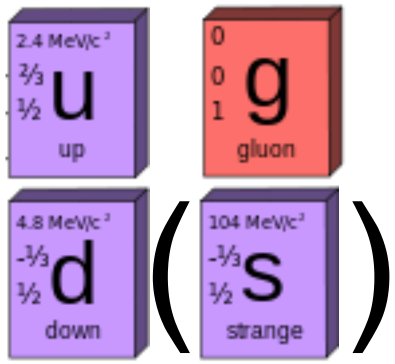
Sign problems and quantum computers

Ground states via spectral combing on a quantum computer
D.K., Natalie Klco, Alessandro Roggero
arXiv:1709.08250 [quant-ph]

Sign problems, noise, and chiral symmetry breaking in a QCD-like theory
Dorota Grabowska, D.K., Amy Nicholson
Phys Rev D87 (2013) 014504
arXiv:1208.5760 [hep-lat]

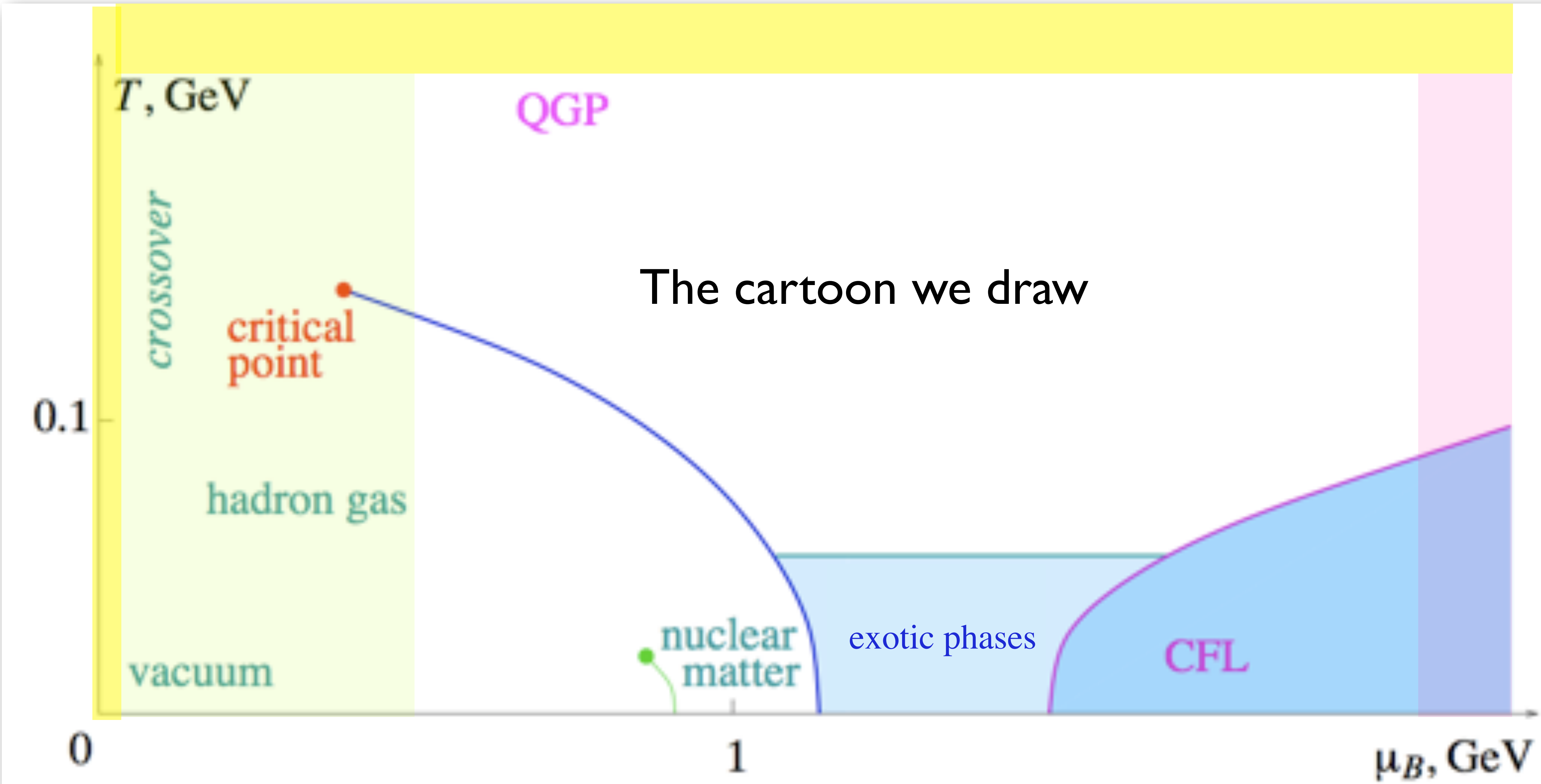
Noise, sign problems, and statistics
Michael Endres, D.K., Jong-Wan Lee, Amy Nicholson
Phys Rev Lett 107 (2011) 201601
arXiv:1106.0073 [hep-lat]



We have no way to reliably characterize the properties of matter from the standard model

Except:

- *asymptotic temperatures & densities*
- *zero, or very small baryon density*



The cartoon we draw

Requires a nonperturbative calculation

…and lattice QCD suffers from a "sign problem"

Requires a nonperturbative calculation
...and lattice QCD suffers from a "sign problem"

- What is the sign problem, and why is it so hard?
- Sign problems = noise in correlation functions
- The relation between noise and the pion
- Quantum computing for taming exponentially hard computations?
- Algorithms for finding the ground state of a many-body quantum mechanical systems

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- 2 degenerate flavors u,d
- chemical potential μ for quark number:

$$Z = \int [DA_\mu]\, e^{-S_{YM}} \det_2 \left[\not{D} + m + \mu\gamma_0 \right]$$

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Requires sampling gauge fields with probability...

$$P(A) \propto e^{-S_{YM}(A)} \det_2 \left[\not{D} + m + \mu\gamma_0 \right]$$

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$$P(A) \propto e^{-S_{YM}(A)} \det{}_2 \left[\not{D} + m + \mu\gamma_0 \right]$$

...but the determinant is complex!

$$\det \left[\not{D} + m + \mu\gamma_0 \right]^\dagger = \det{}_2 \left[\not{D} + m - \mu\gamma_0 \right]$$

Apply dagger, γ_5

Can we write:

$$\det{}_2\left[\not{D}+m+\mu\gamma_0\right]=\underbrace{\left|\det{}_2\left[\not{D}+m+\mu\gamma_0\right]\right|}_{\text{measure}}\,\underbrace{e^{2i\theta}}_{\text{operator}}$$

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Practical only if $e^{2i\theta}$ doesn't fluctuate wildly.

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measure operator

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2 flavors with isospin chemical potential

K. Splittorff
J. Verbaarschot, 2006

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How badly does the phase fluctuate? Consider computing:

$$\frac{\int[DA]e^{-S_{YM}}\det}{\int[DA]e^{-S_{YM}}|\det|} = \frac{\int[DA]e^{-S_{YM}}|\det|e^{i\theta}}{\int[DA]e^{-S_{YM}}|\det|} = \langle e^{i\theta}\rangle_I$$

if very small ⇔ phase is fluctuating wildly.

$$\frac{\int [DA] e^{-S_{YM}} \det}{\int [DA] e^{-S_{YM}} |\det|} = \frac{\int [DA] e^{-S_{YM}} |\det| e^{i\theta}}{\int [DA] e^{-S_{YM}} |\det|} = \langle e^{i\theta} \rangle_I$$

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$$\det = \det{}_2 \left[\not{D} + m + \mu\gamma_0 \right]$$

2 flavors with baryon chemical potential
($\mu_u = \mu_d = \mu$)

$$|\det| = \det{}_2 \left[\not{D} + m + \tau_3 \mu\gamma_0 \right]$$

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$$\boxed{\langle e^{i\theta} \rangle_I = \frac{Z_B}{Z_I} = e^{-VT(\mathcal{F}_B - \mathcal{F}_I)}}$$

If $F_B > F_I$ then there will be a sign problem that is exponentially bad (in the spacetime volume)

Phase of fermion det with quark baryon μ, averaged over isospin ensemble

$$\langle e^{2i\theta}\rangle_I = \frac{Z_B}{Z_I}$$

Partition functions with baryon/isospin chemical potentials

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$\mu < m_\pi/2 :$ (T=0)

$$Z_B = Z_I = 1 \quad \Longrightarrow \quad \langle e^{2i\theta}\rangle_I = 1$$

$m_\pi/2 < \mu < M_N/3 :$ (T=0)

$$Z_B = 1\ ,$$

$$Z_I \sim e^{\underline{VTf_\pi^2\mu^2(1-m_\pi^2/4\mu^2)^2}} \gg 1$$

$$\Longrightarrow \quad \langle e^{2i\theta}\rangle_I \ll 1$$

Free energy due to pion condensation

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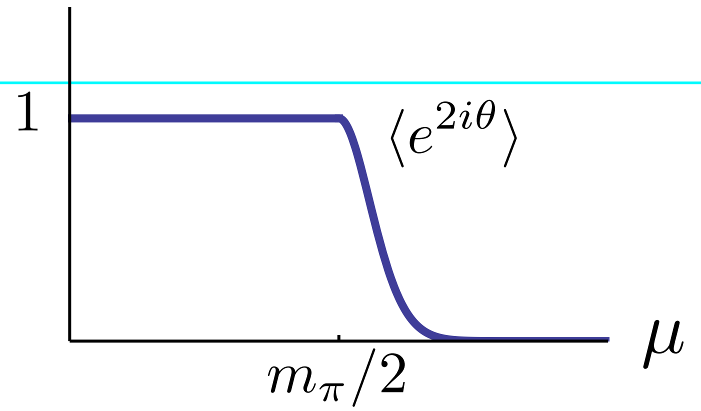

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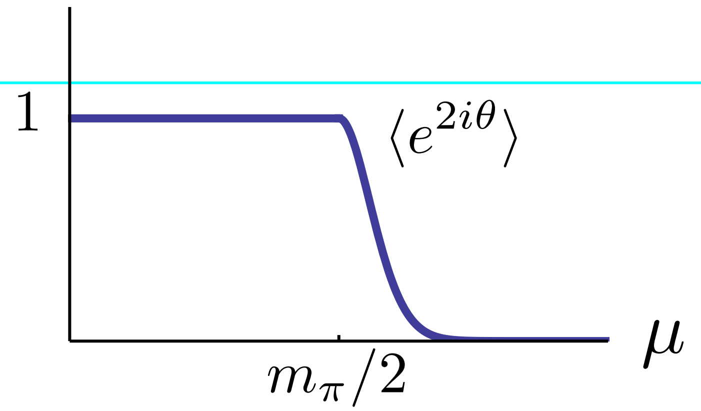


- The phase cancellations are <u>exponentially</u> bad in the spacetime volume
- Turning on μ: onset of the problem occurs before baryons appear!
- Pions are the villains

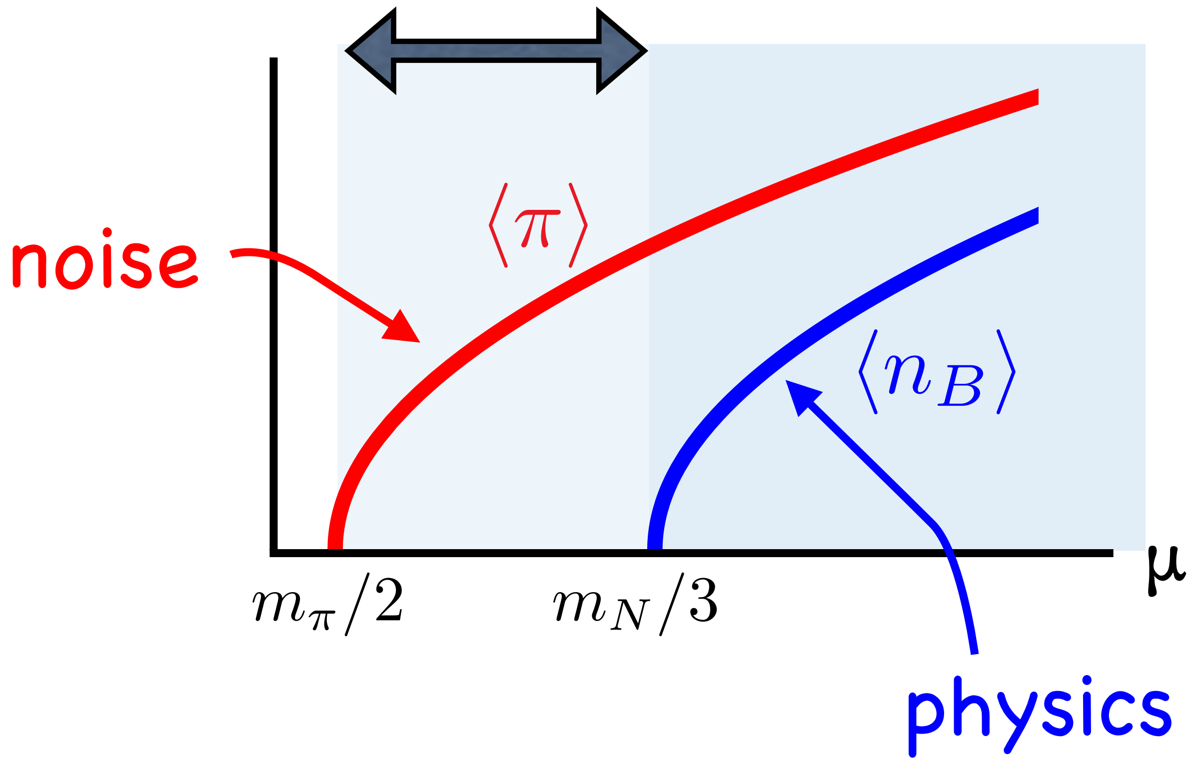
The sign problem in the grand canonical approach:

$\text{Det}(\not{D}+\mu\gamma^0)$ is complex

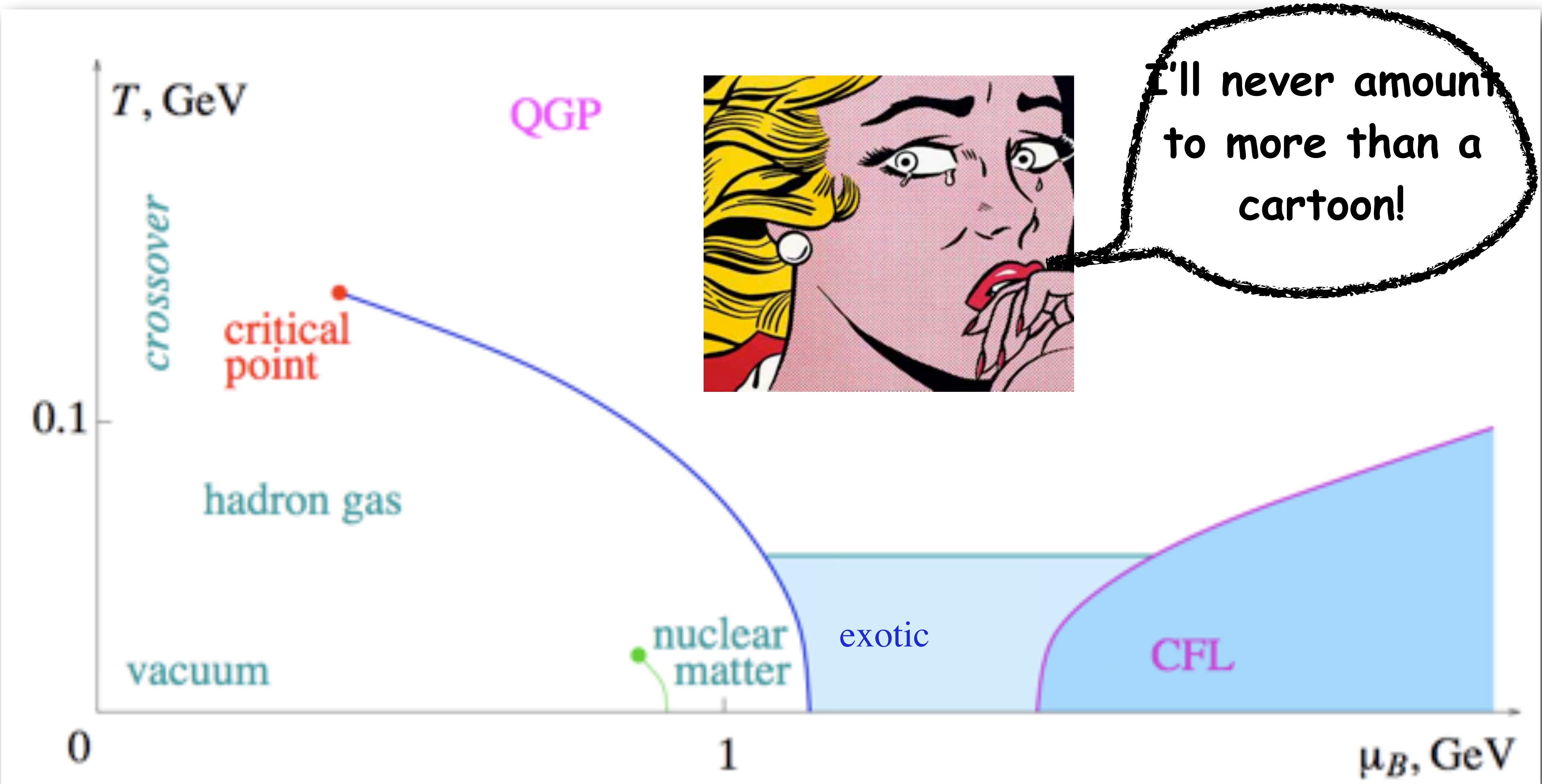
P.E. Gibbs, 1986

- physics happens for $\mu \geq m_N/3$...
- ...but sign problem starts at $\mu = m_\pi/2$!

$$\Delta\mu = \left(\frac{m_N}{3} - \frac{m_\pi}{2}\right)$$



Role of phase: "eliminate pion condensate" for $\mu \geq m_\pi/2$!


