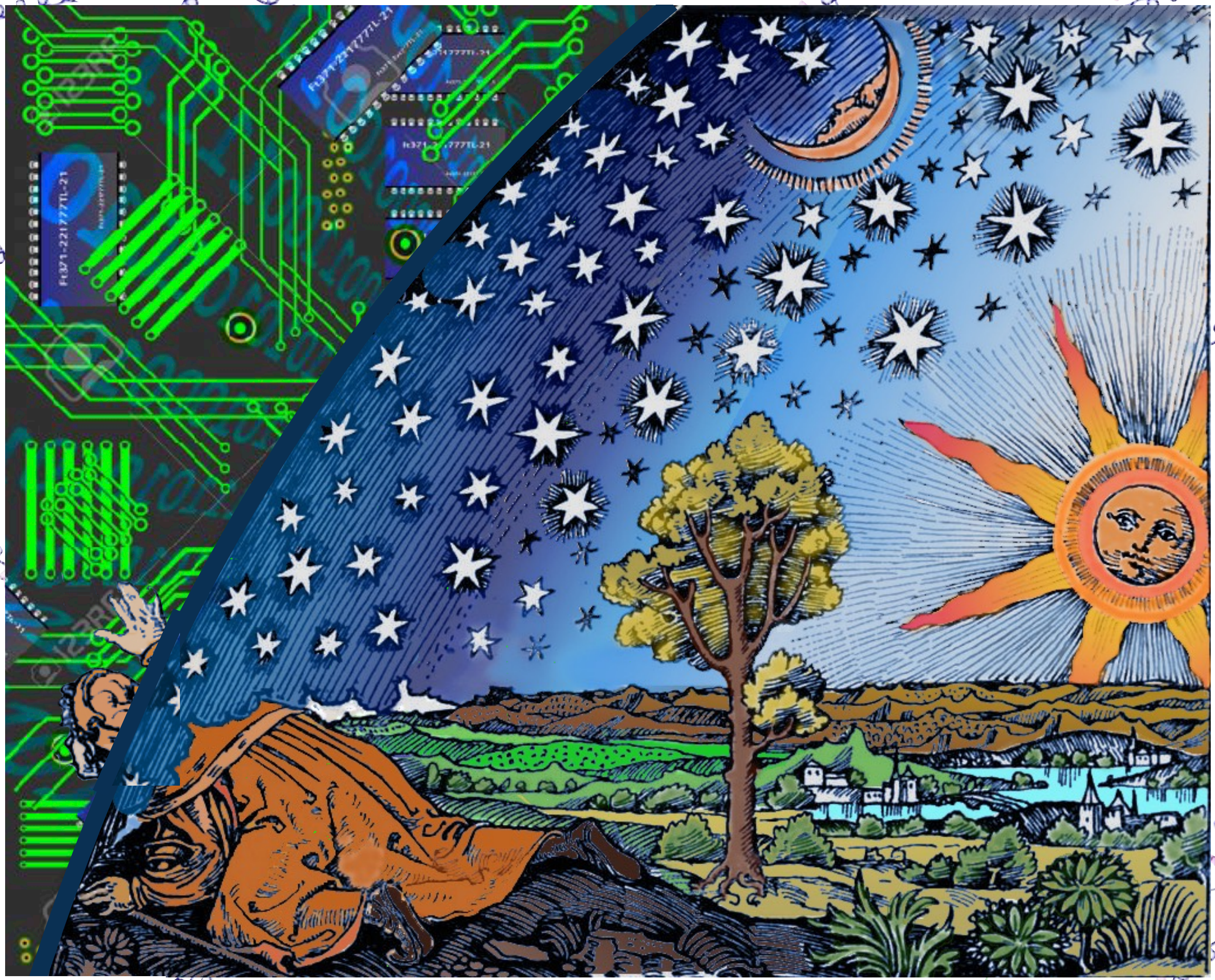
Quantum computers for scientific computing



D. B. Kaplan ~ Beijing “Frontiers in LQCD” ~ 28/6/19

INSTITUTE for NUCLEAR THEORY

Lattice QCD has become a powerful tool:

- hadron spectrum
- weak matrix elements
- g-2
- light nuclei
- properties of hot QCD
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SIGN PROBLEMS

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- 2 degenerate flavors u,d
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$$Z = \int [DA_\mu]\, e^{-S_{YM}} \det{}_2 \left[\not{D} + m + \mu\gamma_0\right]$$

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Requires sampling gauge fields with probability...

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…but the determinant is complex!

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

Apply dagger, γ5

Can we write:

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

?

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Note:

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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.

