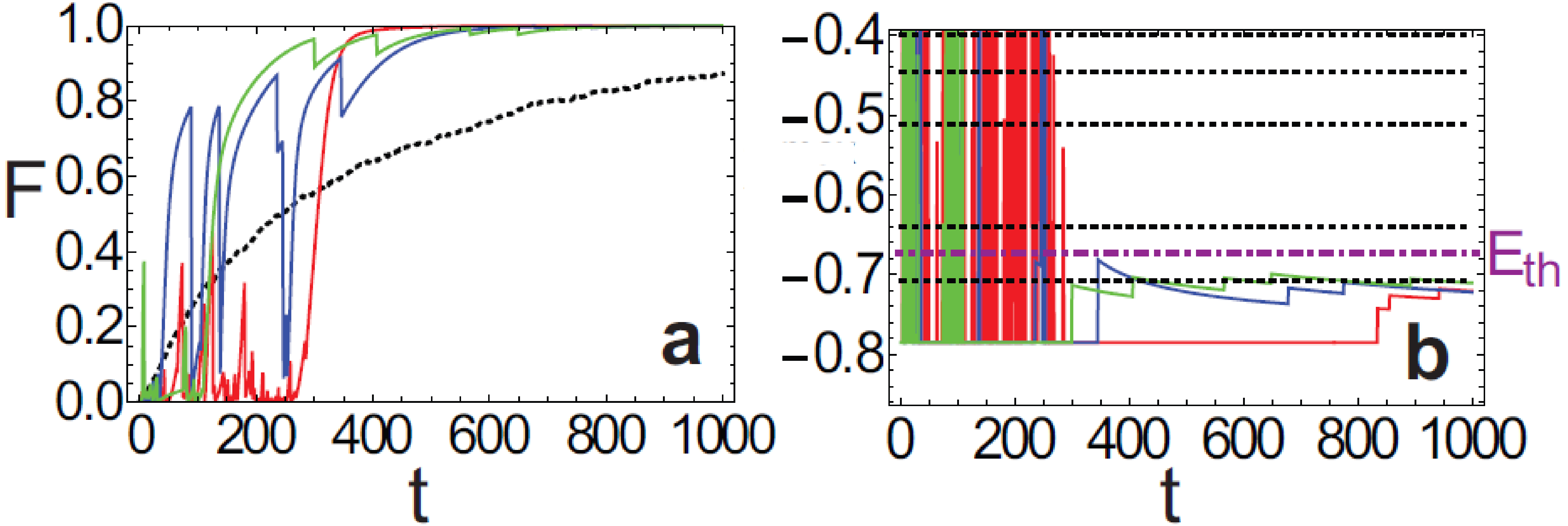
Mao et al. arxiv 2202.09100

Transverse field Ising model

$$H = \sum_{i=1}^{L-1} Z_i Z_{i+1} + \lambda \sum_{i=1}^{L} X_i$$

$$U_C = \otimes_{n=1}^{L} e^{2\pi i(\phi_n^x X_n + \phi_n^y Y_n + \phi_n^z Z_n)}$$

εE_n $L = 5$ $\lambda = 1$ $\epsilon = 0.12$



Mao et al. arxiv 2202.09100

AKLT state

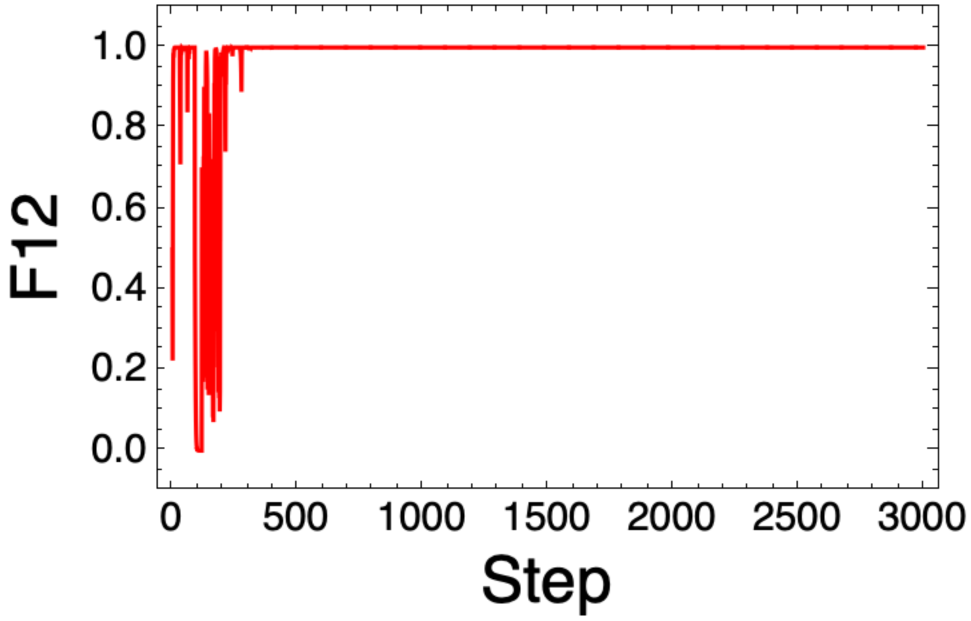
$$H_{AKLT} = \sum_i P_{i,i+1}$$ (S=1 operators)