T, GeV
QGP
crossover
critical point
0.1
hadron gas
nuclear matter
exotic
CFL
vacuum
0
1
μ_B, GeV
I'll never amount to more than a cartoon!

Can one avoid the sign problem by working in the micro canonical ensemble instead?

(E.g., by computing multi-baryon correlates at $\mu=0$)

No! Sign problem $\Rightarrow$ Noise problem…also due to the light pion

Useful to relate the sign problem at $\mu \neq 0$ to the noise in canonical ($\mu = 0$) measurements of hadron masses.

Compute correlator of 3N quarks with $\mu = 0$

No sign problem…but now a <u>noise</u> problem

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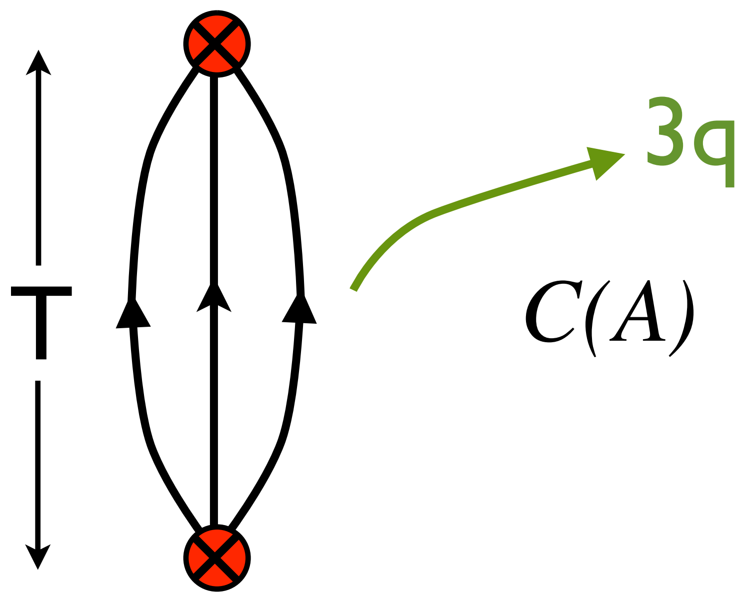

mean of nucleon correlator

signal, large T: $\sim e^{-m_N T}$

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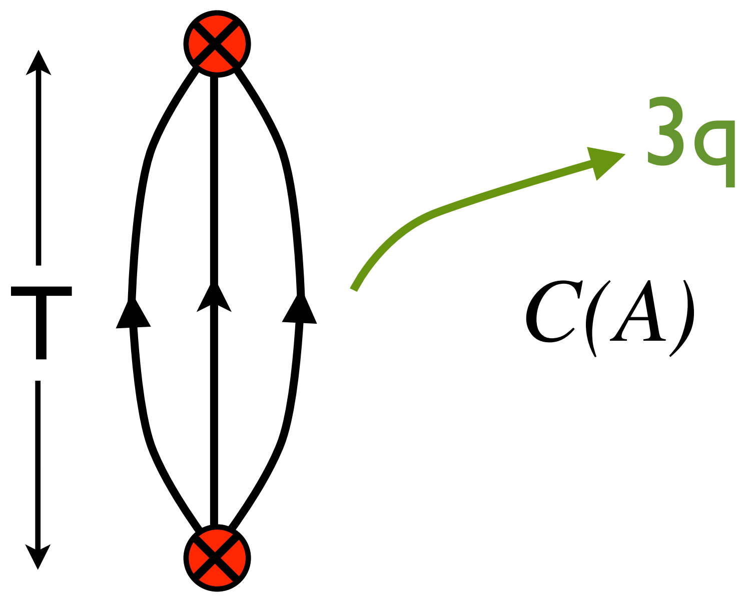
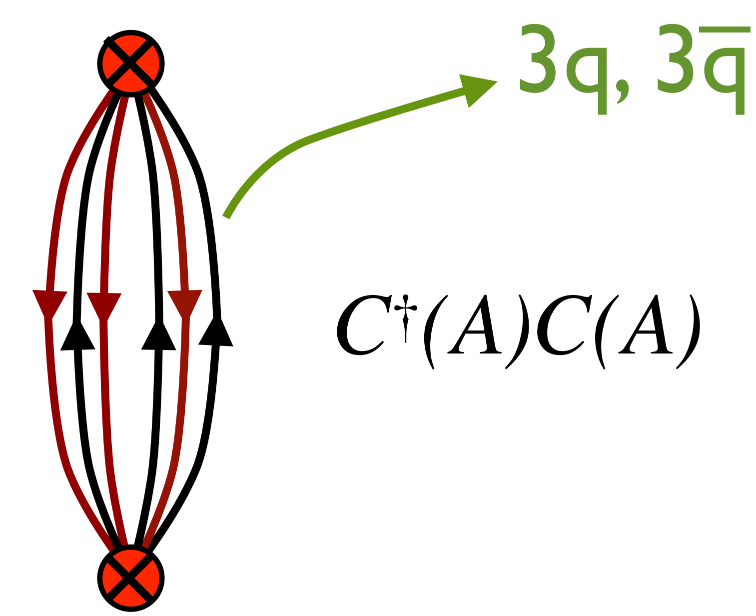
Parisi, Lepage 1980's





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variance of nucleon correlator

noise: $\sim \dfrac{1}{\sqrt{N_{\text{conf.}}}} e^{-\frac{3}{2}m_\pi T}$

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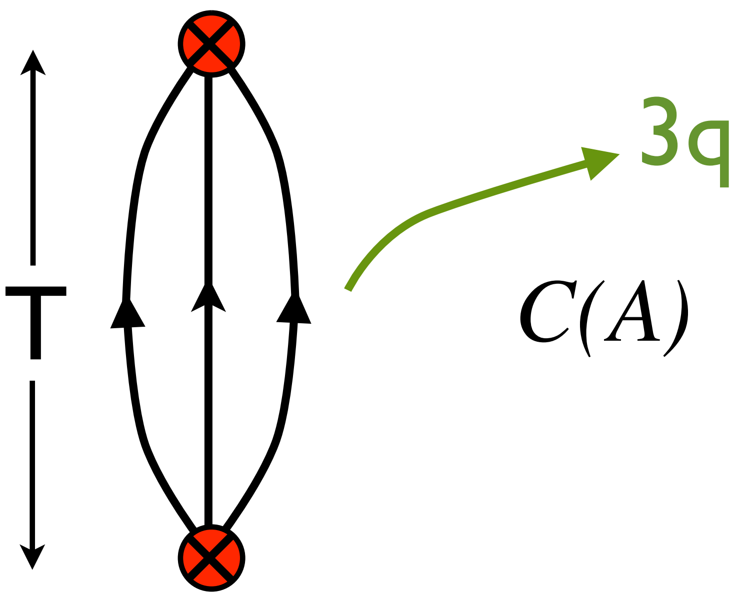

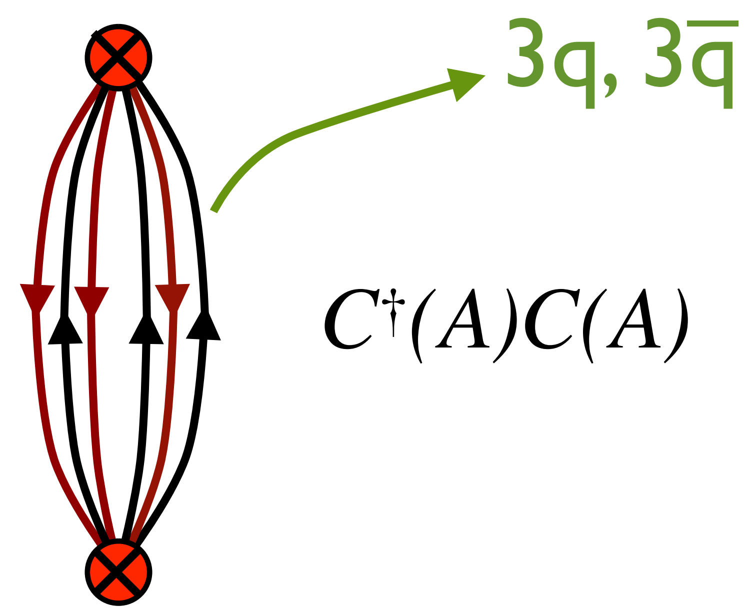

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$$\frac{\text{signal}}{\text{noise}} \sim \sqrt{N_{\text{conf.}}}\, e^{-3T\left(\frac{m_N}{3} - \frac{m_\pi}{2}\right)}$$

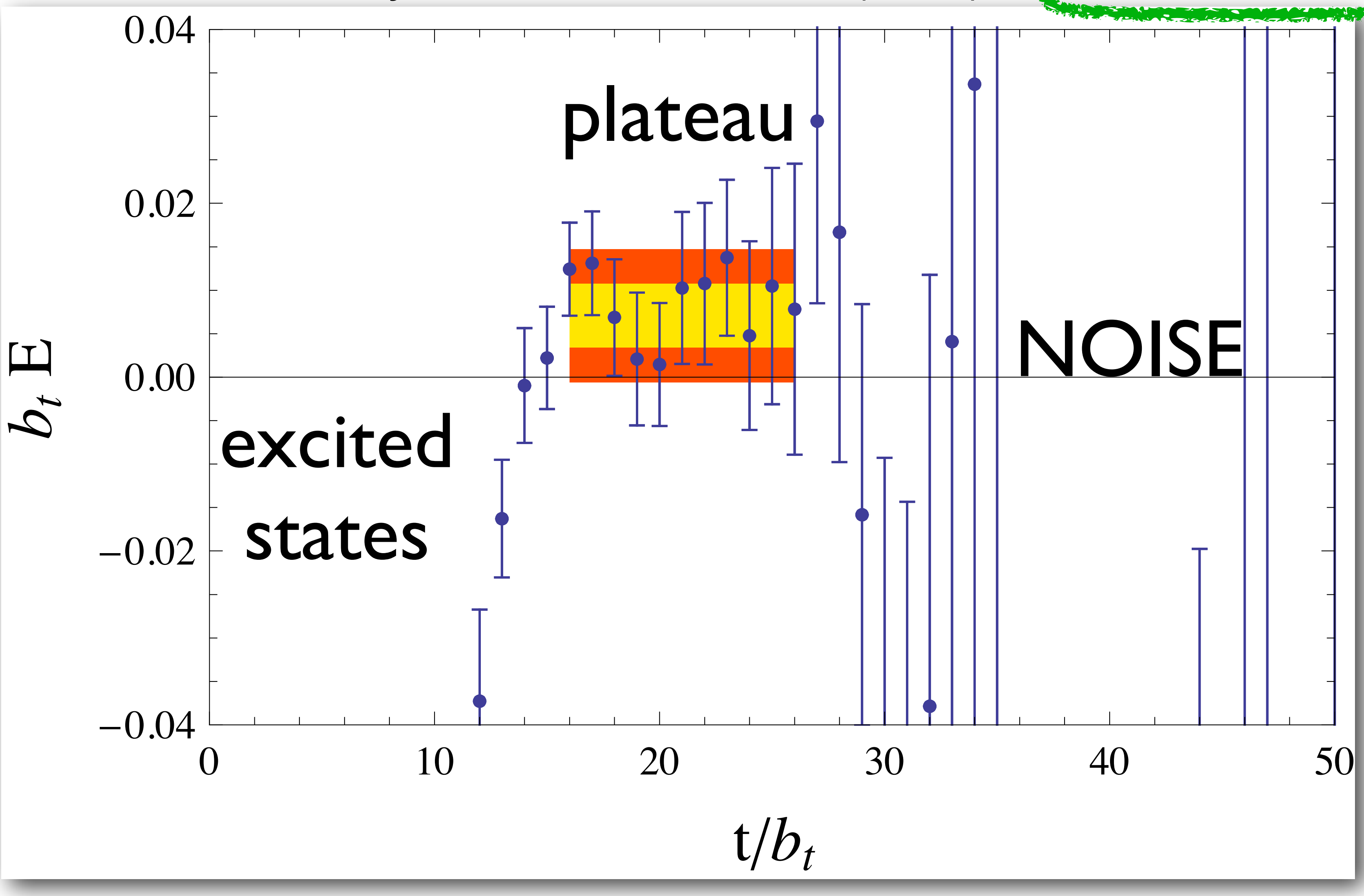
SMALL at large T. Same factor as Δμ in grand canonical

“Pion noise” is seen in real simulations, with roughly expected amplitude. Currently can look at nuclei only for heavy pion

Triton B.E.

S. R. Beane et al. (NPLQCD), Phys. Rev. D 80, 074501 (2009)

$(m_\pi = 390 \text{ MeV})$



Currently:

can go up to ^5He

with $m_\pi \approx 900$ MeV

Large-N NJL model in d=3

$$\mathcal{L} = N\left(\bar\psi_a(\partial\!\!\!/ - m)\psi_a - \frac{C}{2}\left[(\bar\psi_a\psi_a)^2 + (\bar\psi_a i\gamma_5\psi_a)^2\right]\right)$$

- a=1,...,N
- d=4 theory dimensionally reduced to d=3
- ψ = 4 component spinor (like d=4)
- γ-matrices = 4x4 (like d=4)
- Symmetry = $U(N)_V$ x $U(1)_A$ (approximate if m≠0)

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Two equivalent formulations with auxiliary fields:

$$\mathcal{L} = N\left(\frac{1}{2C}\left(\sigma^2 + \pi^2\right) + \bar\psi_a\left[\partial\!\!\!/ - m + \sigma + i\pi\gamma_5\right]\psi_a\right)$$

σ/π

$$\mathcal{L} = N\left(\frac{1}{C}\,\mathrm{Tr}\,\left(V_\mu V_\mu + A_\mu A_\mu\right) + \bar\psi_a\left[\partial\!\!\!/ + iV\!\!\!/ + A\!\!\!/\gamma_5\right]_{ab}\psi_b\right)$$

A/V

(obtained by Fierz rearrangement of 4-fermion interaction)

For even N, the σ/π formulation has no sign problem at μ≠0:

$$(\not\partial + \sigma + i\pi\gamma_5 + \mu\gamma_1)^* = C(\not\partial + \sigma + i\pi\gamma_5 + \mu\gamma_1)C$$

$$\Rightarrow \quad \det(\not\partial + \sigma + i\pi\gamma_5 + \mu\gamma_1)^N$$ = real, positive

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...but the equivalent A/V formulation has a QCD-like sign problem:

$$\det\left[\not\partial + i\not V + \not A\gamma_5 + \mu\gamma_1\right]^N$$ = complex!