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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)

$$Z_B = 1 \ ,$$

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

Free energy due to pion condensation

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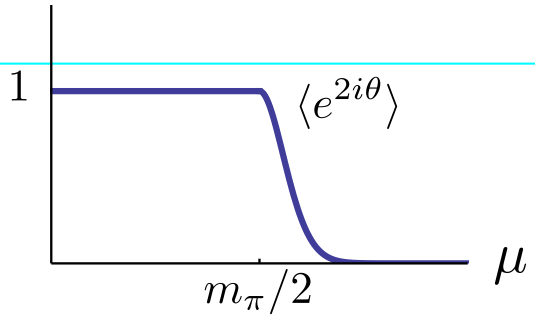

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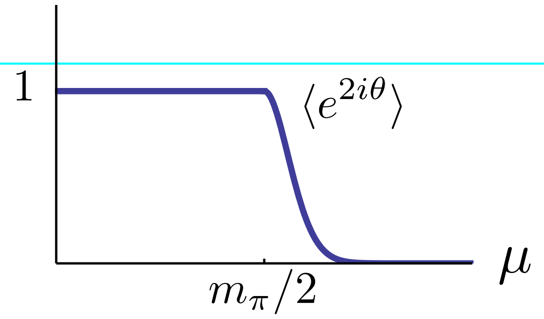

- The phase cancellations are <u>exponentially</u> bad in the spacetime volume

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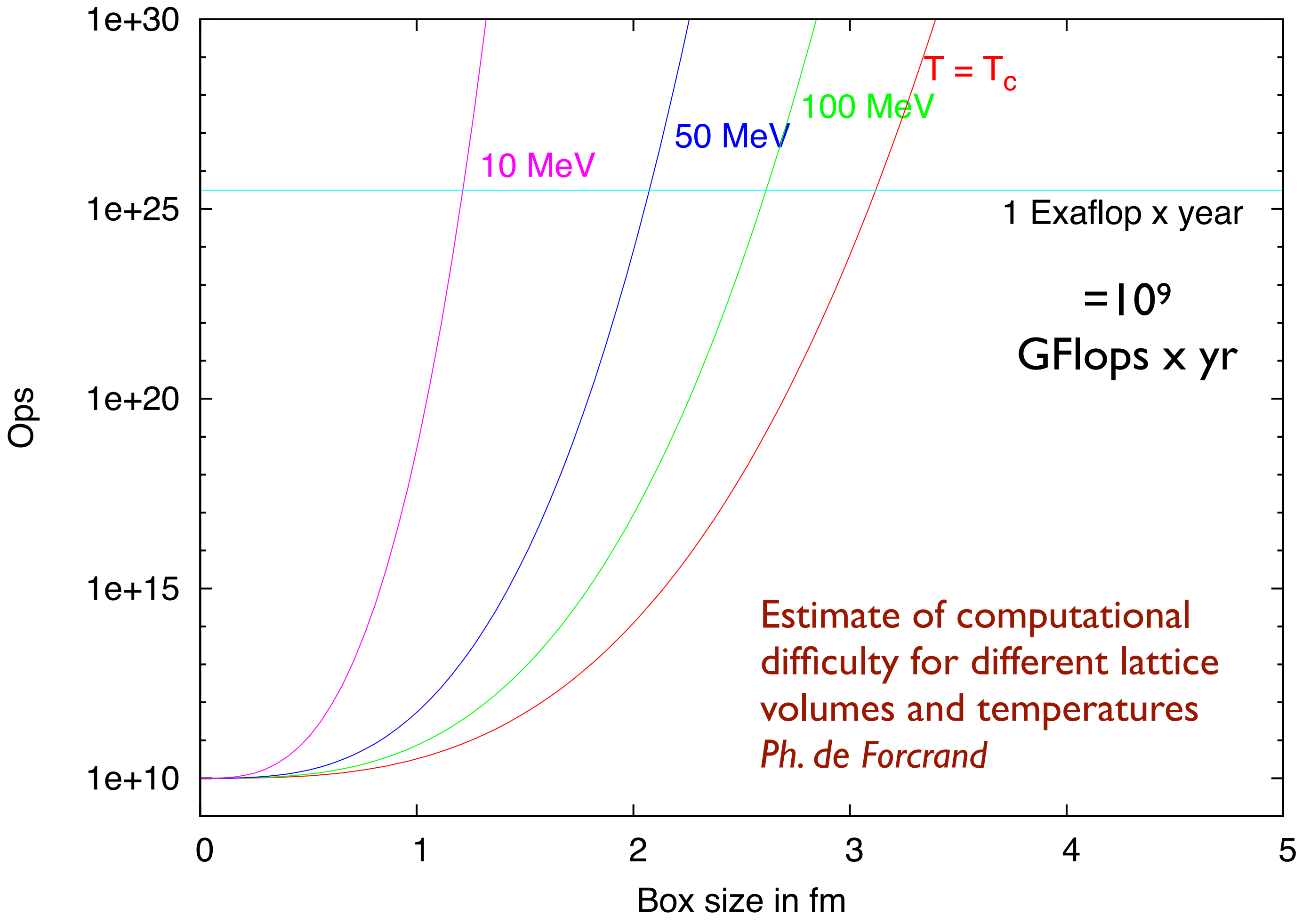
CPU effort to study matter at nuclear density in a box of given size
Give or take a few powers of 10…