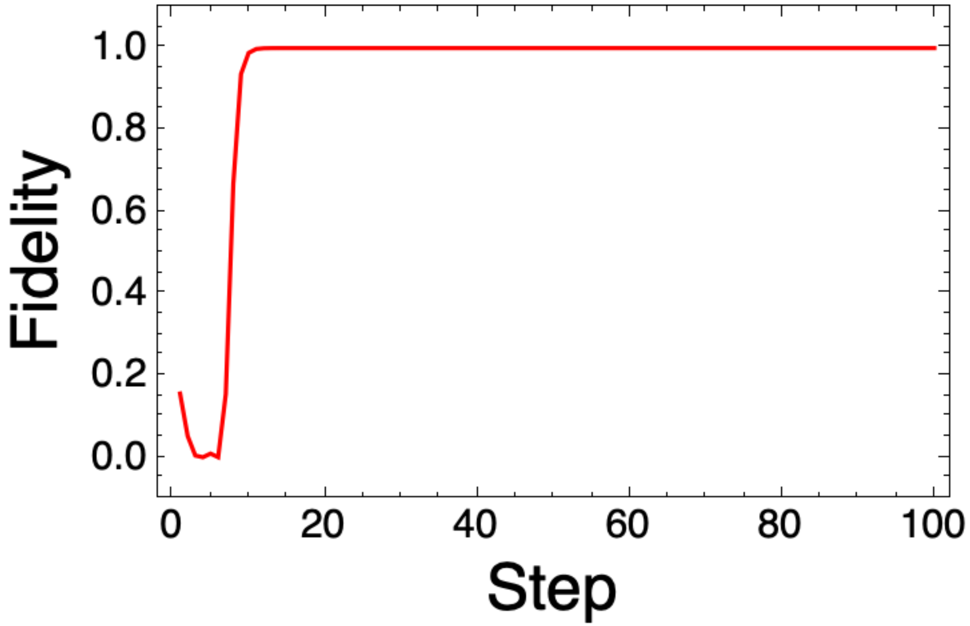
$$P_{i,i+1} = \frac{1}{2}\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{6}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 + \frac{1}{3}$$

Since the ground state satisfies $P_{i,i+1}|AKLT\rangle = 0$

We may apply these in sequence

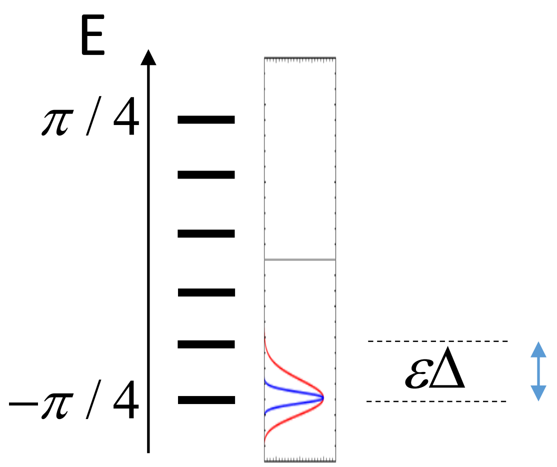
4 site PBC





Tianqi Chen, .. , TB (in preparation)

Scaling



How many steps are required to get to convergence?