(Can give a Splittorff-Verbaarschot argument for why it is complex, relating phase fluctuations of determinant to pion condensation in 2N flavor theory, just as in QCD.)

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Same theory, different formulation.
Having an explicit pion field (a physical state) cures the sign problem

The moral:

- sign problems appear to arise from using degrees of freedom that do not represent the (light) physical degrees of freedom well
- Presumably the energy eigenstates appear as highly correlated states when built out of the wrong degrees of freedom

Trivial example: free particle $$|p\rangle = \int dx\, e^{ipx} |x\rangle$$

- sign problems are due to the difficulty finding the right vectors in the vast Hilbert space, starting from a poor starting point

(You know the exact energy eigenstates? Then $Z = \Sigma\, e^{-\beta E}$, no sign problem!)

If we cannot figure out how to express QCD in terms of mesons & baryons,
‣ need to find a better way to navigate the Hilbert space!

Quantum computers to the rescue?

Certain algorithms on a quantum computer can do in polynomial time wh
takes exponential time on a classical computer.

<u>Example: discrete Fourier transform</u>

Classical Fourier transform on a discrete function with N values

$$\{x_0,\ldots x_{N-1}\} \mapsto \{y_0,\ldots y_{N-1}\}$$

$$y_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} x_j \omega^{jk} \qquad\qquad \omega = e^{\frac{2\pi i}{N}}$$

Computational cost = O(N log N).

When $N = 2^n$, cost (# gate operations) is $O(n\, 2^n)$.

On a quantum computer cost is $O(n^2)$

Fourier transform on a quantum computer

Start with n=2 qubits $|x\rangle = |x_0,x_1\rangle$ where $x_i = 0,1 \ldots$
So $N = 2^2 = 4$ and $\omega = e^{2\pi i/4}$

The Fourier transform is then the unitary transformation on these states

$$\begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix} \to U \begin{pmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix}$$

$$U = \frac{1}{\sqrt{2^2}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega^1 & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{pmatrix} = \frac{1}{\sqrt{2^2}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega^1 & \omega^2 & \omega^3 \\ 1 & \omega^2 & 1 & \omega^2 \\ 1 & \omega^3 & \omega^2 & \omega \end{pmatrix}$$

Then

$$|\psi\rangle = \sum_k x_k |k\rangle \to U\psi = \sum_{j,k} x_j U_{jk} |k\rangle \equiv \sum_k y_k |k\rangle \ , \qquad \text{so } y_k = \sum_j x_j \omega^{jk}$$

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ω^0

$\omega^{x_2+2x_1}$

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$$\begin{array}{rcccc} 2x_1+x_2: & 0 & 1 & 2 & 3 \\ \{x_1x_2\} = & \{00\} & \{01\} & \{10\} & \{11\} \end{array}$$

$$U = \frac{1}{\sqrt{2^2}} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{pmatrix}$$

ω^0

$\omega^{x_2+2x_1}$

$\omega^{2(x_2+2x_1)}$

Then

$$|\psi\rangle = \sum_k x_k |k\rangle \to U\psi = \sum_{j,k} x_j U_{jk} |k\rangle \equiv \sum_k y_k |k\rangle \ , \qquad \text{so } y_k = \sum_j x_j \omega^{jk}$$

The coefficients of the qubits in the final state will be the Fourier transform of the coefficients of the qubits in the initial state

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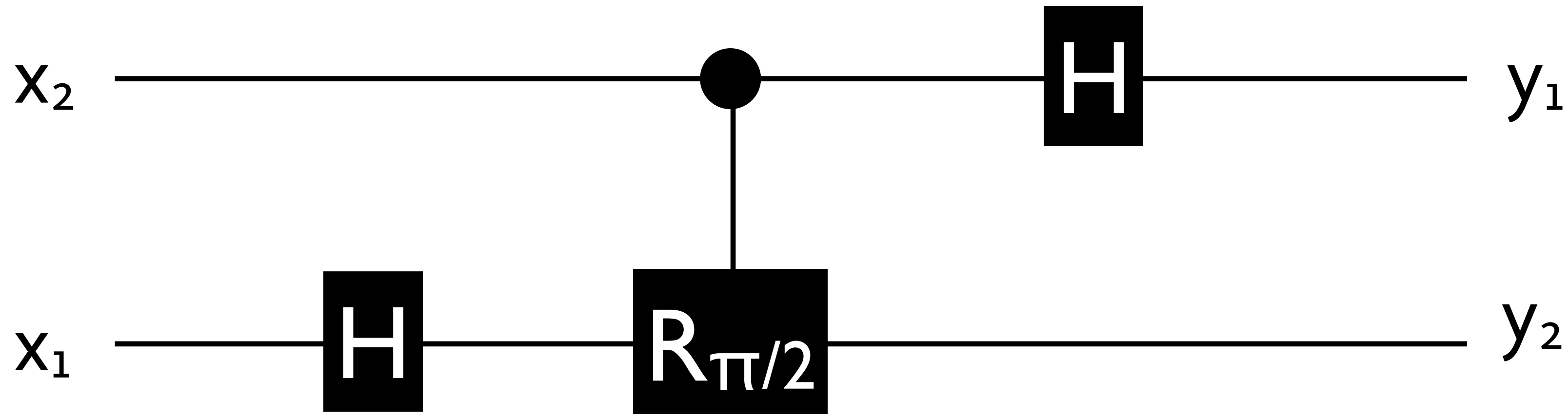
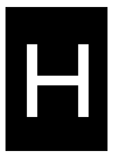
$$\boxed{|y\rangle = U|x\rangle = \frac{1}{2}\left(|0\rangle + \omega^{2x_2}|1\rangle\right)\left(|0\rangle + \omega^{2x_1+x_2}|1\rangle\right)}$$

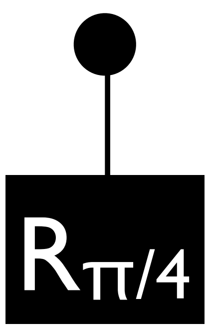
$\omega^4 = 1$

This can be effected (up to overall phase) with 3 basic gates:





= Hadamard gate: $$|0\rangle \to \frac{|0\rangle + |1\rangle}{\sqrt{2}}\ , \quad |1\rangle \to \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

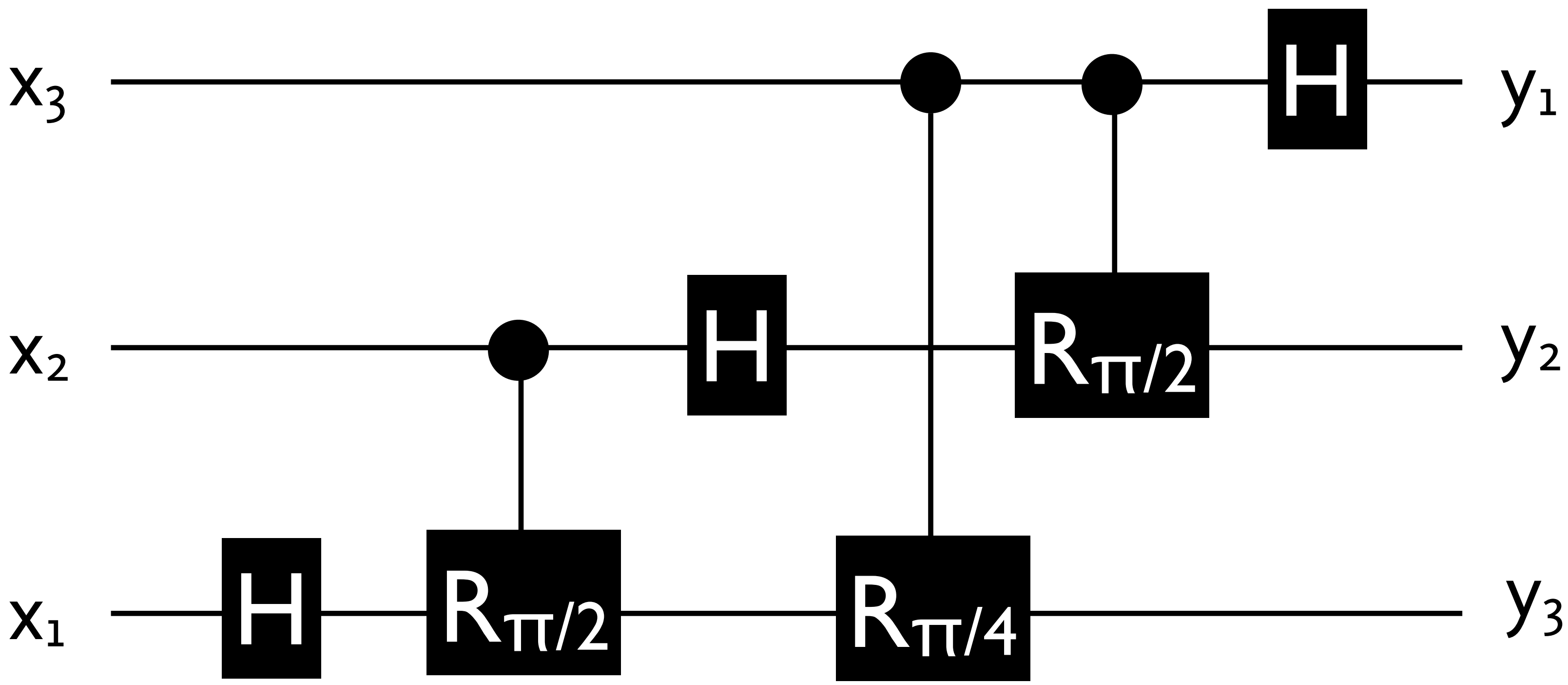


= Controlled Phase Rotation: $$|x_1\rangle \to \omega^{x_1}|x_1\rangle \quad \text{iff } x_2 = 1$$

$$|x_1\, x_2\rangle \xrightarrow{H} \left(\frac{|0\rangle + \omega^{2x_1}|1\rangle}{\sqrt{2}}\right)|x_2\rangle \xrightarrow{R_{\pi/2}} \left(\frac{|0\rangle + \omega^{2x_1+x_2}|1\rangle}{\sqrt{2}}\right)|x_2\rangle \xrightarrow{H} \left(\frac{|0\rangle + \omega^{2x_1+x_2}|1\rangle}{\sqrt{2}}\right)\left(\frac{|0\rangle + \omega^{2x_2}|1\rangle}{\sqrt{2}}\right)$$

$$|y_1 y_2\rangle = \left(\frac{|0\rangle + \omega^{2x_2}|1\rangle}{\sqrt{2}}\right)\left(\frac{|0\rangle + \omega^{2x_1+x_2}|1\rangle}{\sqrt{2}}\right)$$

The “score” for the n=3 Fourier transform:



3 gates for the n=2 case; 6 gates for n=3. Scales like n^2 for large n

- n H-gates
- n(n+1)/2 R-gates

Same discrete FT scales like ($n\ 2^n$) on a classical computer.

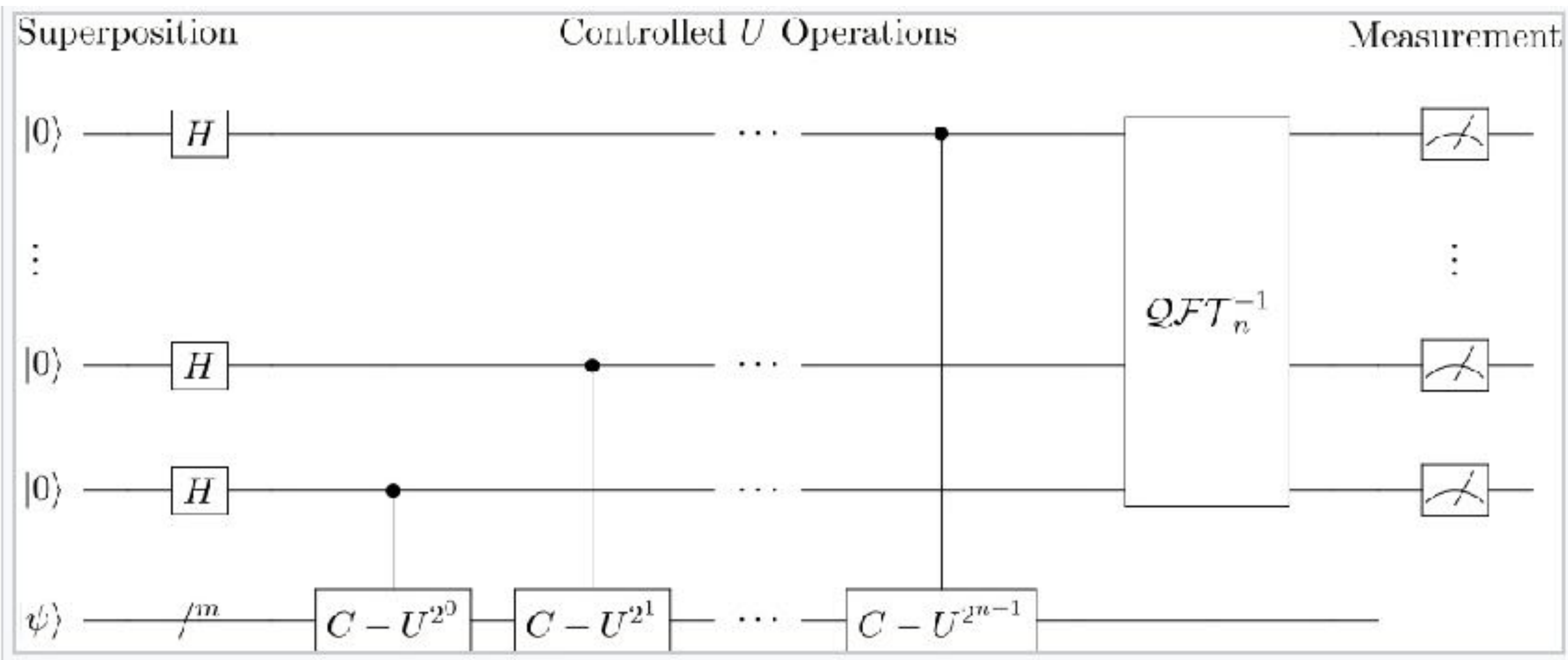
How can you use this for physics?