$=10^9$
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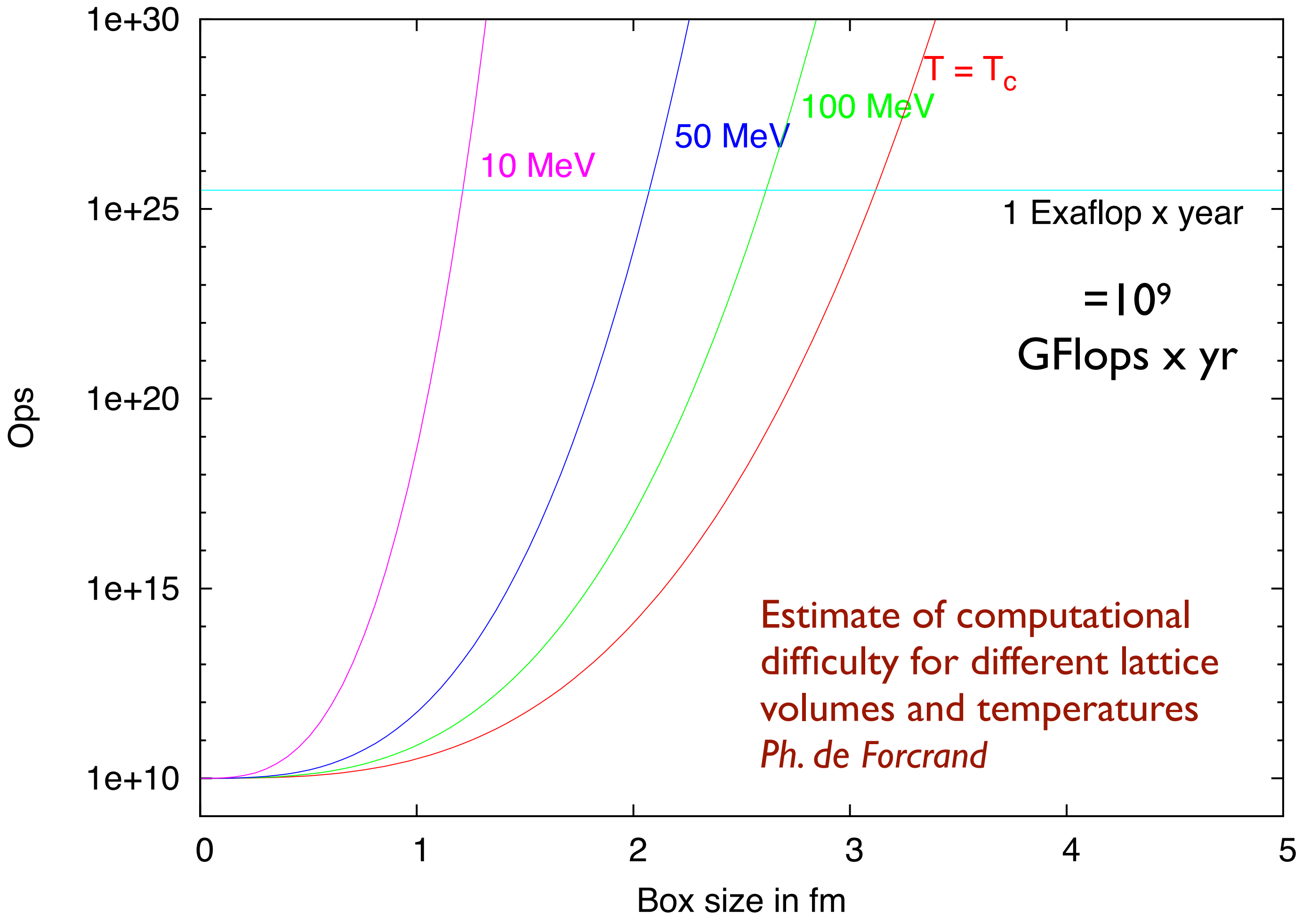

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Estimate of computational difficulty for different lattice volumes and temperatures
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e.g.: T=10 MeV, L=3fm, ρ=nuclear density: > $10^{10\text{-}20}$ exaflop-yrs?!

Practical implementation of Wilson's formulation of the Feynman path integral on a classical computer:

32^3 x 64 lattice size: millions of degrees of freedom
Hilbert space size ~ e^{millions}. Lattice QFT: sample it!

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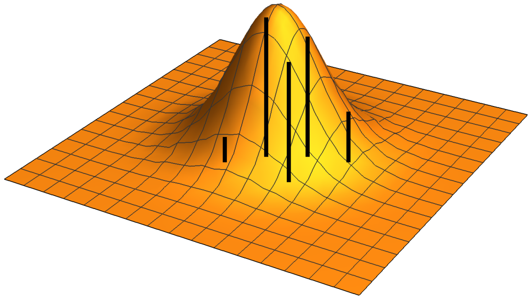

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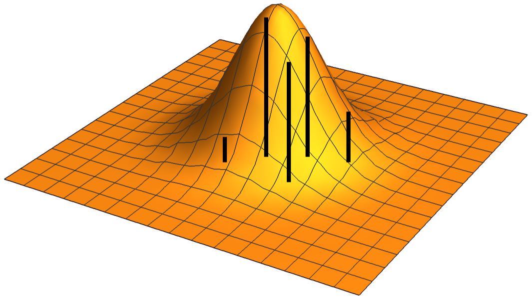

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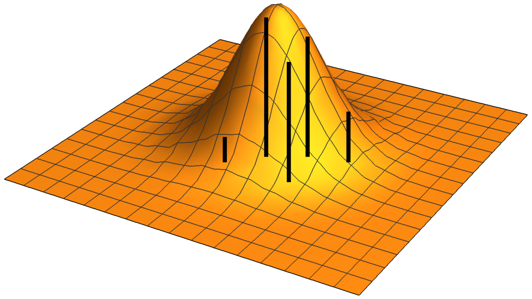