Consider a prototype example: Uniformly spaced non-degenerate Hamiltonian:

From a uniformly distributed initial state $|\psi_0\rangle = \frac{1}{\sqrt{D}} \sum_{n=0}^{D-1} |E_n\rangle.$

The probability of getting k consecutive M0 outcomes is

$$p_k = \langle\psi_0|(M_0^\dagger)^k M_0^k|\psi_0\rangle$$

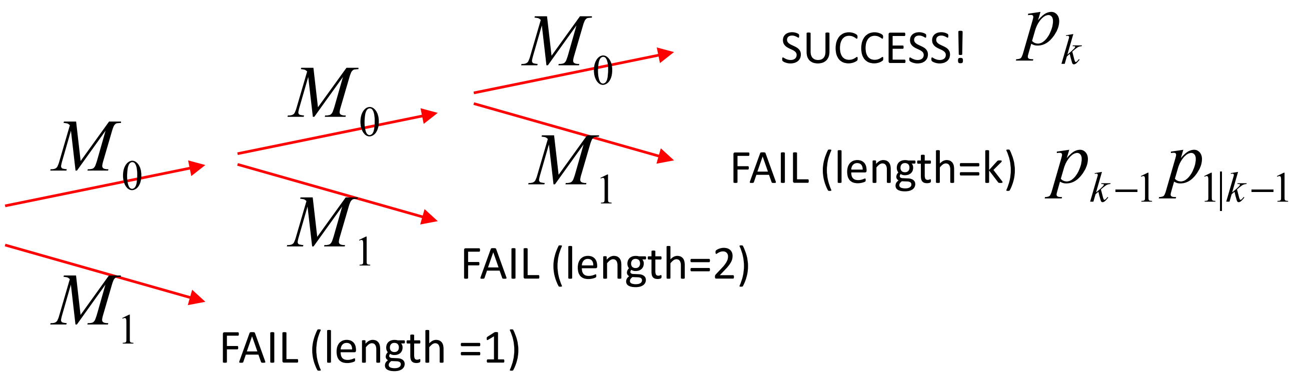
$$= \frac{1}{D} \sum_{n=0}^{D-1} \cos^{2k}(\epsilon E_n + \pi/4) = \frac{1}{4^k}\binom{2k}{k} \approx \frac{1}{\sqrt{k\pi}}$$

NOT $1/2^k$ As from a random distribution

→ "Self-enhancing" effect

How big should k be such that convergence is attained? $\varepsilon\Delta \sim 2/\sqrt{k}$ Such that the gaussian suppresses the first excited state

What is the average length of a failed sequence before we get k M0’s?



$$p_k = \frac{1}{4^k}\binom{2k}{k}$$

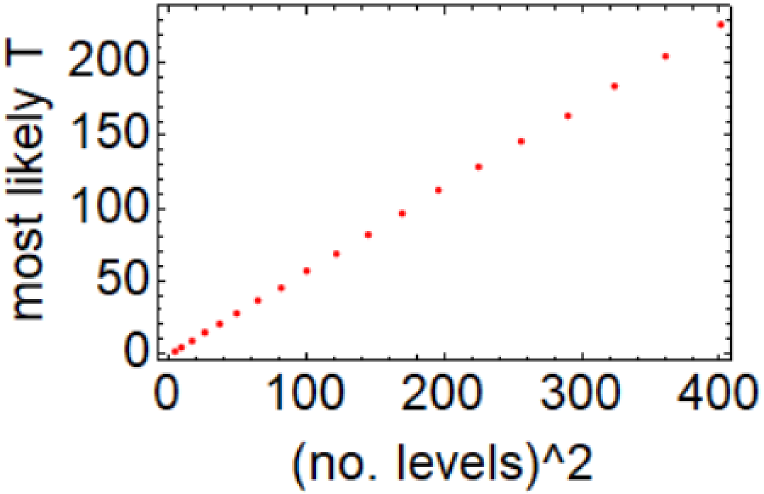
$$p_{1|k} = 1 - p_{0|k} = \frac{1}{2(k+1)}$$

Average length of a failed sequence $$T_k^{\text{fail}} = \sum_{k'=1}^{k} k' p_{1|k'-1} p_{k'-1} = \frac{k}{4^k}\binom{2k}{k} \approx \sqrt{\frac{k}{\pi}}$$