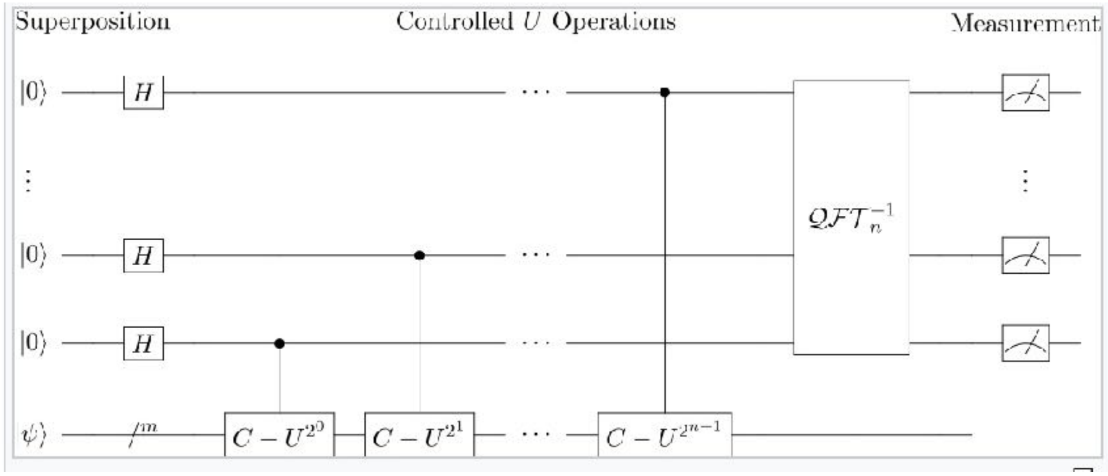
Example: phase estimation algorithm

Suppose $|\psi>$ is the eigenvector of a unitary operator U (= e^{-iHt}), represented by m qubits:

$$U\,|\psi> = e^{2\pi i\theta}\,|\psi>$$

and you want to determine θ to accuracy $1{:}2^{-n}$





Hadamard gates give you the state: $2^{-n/2}(|0\rangle + |1\rangle)^{\otimes n}\,|\psi\rangle$

Controlled phase rotations by U then give you the state

$$\frac{1}{2^{\frac{n}{2}}}\underbrace{\left(|0\rangle + e^{2\pi i 2^{n-1}\theta}|1\rangle\right)}_{1^{st}\ qubit} \otimes \cdots \otimes \underbrace{\left(|0\rangle + e^{2\pi i 2^{1}\theta}|1\rangle\right)}_{n-1^{th}\ qubit} \otimes \underbrace{\left(|0\rangle + e^{2\pi i 2^{0}\theta}|1\rangle\right)}_{n^{th}\ qubit} = \frac{1}{2^{\frac{n}{2}}}\sum_{k=0}^{2^n-1} e^{2\pi i\theta k}|k\rangle.$$

If $\theta = a\, 2^{-n}$ for integer a, then the inverse Fourier Transform will yield an eigenstate of spin for each of the final qubits $|y\rangle$

Measuring $|y\rangle$ yields the exact answer for a:

$a = 2^0 y_0 + 2^1 y_1 + 2^2 y_2 + \ldots + 2^{n-1} y_{n-1}$,

all y_i measured to be 0 or 1

If $\theta = a\, 2^{-n} + \delta$ for integer a, then the probability for measuring a particular value of a is peaked around the true value.

The probability of determining the correct value of a

$$\begin{aligned} P(a) &= \frac{1}{2^{2n}} \frac{\left|2\sin(\pi 2^n \delta)\right|^2}{\left|\sin \pi\delta\right|^2} \\ &\geq \frac{4}{\pi^2} = 0.41 \quad \text{for} \quad |\delta| \leq 2^{-n-1} \end{aligned}$$

If $|\psi\rangle$ is a linear combination of two eigenstates

$$|\psi\rangle = \alpha\,|\theta = a 2^{-n}\rangle + \beta\,|\theta = b 2^{-n}\rangle$$

with a,b integers, measurement of the auxiliary qubits will

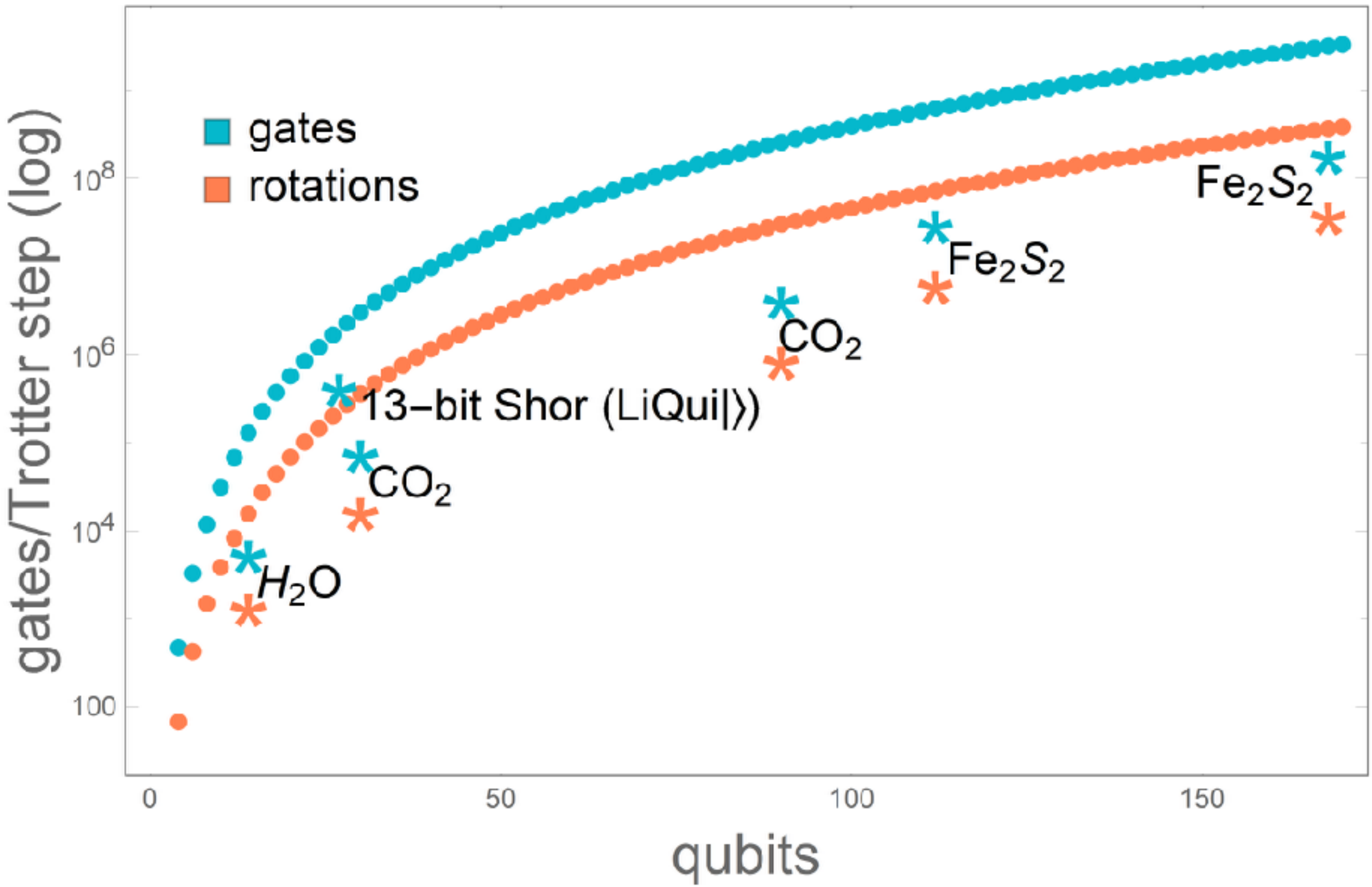
- yield a with probability $|\alpha|^2$ or b with probability $|\beta|^2$
- after measurement, $|\psi\rangle$ collapses to eigenstate

More general $|\psi\rangle$, QPE measures the spectrum of $|\psi\rangle$

Quantum phase estimation is a method for solving for energy levels of a quantum many-body system:

1. Initialize qubits with a trial wave function $|\psi_i\rangle$
2. Use $U = e^{-iHt}$ for Quantum Phase Estimation (QPE) with choice of t such that $0 \leq Et \leq 2\pi$
   - Break U up into project of short time evolution operators (Trotter)
   - Express these in terms of gate operations
3. Measurements at end of QPE will give the spectrum of Et, weighted by overlap of $|\langle E|\psi_i\rangle|^2$
4. After each measurement, output qubits will represent the eigenfunction corresponding to the measured Et.
5. Can use this wave function to compute matrix elements

Need a good trial wave function to find the ground state e.g.: some quantum chemistry problems



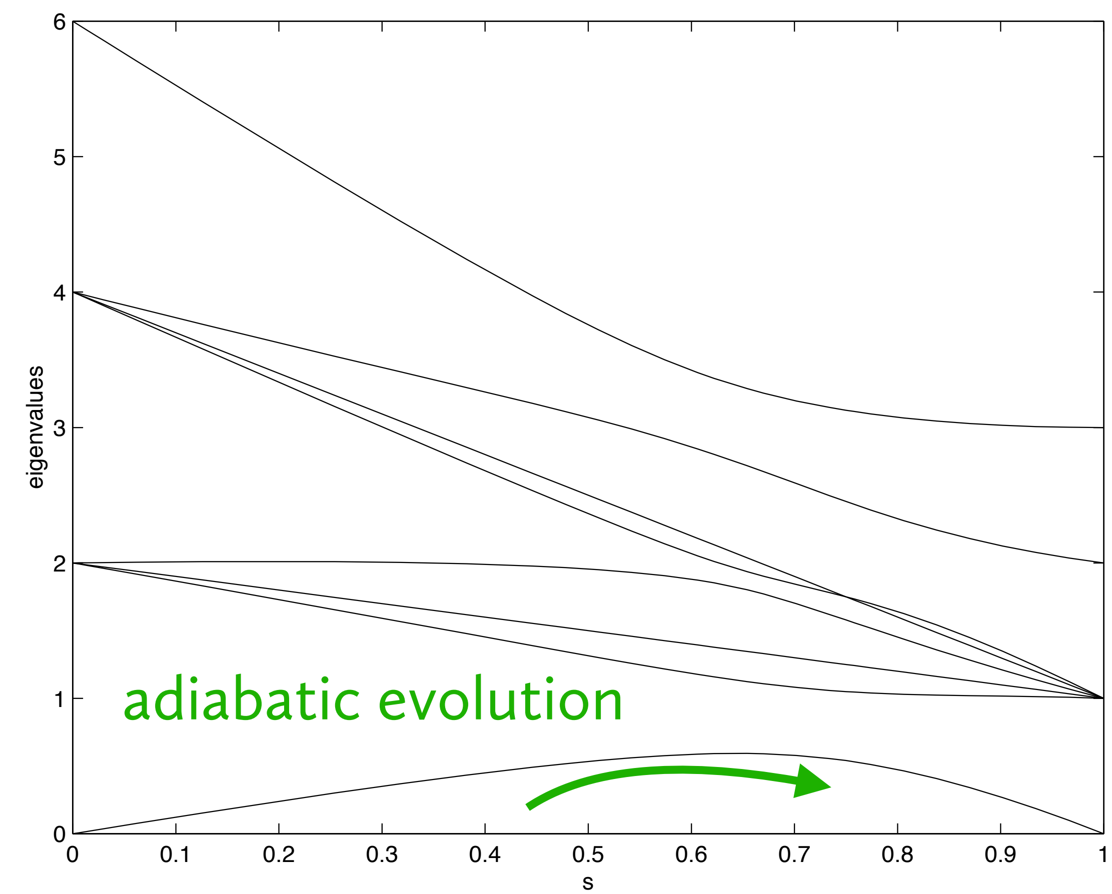
Gate-count estimates for performing quantum chemistry on small quantum computers

Dave Wecker, Bela Bauer, Bryan K. Clark, Matthew B. Hastings, and Matthias Troyer
Phys. Rev. A 90, 022305 – Published 6 August 2014

Other ways to find the ground state
(Quantum computer works with unitary evolution, unlike Euclidian time)

Quantum Adiabatic Algorithm:

$$H(s) = (1-s)H_0 + sH_1 \qquad 0 \le s \le 1$$



Edward Farhi, Jeffrey Goldstone, Sam Gutmann, Michael arXiv:quant-ph/0001106

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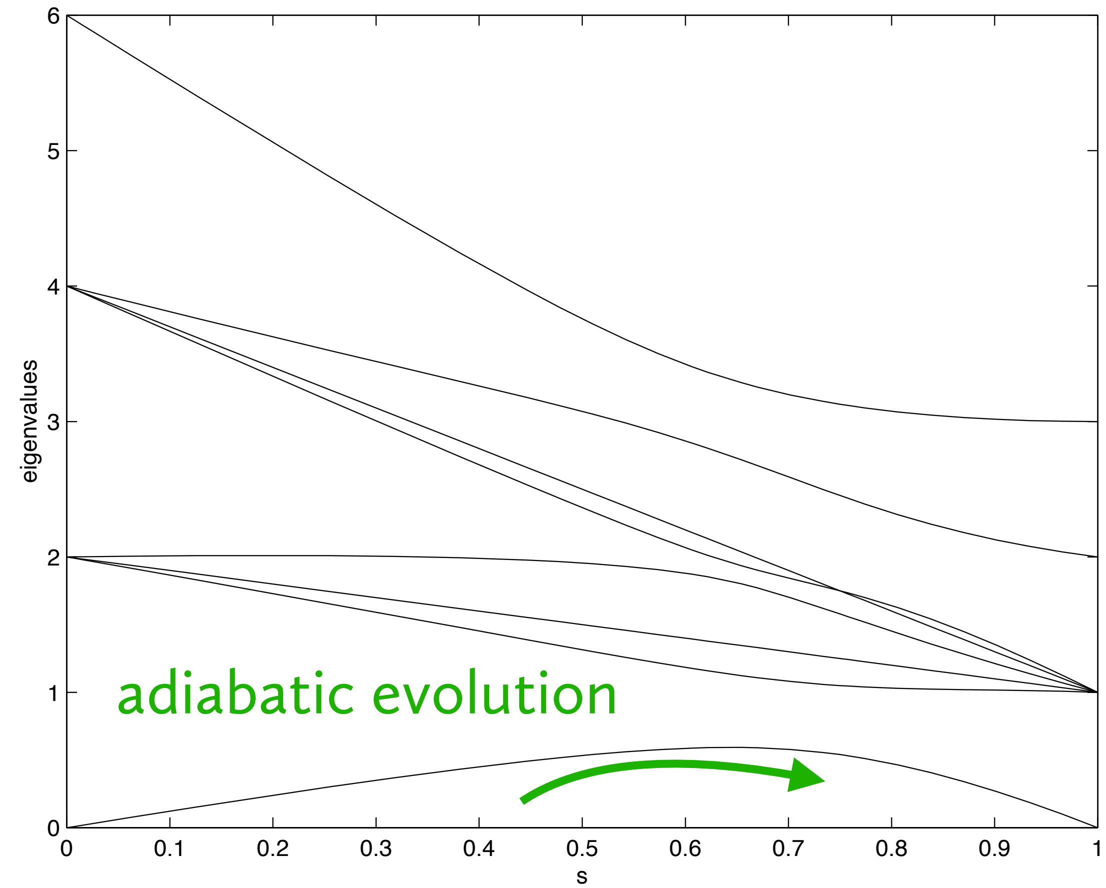
simple Hamiltonian