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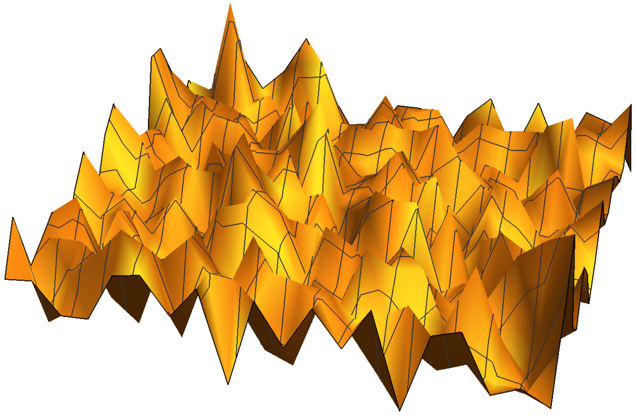
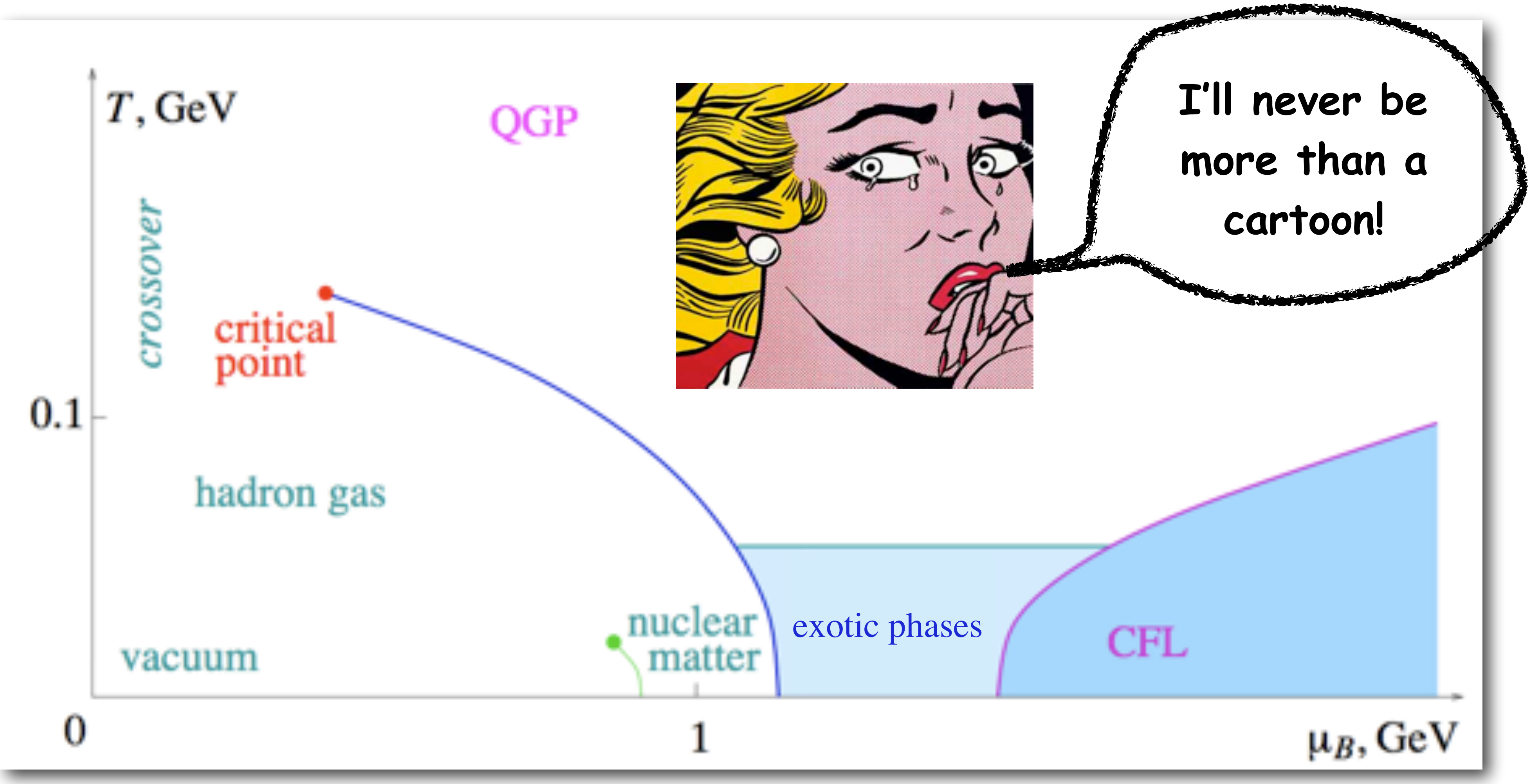
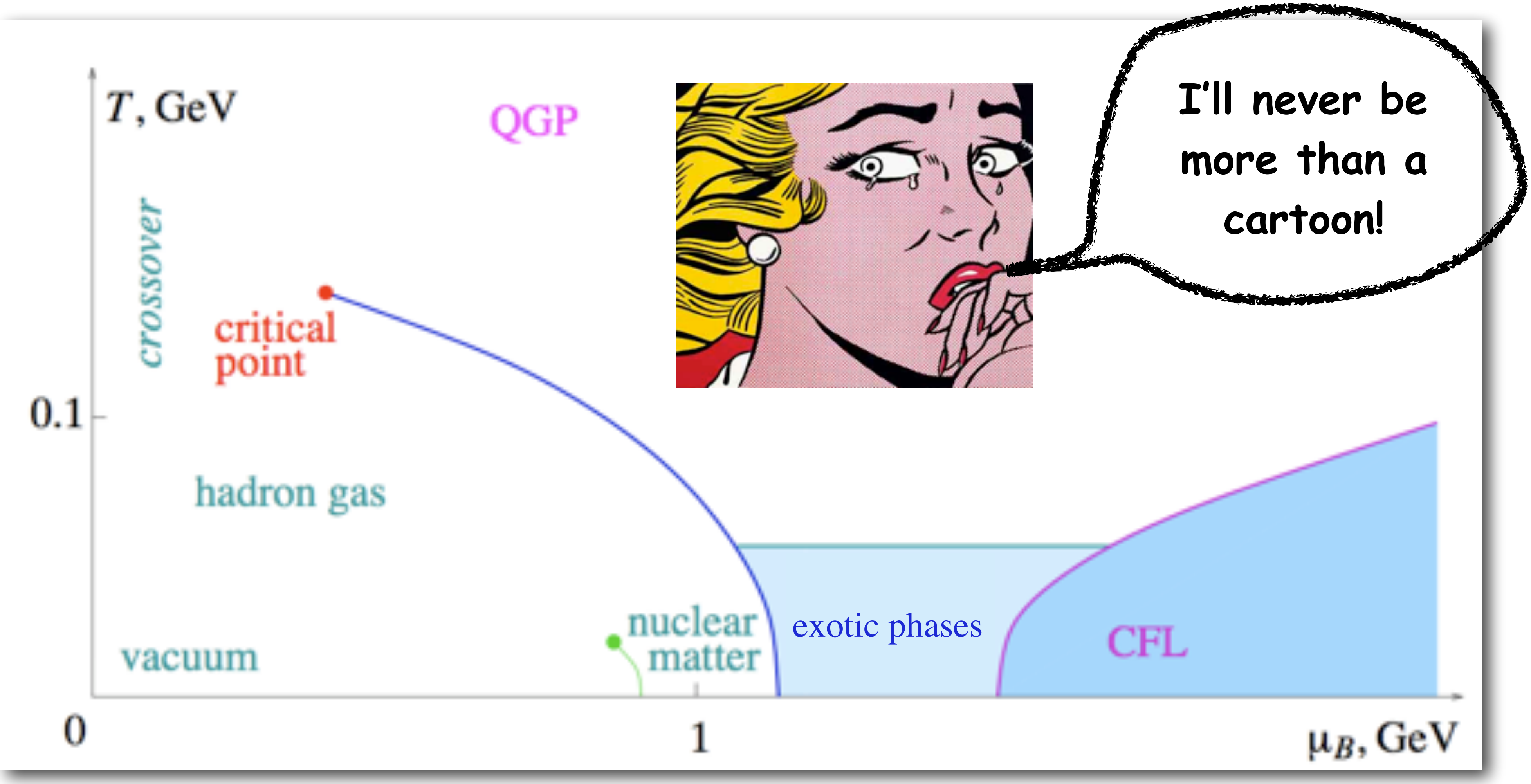