Then the total number of failed sequences is $$T = \frac{T_k^{\text{fail}}}{p_k} + k \approx 2k$$

Putting this together with the necessary k we have $$T \approx \frac{8}{\epsilon^2 \Delta^2}$$

Numerical simulation:



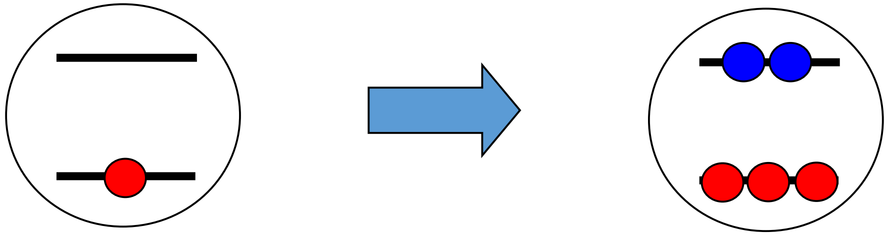
Spinor quantum computing

The analogy between spin coherent states and qubits suggests we try and encoding like

Want to encode | ***Physically we actually do***

$\alpha|\uparrow\rangle + \beta|\downarrow\rangle$

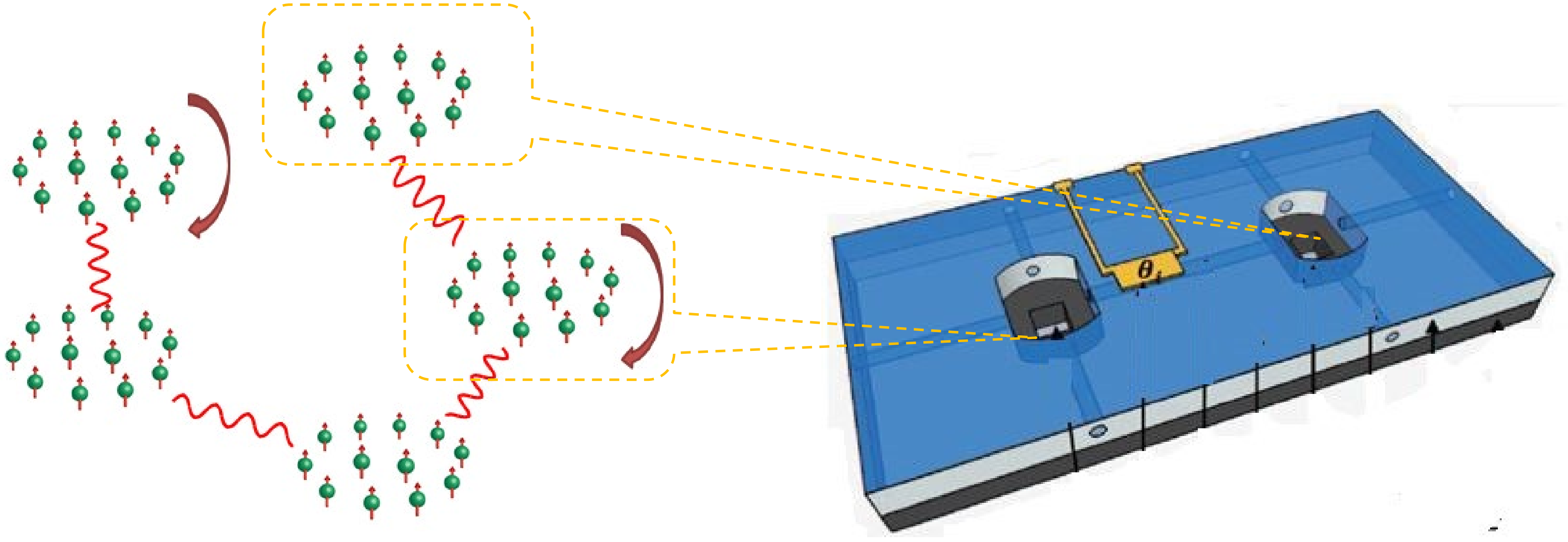
Qubit



$$|\alpha,\beta\rangle\rangle \equiv \frac{1}{\sqrt{N!}}\left(\alpha a^\dagger + \beta b^\dagger\right)^N |0\rangle$$

Spin coherent state

We scale up by having many spin coherent states, which are in general entangled with each other