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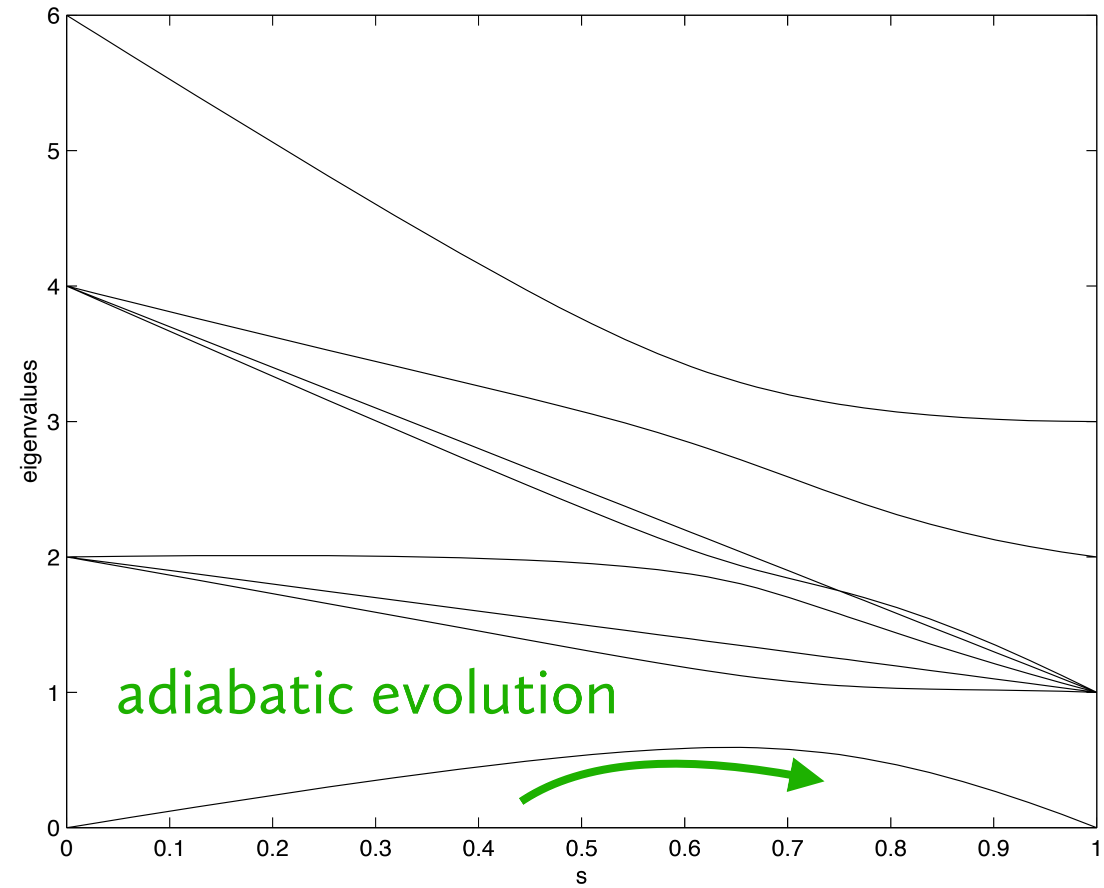

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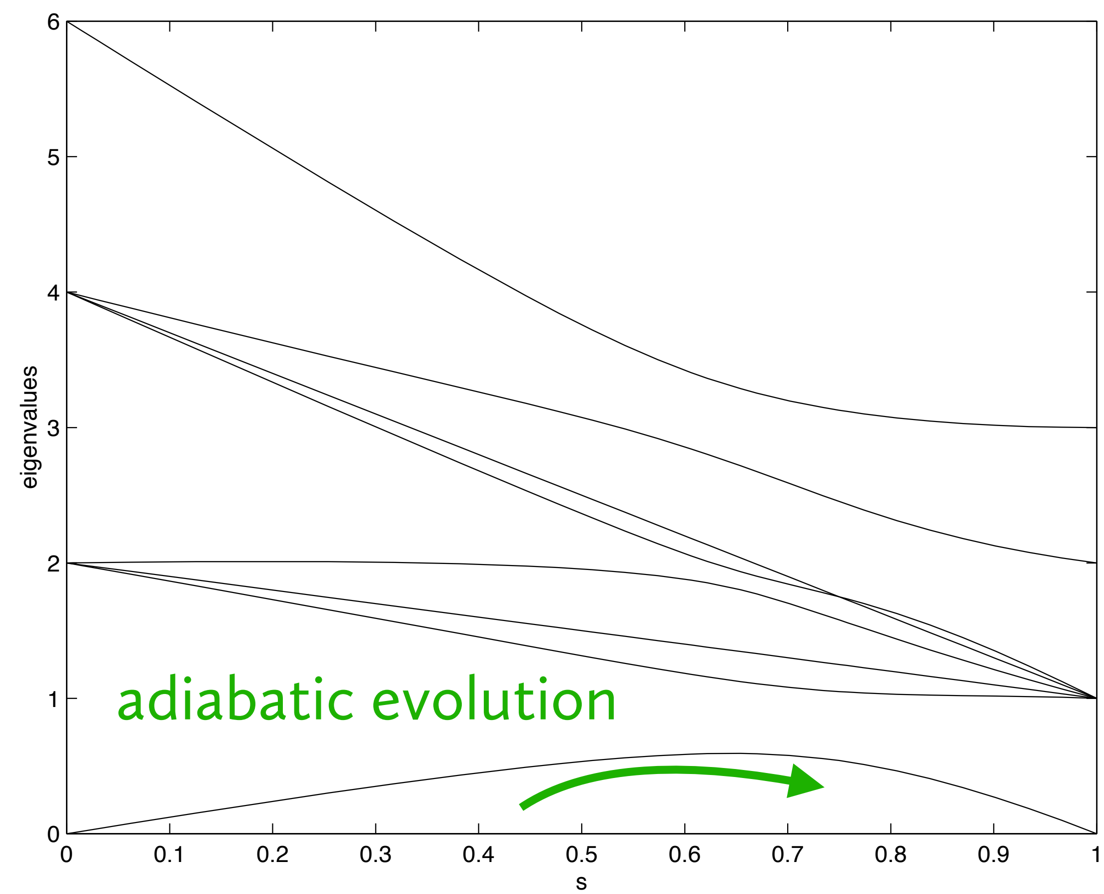
- Initialize qubits for known ground state of H_0



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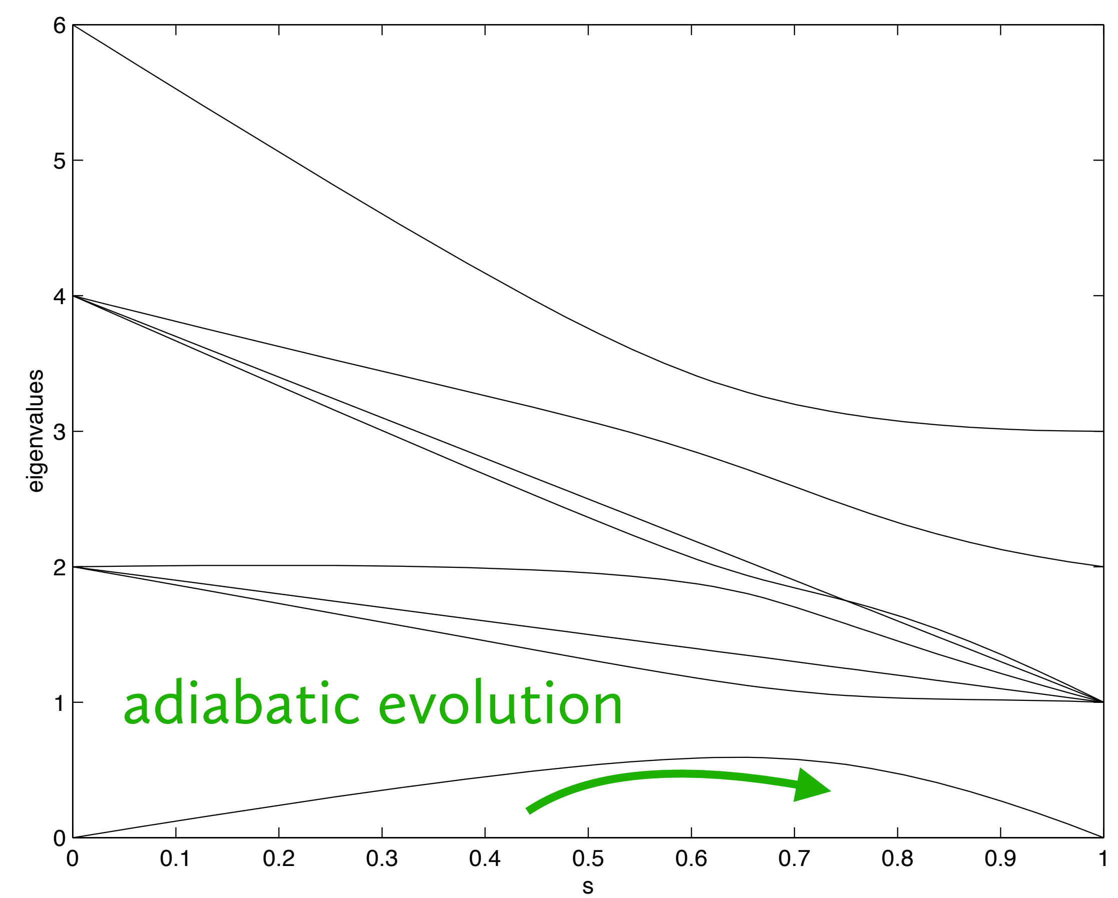
- Initialize qubits for known ground state of H_0
- Evolve according to $H(s)$, varying s slowly from 0 to 1



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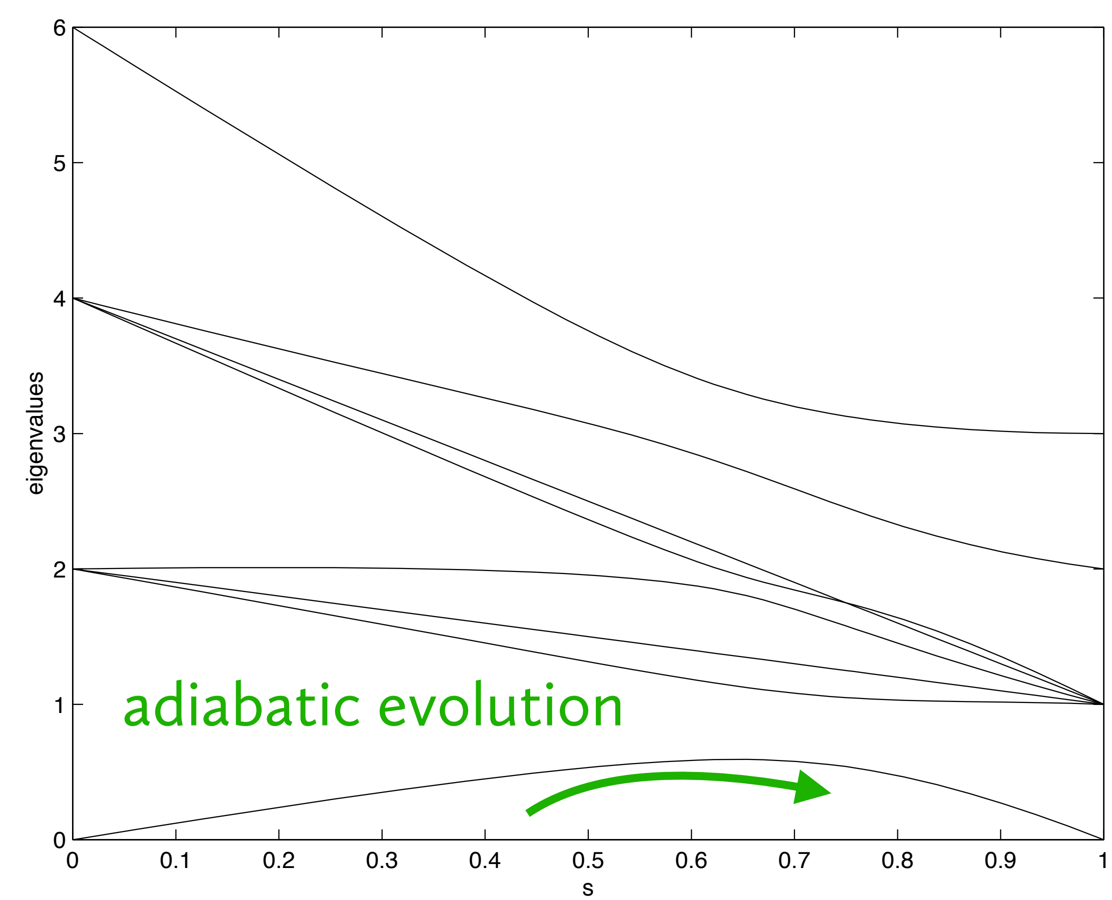
- Adiabatic theorem: ground state of H_0 will evolve into ground state of H_1



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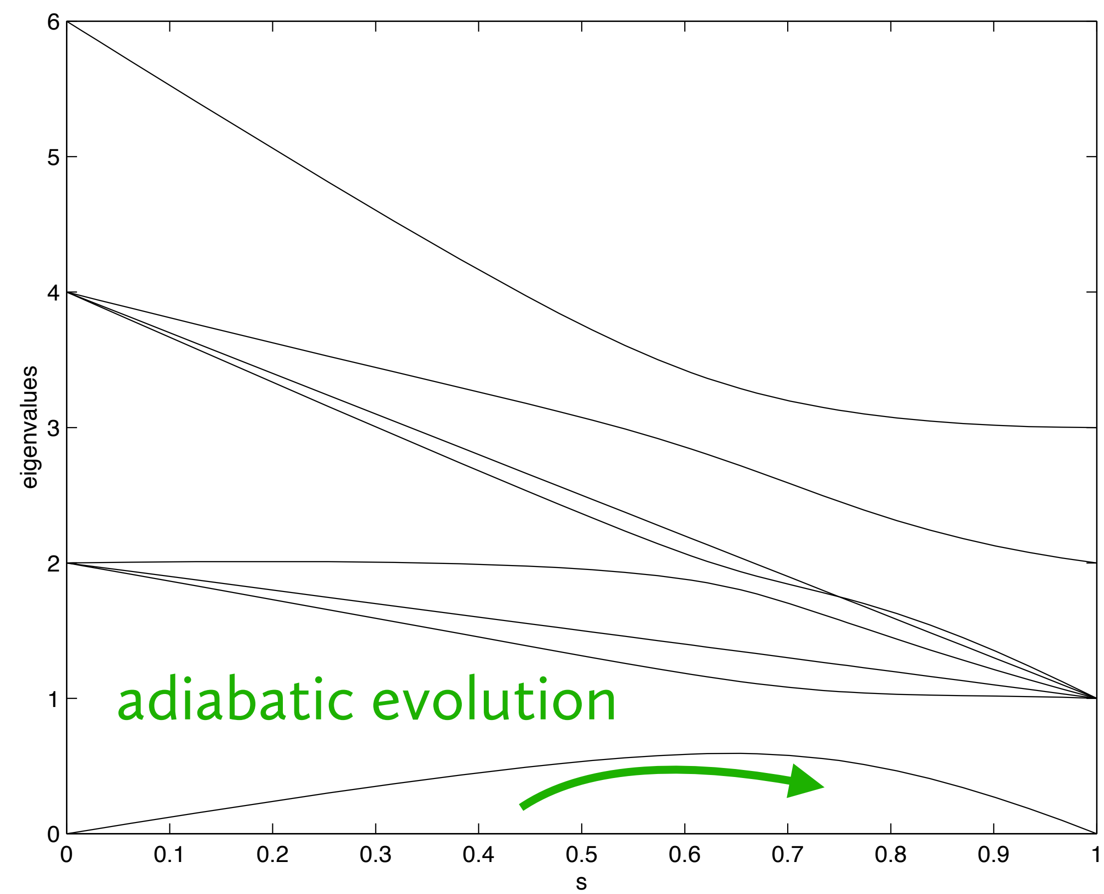
- Initialize qubits for known ground state of H_0
- Evolve according to $H(s)$, varying s slowly from 0 to 1
- Adiabatic theorem: ground state of H_0 will evolve into ground state of H_1
- Measure desired matrix elements