…but not at $\mu\neq0$

…


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



Quantum computers to the rescue?

2 classical bits

state 1: 00

state 2: 01

bit flip = 2x2 matrix acting on 2nd bit

can get from any initial state to any final one by a sequence of single-bit flips

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2 “qubits”

state 1: $|00\rangle$

state 2: $(|00\rangle+|11\rangle)/\sqrt{2}$

requires 4x4 matrix acting on both qubits

cannot get from initial state to final state by a sequence of individual bit flips due to <u>entanglement</u>

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N classical bits: N 2x2 matrices needed to get from one state to the next

N qubits: 2^Nx 2^N matrix needed to get from one state to the next

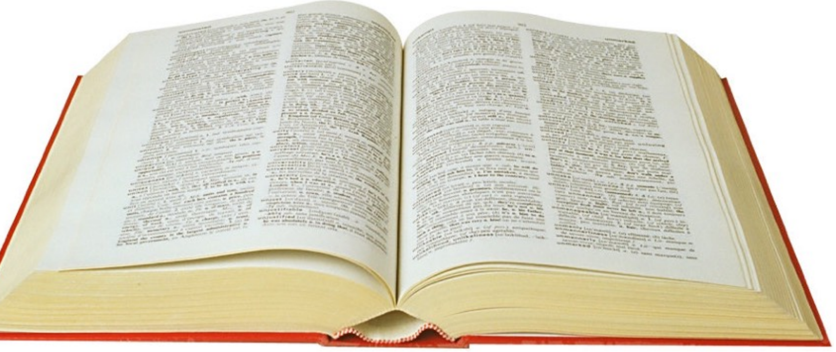
Classical bit stream

1101110010001101011011110…

Classical bit stream

110110010001101011011110...