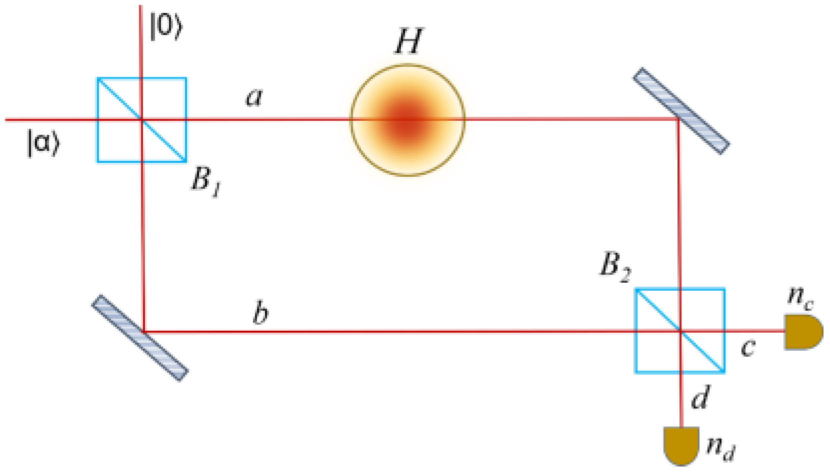
TB .. Yamamoto, Phys. Rev A 85 040306(R) (2012)

Mohseni … TB, npj Quantum Information 7, 71 (2021).

Natural way to perform error suppression!

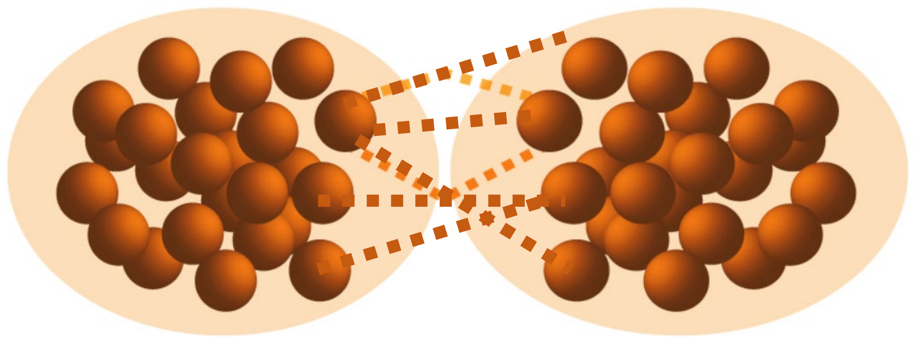
Applications

Actually the measurement can be any kind of weak measurement, including QND measurements:

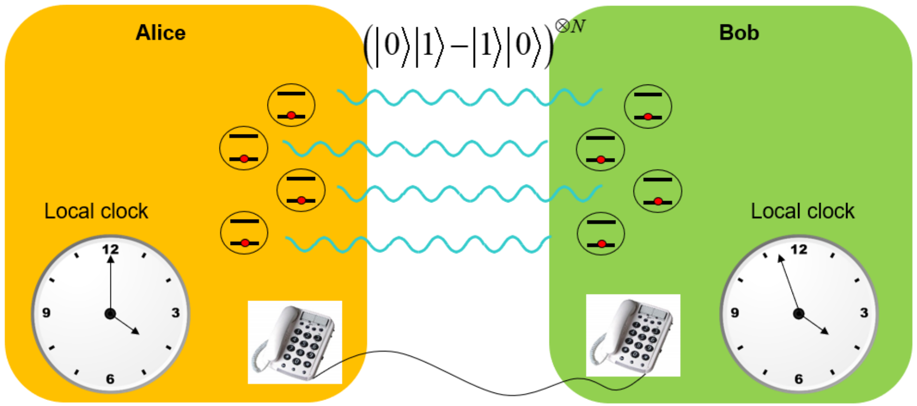


Kondappan, … TB, Phys. Rev. A 107, 042616 (2023)

The ITE operation can be used to deterministically produce a maximally entangled state (macroscopic singlet state)



Ilo-Okeke … TB, Phys. Rev. A 106, 033314 (2022)
Chaudhary, .. TB, arxiv 2302.07526



Ilo-Okeke… TB, Nature Partner Journal Quantum Information 4, 40 (2018)

Summary and conclusions

- Imaginary time evolution is a versatile general algorithm to find the ground state of a Hamiltonian.