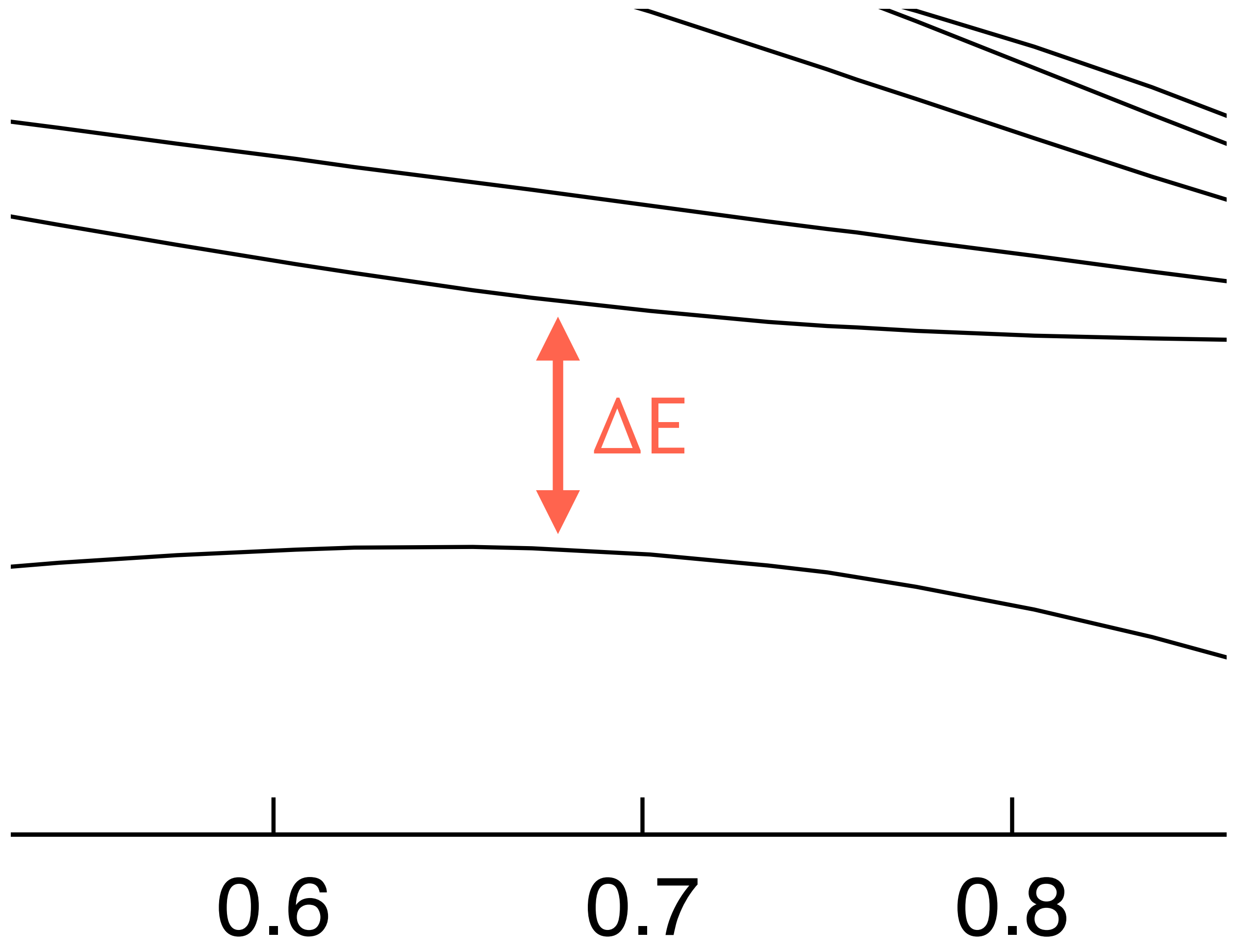


Edward Farhi, Jeffrey Goldstone, Sam Gutmann, Michael   arXiv:quant-ph/0001106

Drawback of the Quantum Adiabatic Algorithm:

Adiabatic theorem requires evolution time scales as

$$t \sim \frac{1}{\Delta E^2}$$



Cooked up example of bad scaling behavior: Take Ising model with small transverse field

$$\mathcal{H}^B_{\rm targ} = -h\sum_{i=1}^{N_t}\sigma^x_i - \sum_{i=1}^{N_t}\sigma^z_i\sigma^z_{i+1} + B\sum_{i=1}^{N_t}\sigma^z_i\ .$$

Take h small, H_0 = above with $B=+B_0$ H_1 = above with $B=-B_0$

$$\mathcal{H}_\pm = -h\sum_i \sigma_i^x - \sum_i \sigma_i^z\sigma_{i+1}^z \pm B_0 \sum_i \sigma_i^z$$

Consider adiabatic method for h small, $H_0 = H_+$, $H_1 = H_-$

Why is this hard for the adiabatic method?

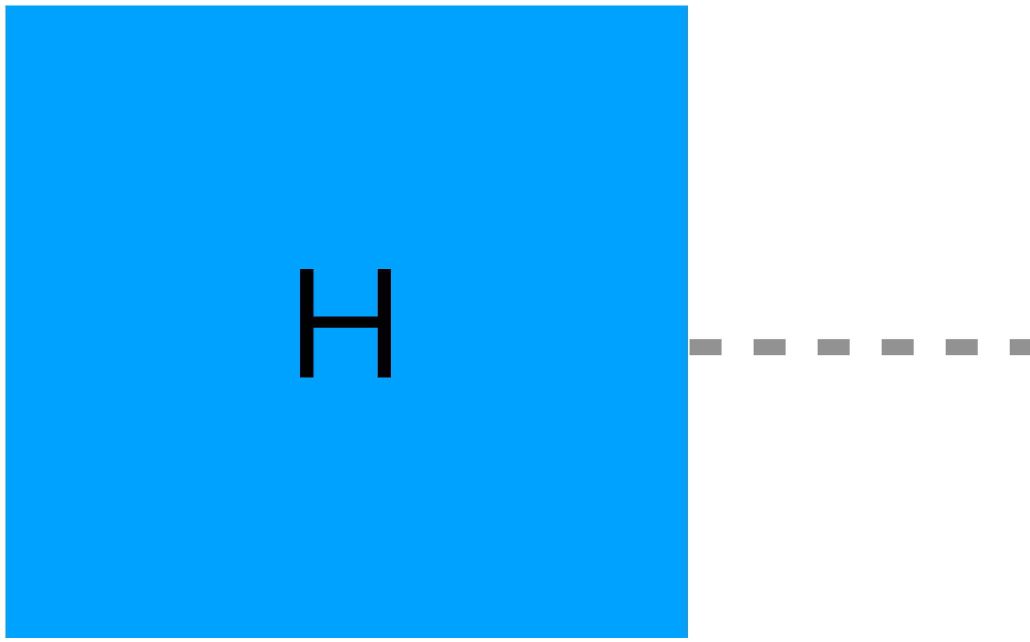
When h=B=0, ground states are degenerate, $|\uparrow\uparrow\cdots\uparrow\rangle$ & $|\downarrow\downarrow\cdots\downarrow\rangle$

When h≠0, there is tunneling between the two and splitting proportional to h^N, N= # spins

When then taking $B = + B_0 \blacktriangleright B = -B_0$ there is therefore 1st order transition (for large N) and a small gap encountered at B=0 proportional to h^N

It has been argued that quantum field theories will always encounter an exponentially small gap (Preskill)

Simulate a "heat bath"?



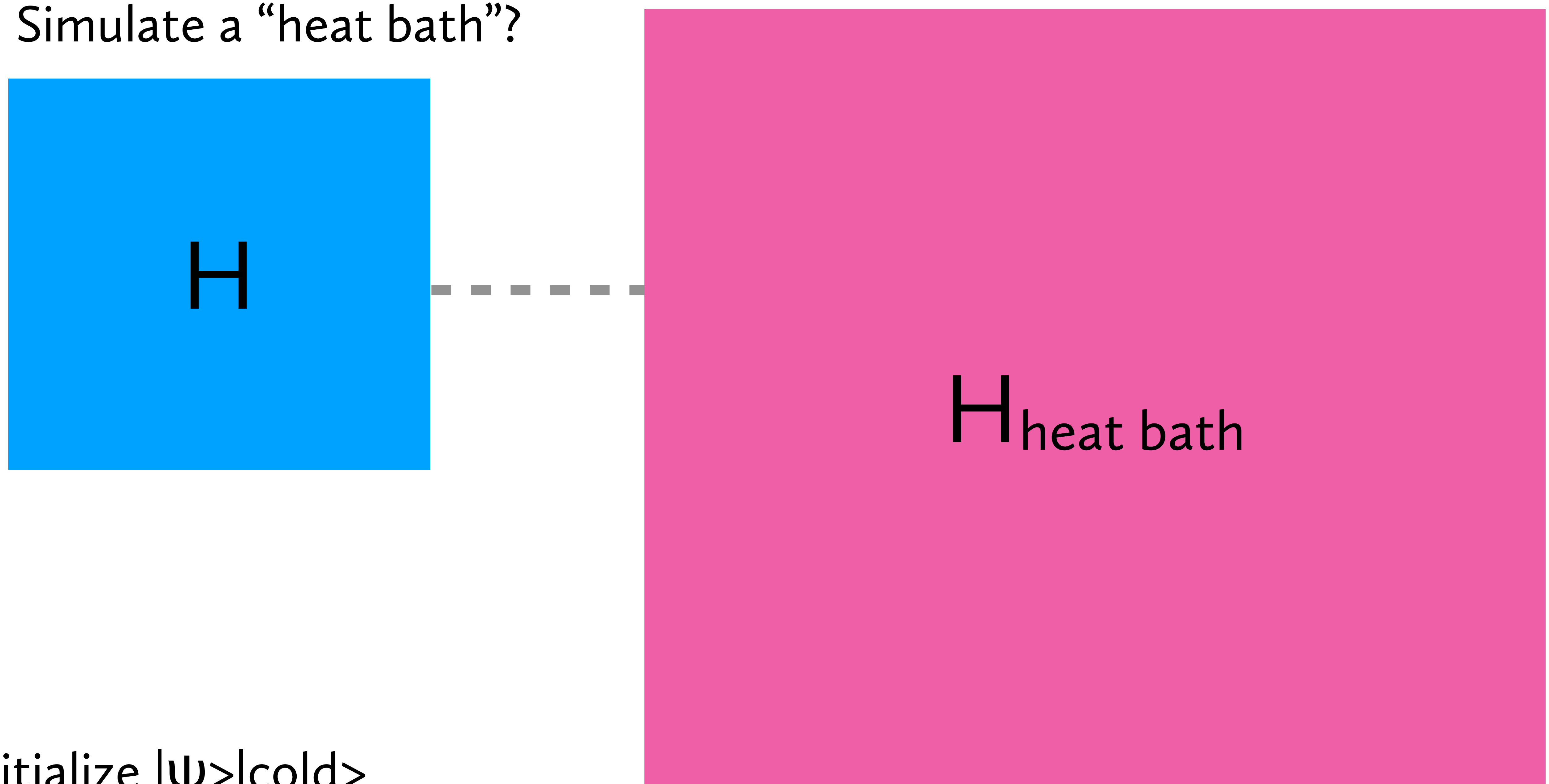
Initialize $|\psi\rangle|\text{cold}\rangle$

Evolves unitarily to entangled state ~ $|\psi_0\rangle|\text{warm}\rangle$

Another possible algorithm: “Spectral Combing”

DBK, N Klco, A Roggerro, E-print 1709.08250 (quant-ph)

Simulate a “heat bath”?

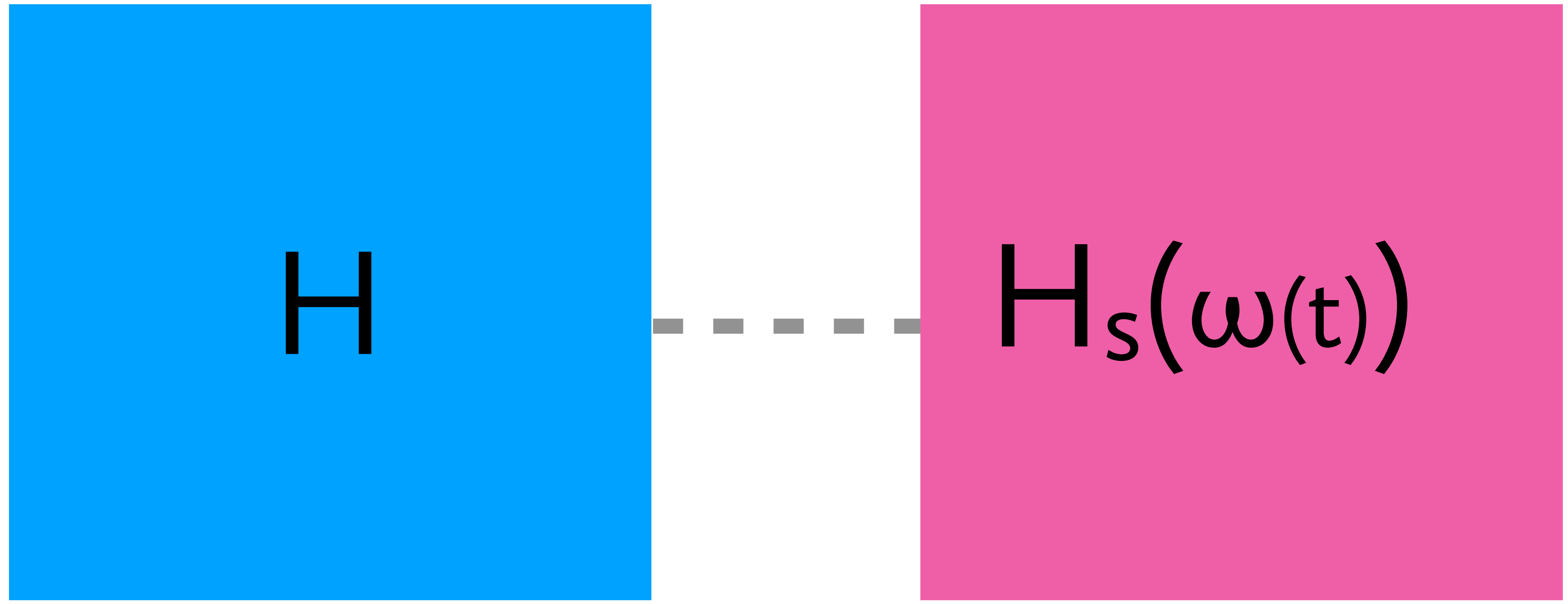


Initialize $|\psi\rangle|\text{cold}\rangle$

Evolves unitarily to entangled state ~ $|\psi_0\rangle|\text{warm}\rangle$

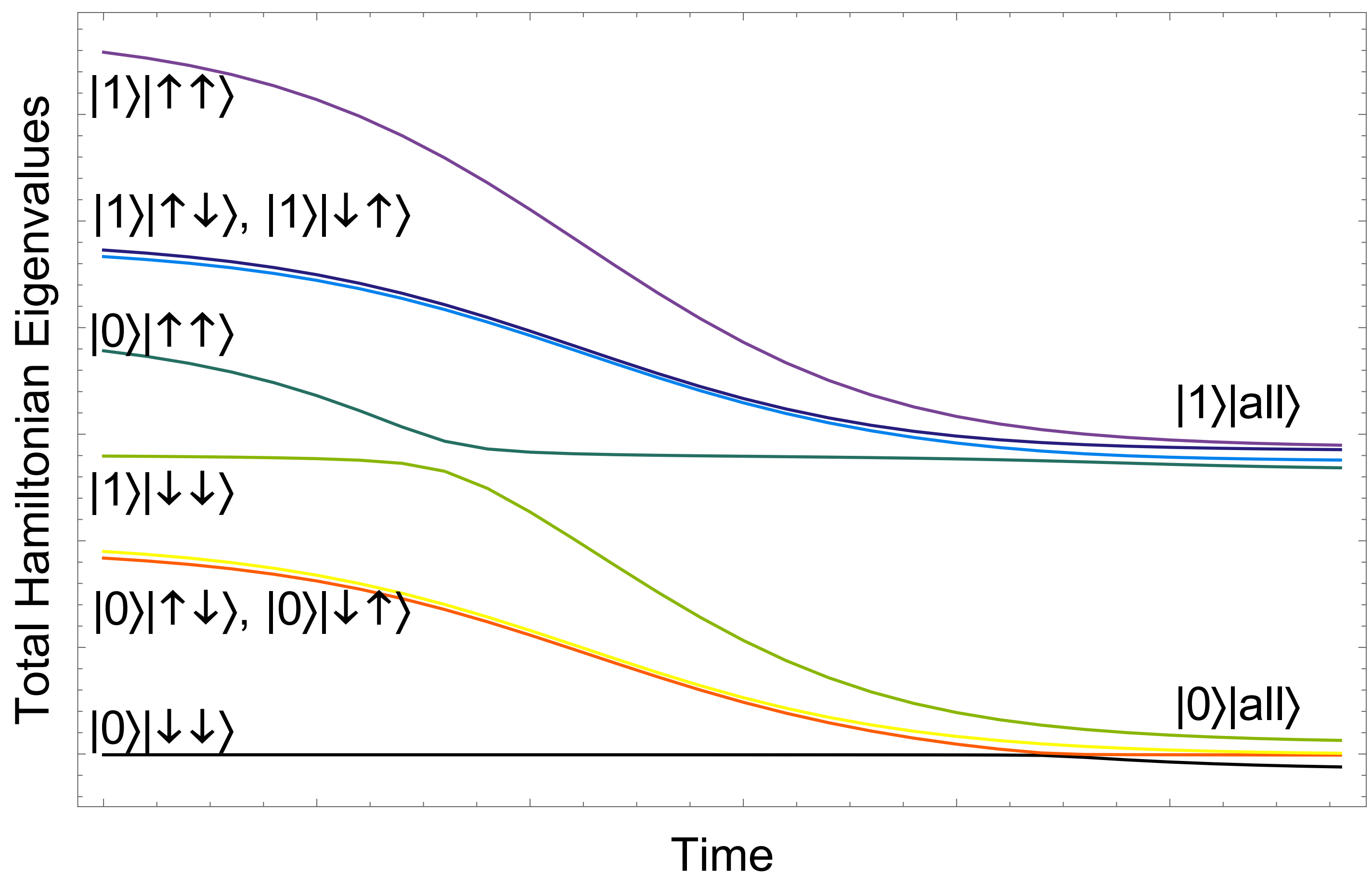
Heat bath does not seem to work well: needs to be very big (eg, many more qubits than the target system)