Classical book



Tear out 1% of the pages and
you lose 1% of the information

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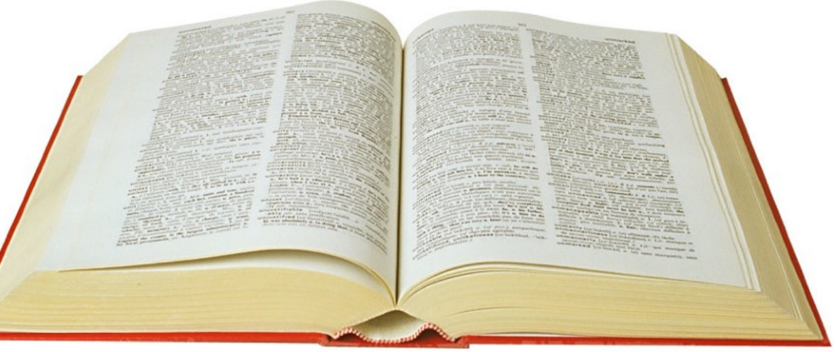

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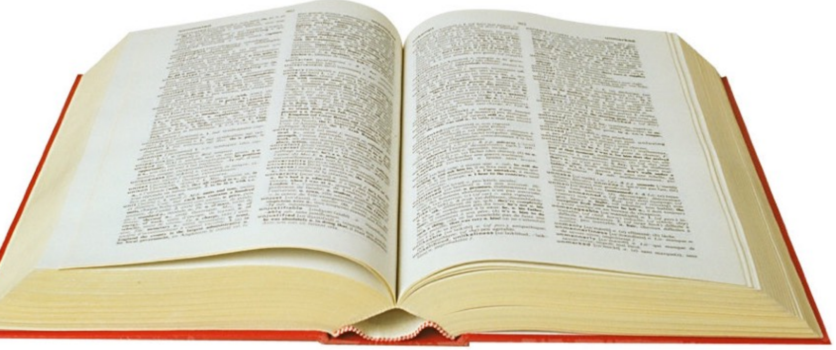
Qbit stream

$$c_1|110010111\dots\rangle \\ +c_2|001000110\dots\rangle \\ +c_3|101010001\dots\rangle + \dots$$

Classical bit stream

110111001000110101011011110...

Classical book



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Entanglement!

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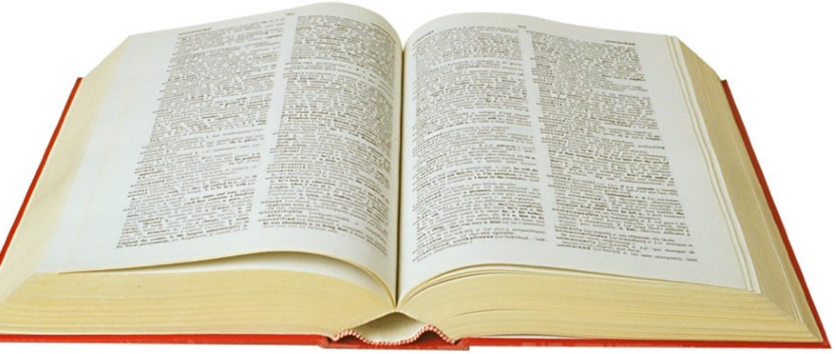

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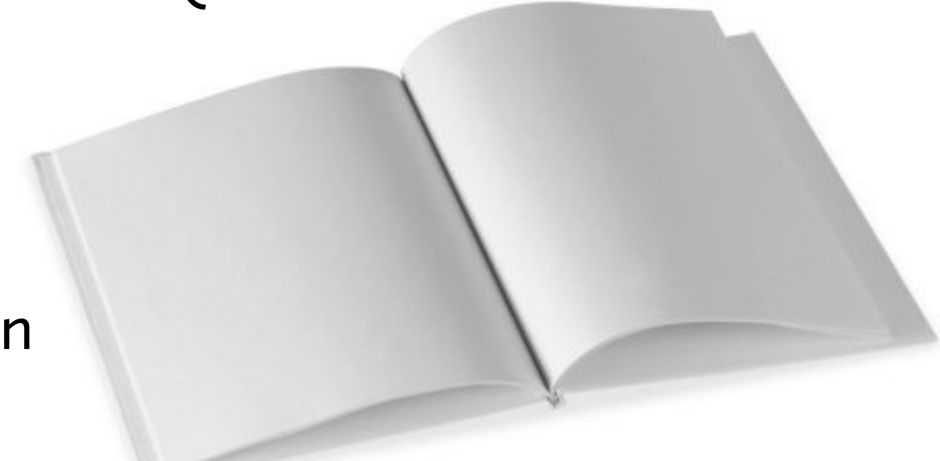

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No information on any one page of the quantum book...tearing out a page is like losing resolution in a photograph...but each page tells you something about what is on the other pages

Classical bit stream

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Qbit stream

$$\begin{gathered} c_1|110010111\ldots\rangle \\ +c_2|001000110\ldots\rangle \\ +c_3|101010001\ldots\rangle + \ldots \end{gathered}$$