- For a simple uniform density of states model the scaling is found to be

$$T \propto \frac{1}{(\varepsilon\Delta)^2}$$

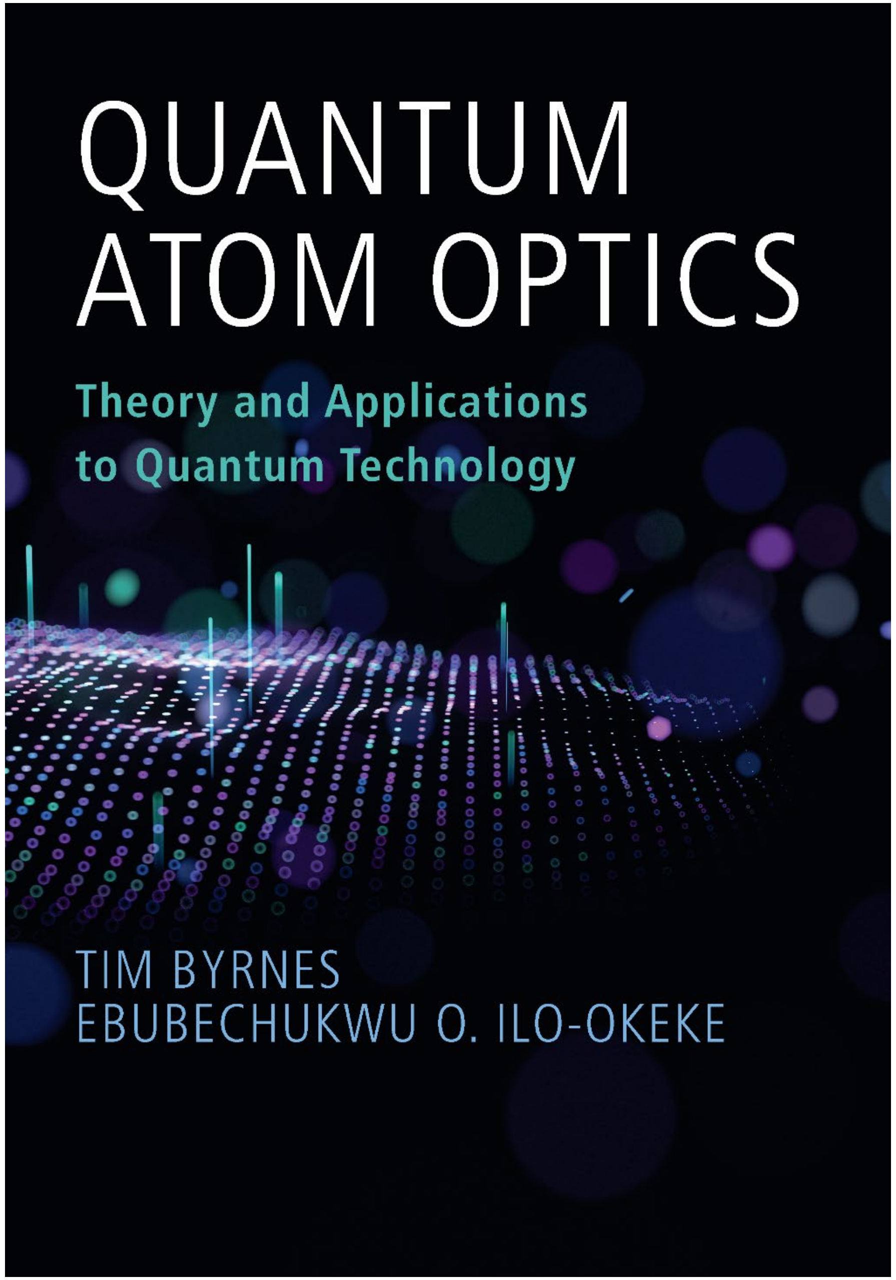
- Useful for state preparation and can be used with any energy estimation measurement (e.g. QND).