Spectral combing:



Couple "target' hamiltonian to a spin system with characteristic energy $\omega(t)$ which decreases with time.

Example: H is a 2-state system |0>, |1>; H_s is a 2-spin system



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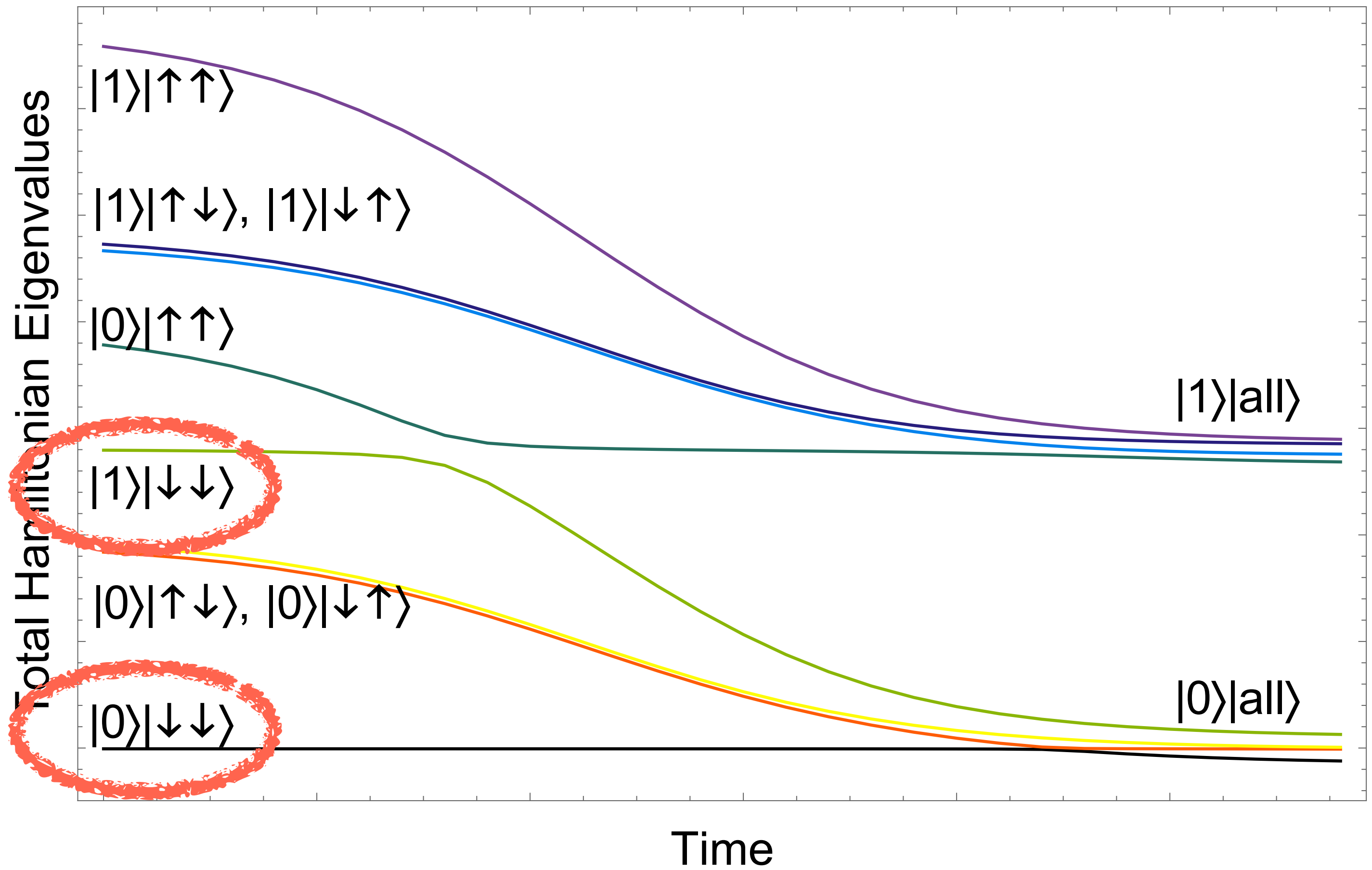

start in arbitrary linear combination of eigenstates |0> and |1> of H

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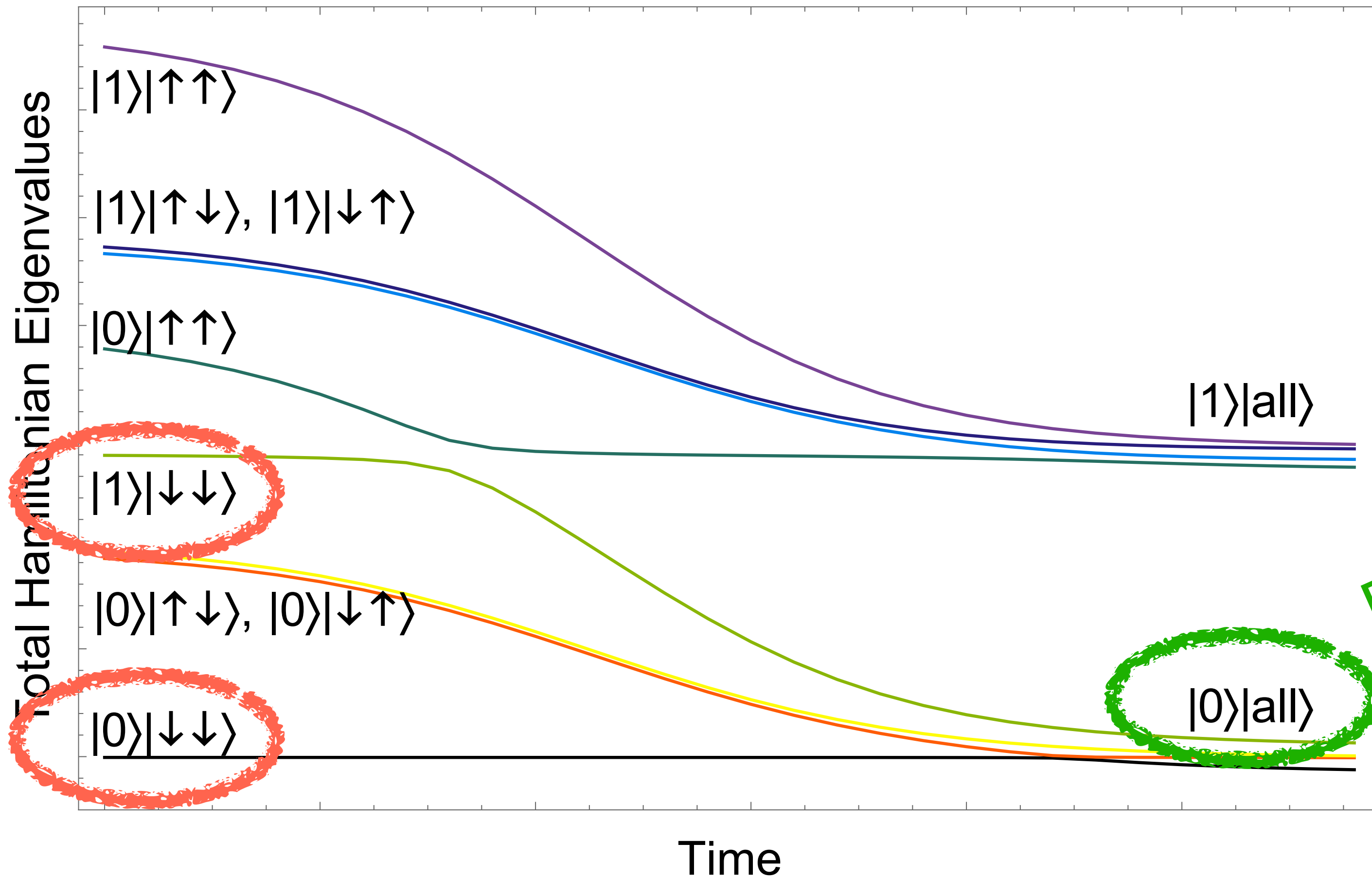

start in arbitrary linear combination of eigenstates |0> and |1> of H

End in |0> of H, with excitations in the spin system

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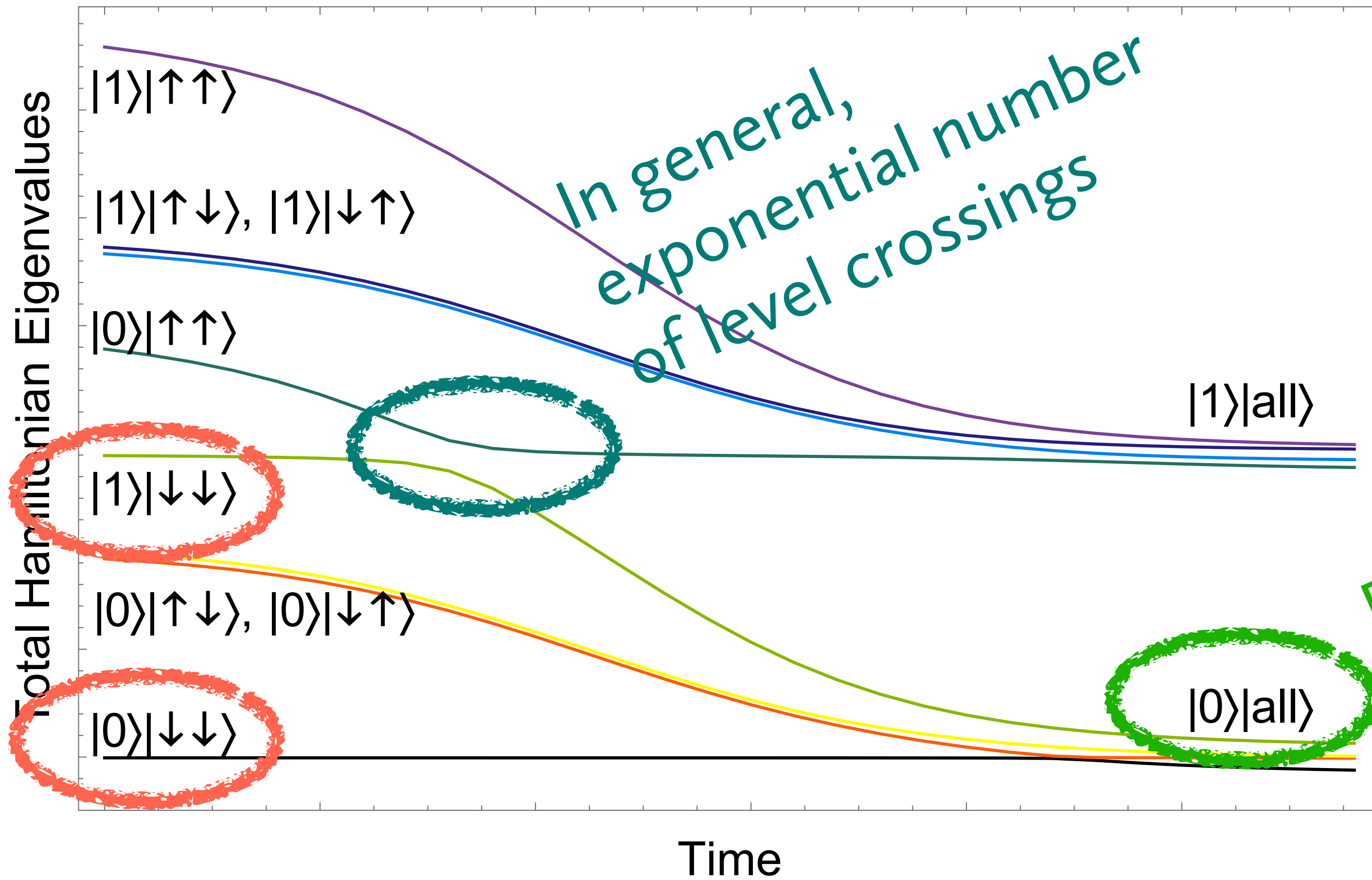
start in arbitrary linear combination of eigenstates |0> and |1> of H