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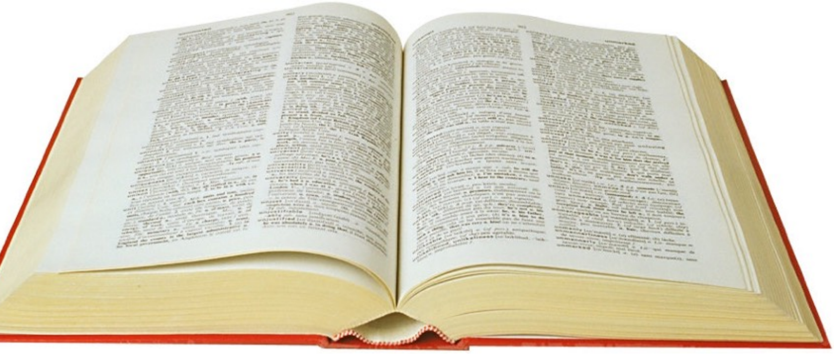
Classical book



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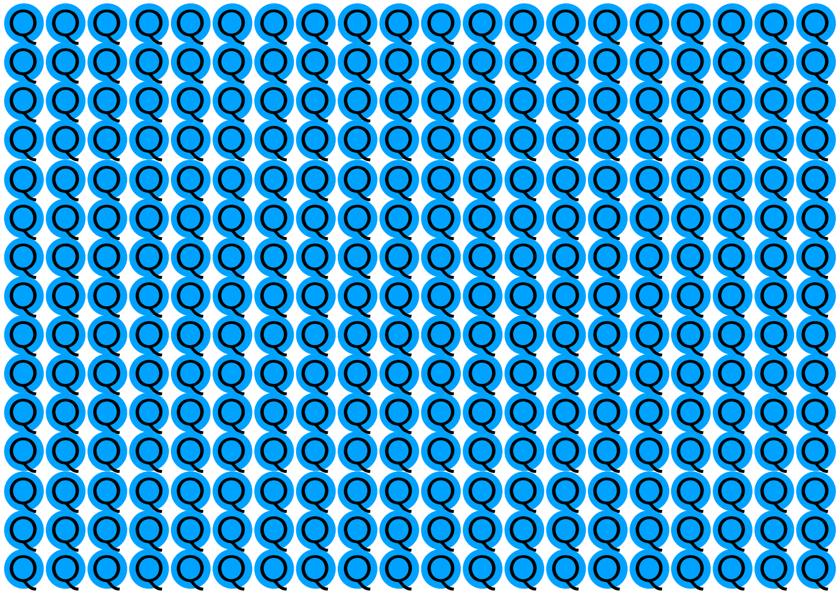

300 qubits

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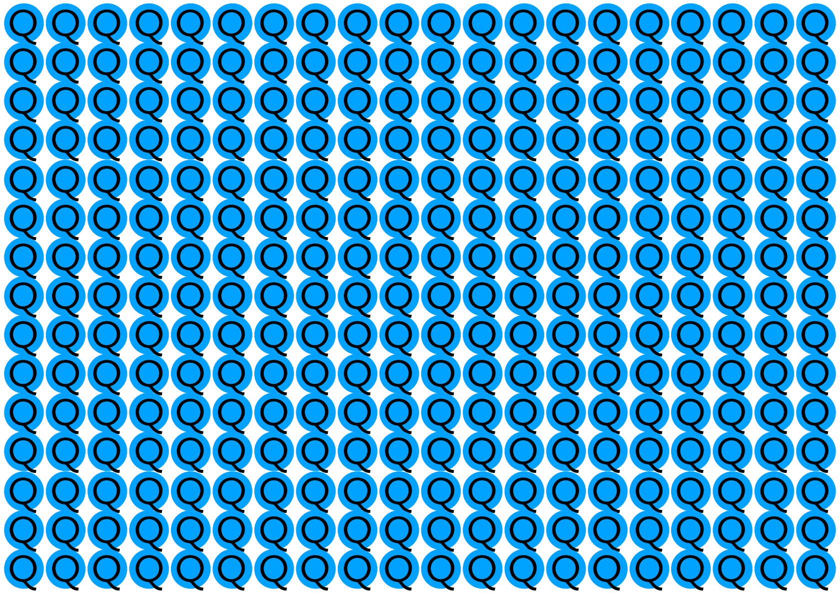

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The number of classical bits required to encode the information in 300 qubits is more than the total number of atoms in the Universe!

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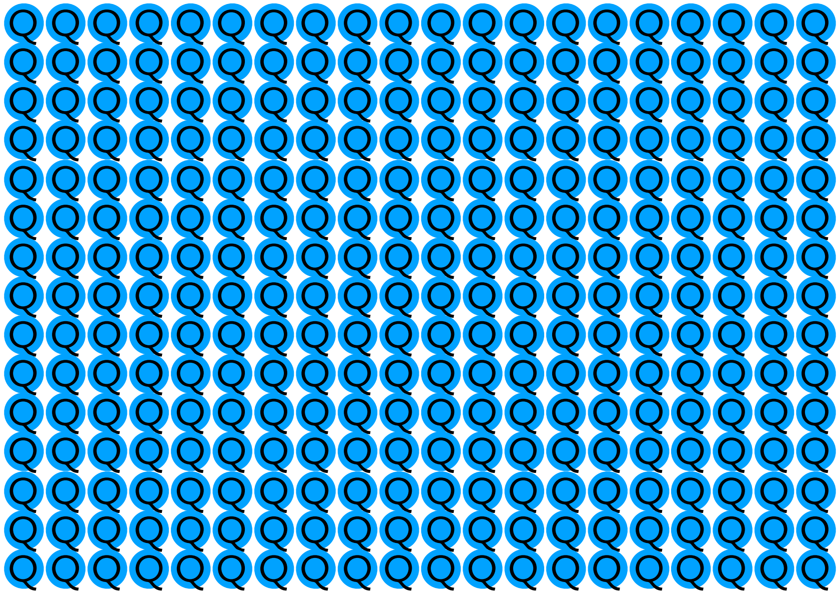

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qubits

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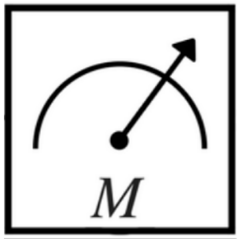

$|\Psi_i\rangle$

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Initialize qubits

Perform gate operations on qubits

Measure (convert to classical bits)

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Classical Fourier transform on a discrete function with N values

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

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

Computational cost = O(N log N).