References

Imaginary time evolution theory: Yuping Mao, Manish Chaudhary, Manikandan Kondappan, Junheng Shi, Ebubechukwu O. Ilo-Okeke, Valentin Ivannikov, Tim Byrnes, arxiv 2202.09100

Quantum nondemolition: Manikandan Kondappan, Manish Chaudhary, Ebubechukwu O. Ilo-Okeke, Valentin Ivannikov, and Tim Byrnes Phys. Rev. A 107, 042616 (2023)

Supersinglet preparation: Ebubechukwu O. Ilo-Okeke, Yangxu Ji, Ping Chen, Yuping Mao, Manikandan Kondappan, Valentin Ivannikov, Yanhong Xiao, and Tim Byrnes, Phys. Rev. A **106**, 033314 (2022)



Prepublication version:
https://arxiv.org/abs/2007.14601

CAMBRIDGE
UNIVERSITY PRESS

Acknowledgments

Postdoc positions available in Machine Learning and other topics!

Funding
National Natural Science Foundation of China (62071301); NYU-ECNU Institute of Physics at NYU Shanghai; Shanghai Frontiers Science Center of Artificial Intelligence and Deep Learning; the Joint Physics Research Institute Challenge Grant; the Science and Technology Commission of Shanghai Municipality (19XD1423000,22ZR1444600); the NYU Shanghai Boost Fund; the China Foreign Experts Program (G2021013002L); the NYU Shanghai Major-Grants Seed Fund; Tamkeen under the NYU Abu Dhabi Research Institute grant CG008; and the SMEC Scientific Research Innovation Project (2023ZKZD55).

Methods to perform imaginary time evolution

Variational Imaginary Time evolution

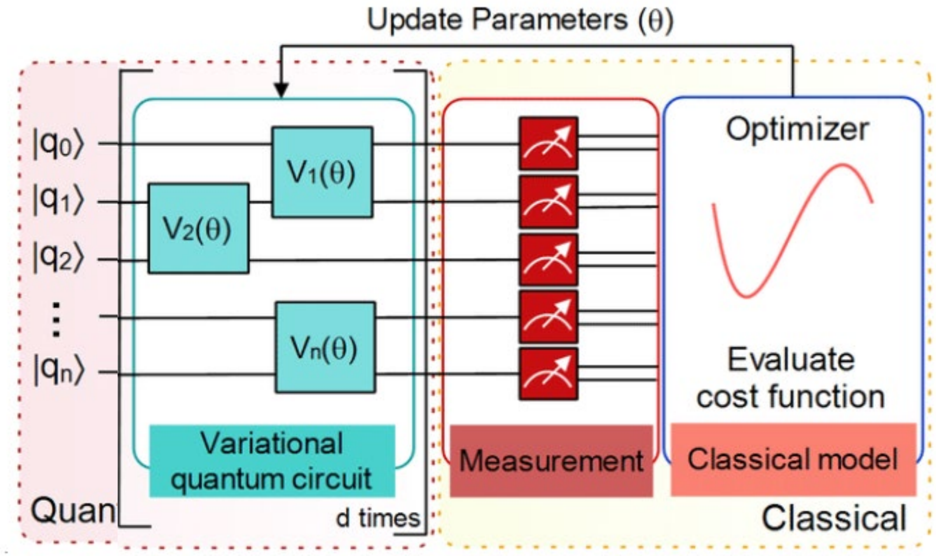
S. McArdle,.., X. Yuan, npj Quantum Information 5, 1 (2019).

Using a parameterized state, use a hybrid quantum-classical approach to measure the parameters A, C of the evolution equations

$$\sum_j A_{ij}\dot{\theta}_j = C_i$$

$$|\phi(\vec{\theta}(\tau))\rangle$$

$$\vec{\theta}(\tau) = (\theta_1(\tau), \theta_2(\tau), \ldots, \theta_N(\tau))$$



Quantum Imaginary Time evolution

M. Motta, … G. K.-L. Chan, Nature Physics 16, 205 (2020).

Decompose Hamiltonian into Trotter steps $$e^{-Ht} = \left(e^{-H_1 t/m} e^{-H_2 t/m} \cdots e^{-H_M t/m}\right)^m$$

Find unitary corresponding to Trotter step $$e^{-H_1 t/m} \rightarrow U$$

Probabilistic Imaginary Time evolution

Colin P. Williams, "Probabilistic nonunitary quantum computing" Proc. SPIE 5436 (2004)

Perform measurement in basis of H and repeat until success ➡ Low success rate for large systems