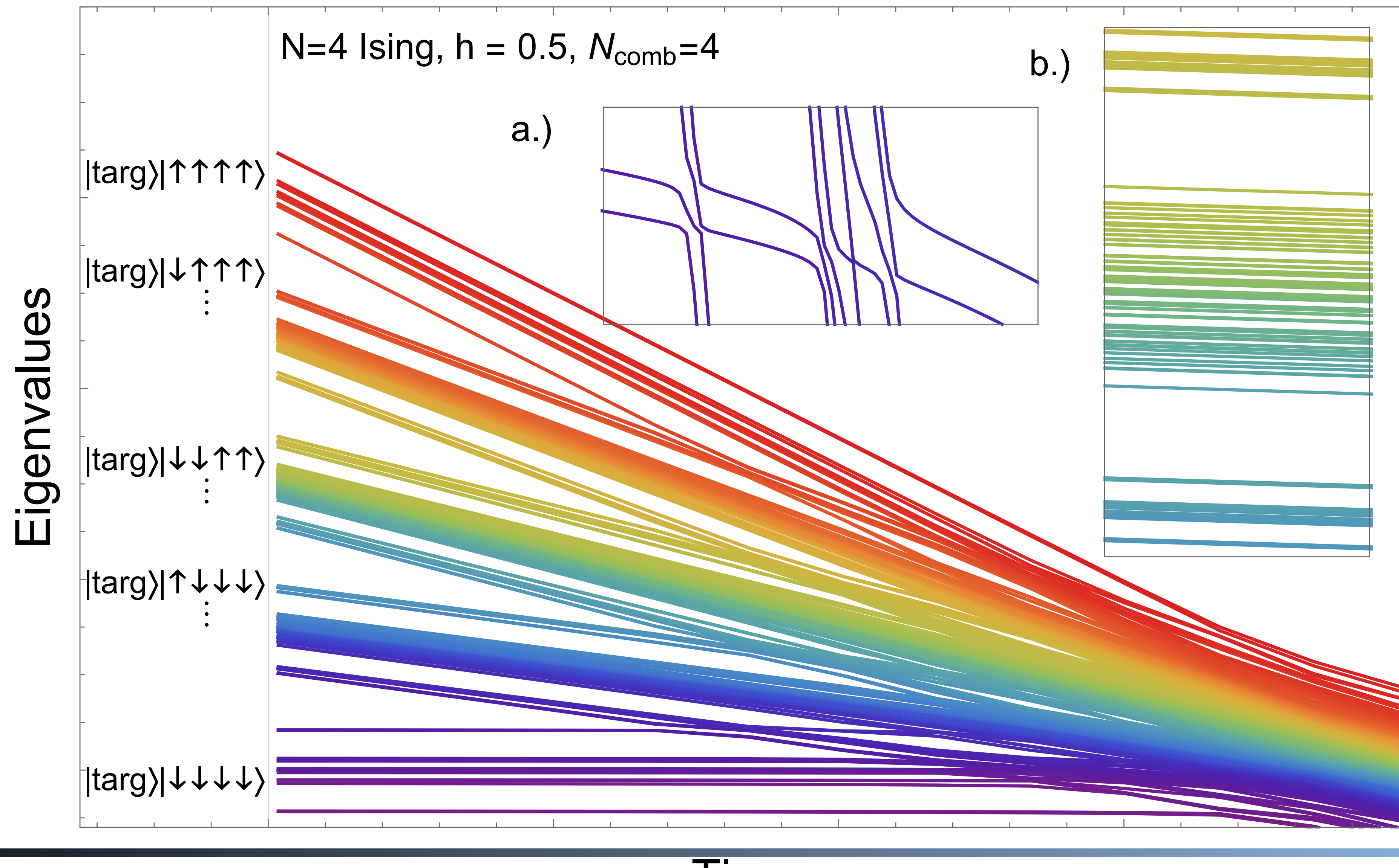
End in |0> of H, with excitations in the spin system

$$\mathcal{H}_{\rm comb}(t) = \sum_{i=1}^{N_c} \nu(t)\sigma_i^+\sigma_i^- + \kappa\phi_i \sum_{cyc}\left(\sigma_i^+\sigma_{i+1}^-\sigma_{i+2}^- + h.c.\right) \; .$$

random

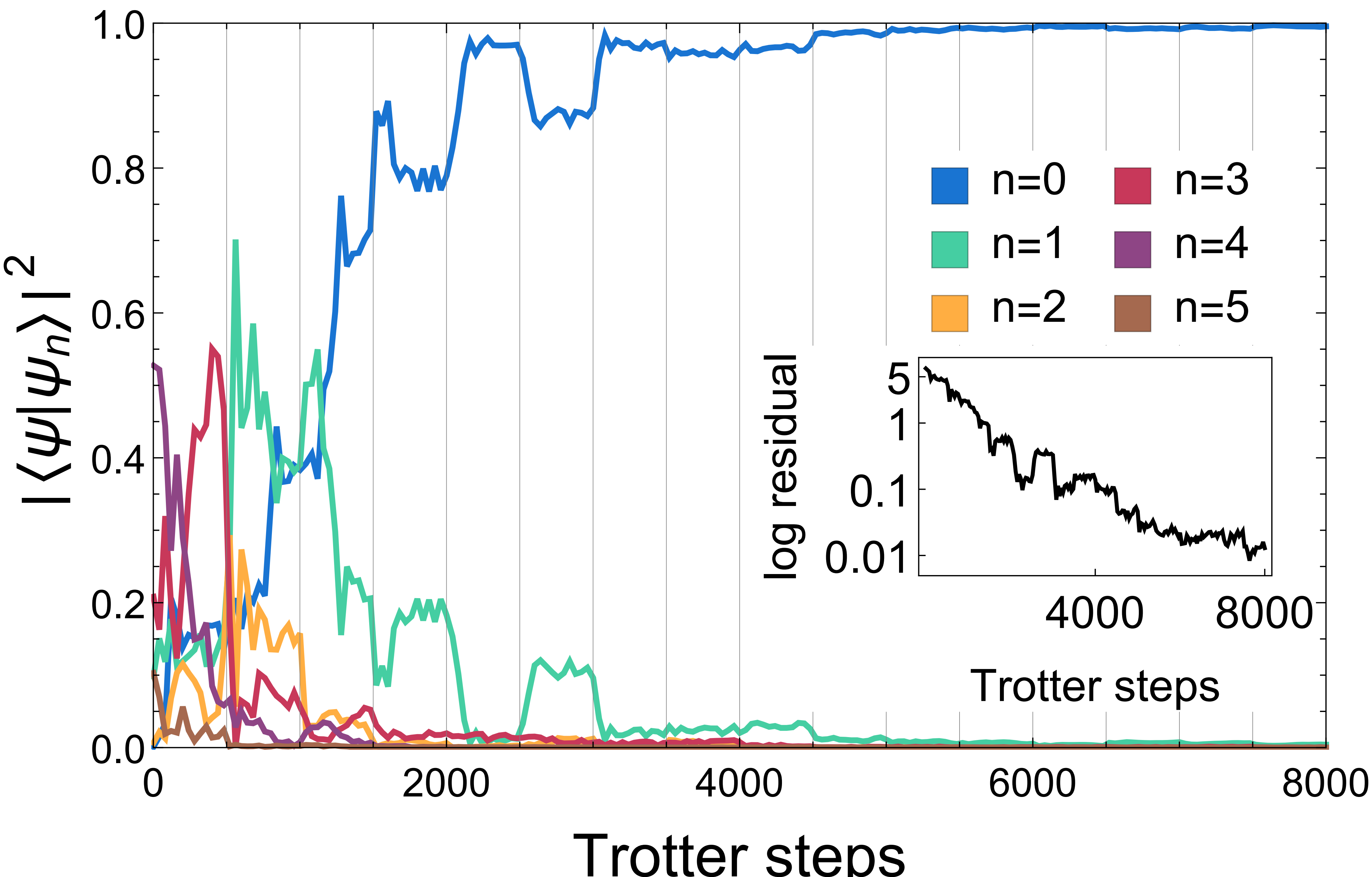
$$\nu(t) = \nu_0(1 - t/t_f)\;, \qquad \nu_0 > 0\;, \quad 0 \le t \le t_f \; .$$

A less toy example exponential number of level crossings:



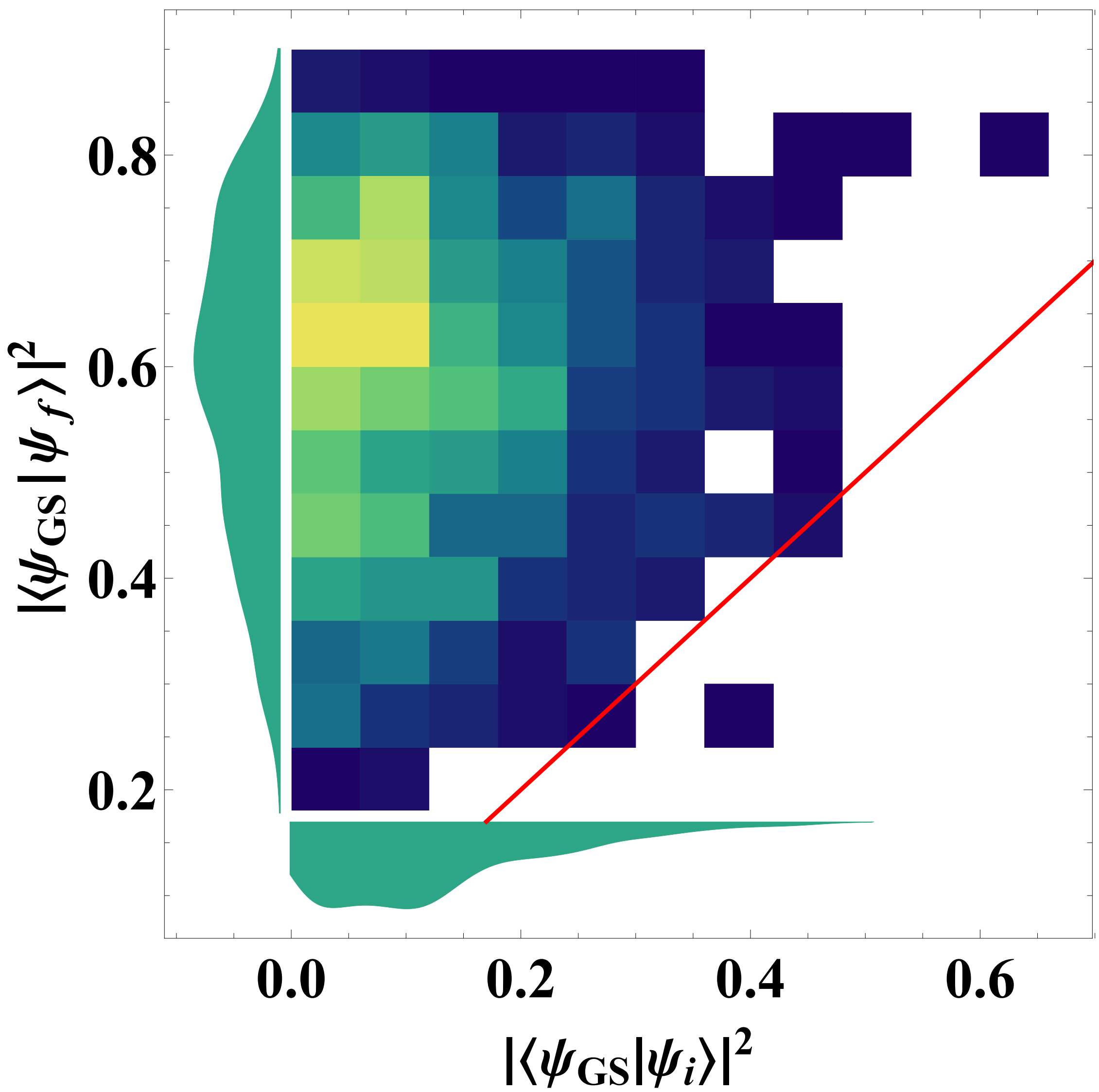
Does it work?

Here: target Hamiltonian is N=3 1d Ising model, N_s=3 spins in the comb, random initial state



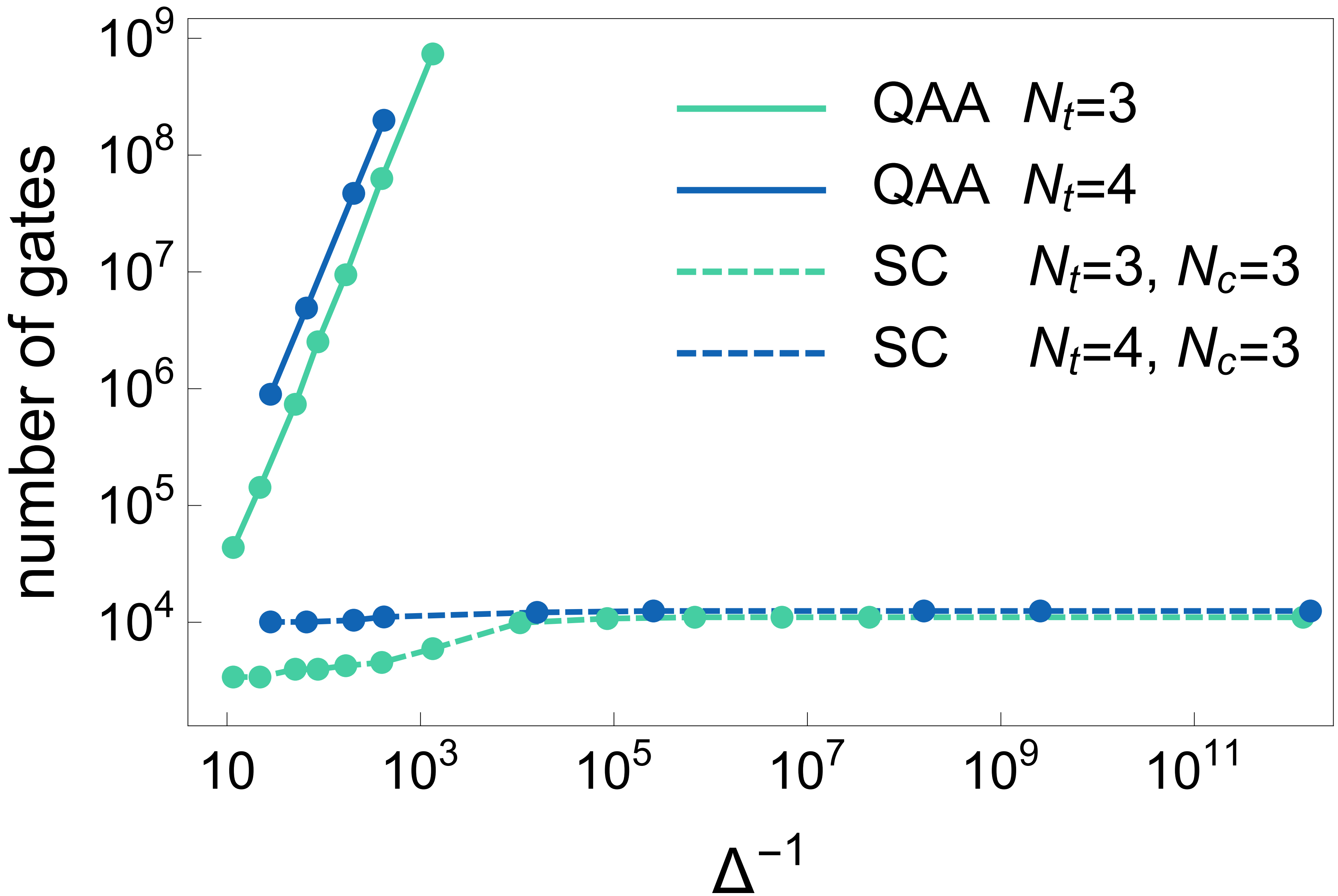
Spectral combing for transverse Ising model with B=0, h=0.5, limiting to 2000 Trotter steps

$$\mathcal{H}^{B}_{\text{targ}} = -h\sum_{i=1}^{N_t}\sigma^x_i - \sum_{i=1}^{N_t}\sigma^z_i\sigma^z_{i+1} + B\sum_{i=1}^{N_t}\sigma^z_i \; .$$



$$\mathcal{H}^B_{\text{targ}} = -h \sum_{i=1}^{N_t} \sigma^x_i - \sum_{i=1}^{N_t} \sigma^z_i \sigma^z_{i+1} + B \sum_{i=1}^{N_t} \sigma^z_i \ .$$

How does it compare with the pathological case for the Quantum Adiabatic algorithm, where one starts in the metastable state (tuning h to make the gap small)?



So: Spectral Combing looks interesting, need to determine its scaling properties for larger systems. In any case, gate count scales like a power of the number N of qubits, NOT the size of the Hilbert space, 2^N

Would like to better understand “thermalization” in closed quantum systems, in order to inform scaling arguments

Just an example of how physicists can contribute in this field.

Many open problems: like, how to simulate gauge theories, Matrix Models, CFTs, etc!

Summary:

Sign problems are severe in interesting theories, and are rooted in the dynamics of the theory, probably not fixable for QCD by new algorithms for classical computers

There are LOTS of hardware obstacles to overcome...
...but if quantum computing becomes a reality, we may be able to solve these outstanding problems ▸ with the potential to revolutionize physics and technology

In the meantime, things for theorists to do...