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

Fourier transform on a quantum computer

Start with n=2 qubits |x> = |x$_0$,x$_1$> where x$_i$ = 0,1 …
So $N = 2^2 = 4$ and $\omega = e^{2\pi i/4}$

The Fourier transform is then the unitary transformation on these states

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

$$U = \frac{1}{\sqrt{2^2}} \begin{pmatrix} \omega^0 & \omega^0 & \omega^0 & \omega^0 \\ \omega^0 & \omega^1 & \omega^2 & \omega^3 \\ \omega^0 & \omega^2 & \omega^4 & \omega^6 \\ \omega^0 & \omega^3 & \omega^6 & \omega^9 \end{pmatrix}$$

Then

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

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

In the basis:

Then

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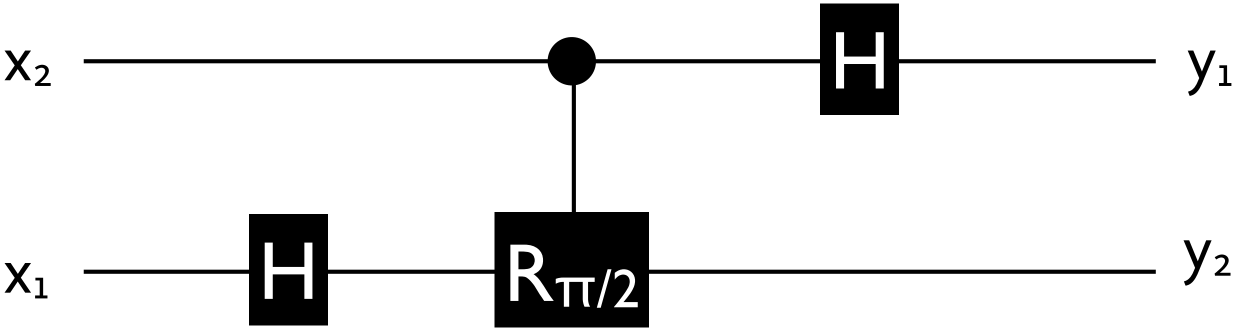
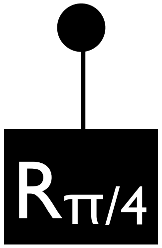
$$\boxed{|y\rangle = U|x\rangle = \frac{1}{2}\left(|0\rangle + \omega^{2x_2}|1\rangle\right)\left(|0\rangle + \omega^{2x_1+x_2}|1\rangle\right)}$$

$\omega^4 = 1$

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



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



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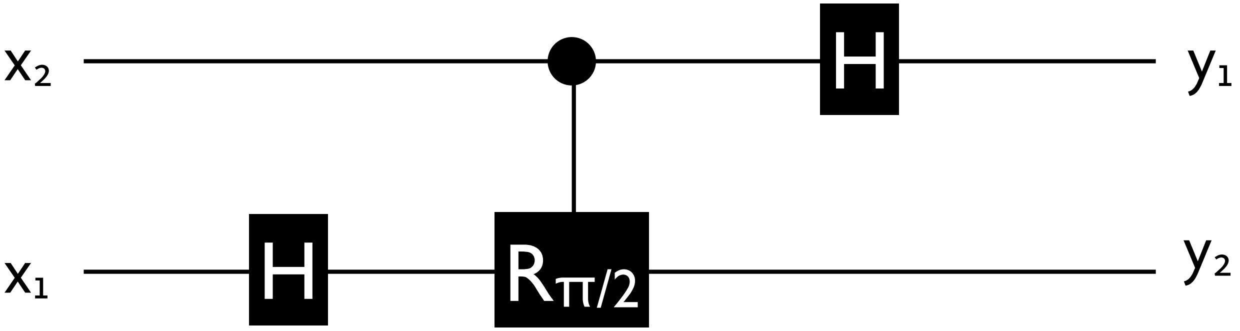

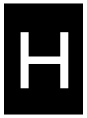

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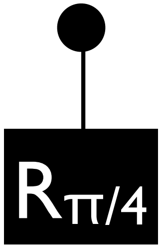

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$$|x_1\, x_2\rangle \xrightarrow{H} \left(\frac{|0\rangle + \omega^{2x_1}|1\rangle}{\sqrt{2}}\right)|x_2\rangle \xrightarrow{R_{\pi/2}} \left(\frac{|0\rangle + \omega^{2x_1+x_2}|1\rangle}{\sqrt{2}}\right)|x_2\rangle \xrightarrow{H} \left(\frac{|0\rangle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

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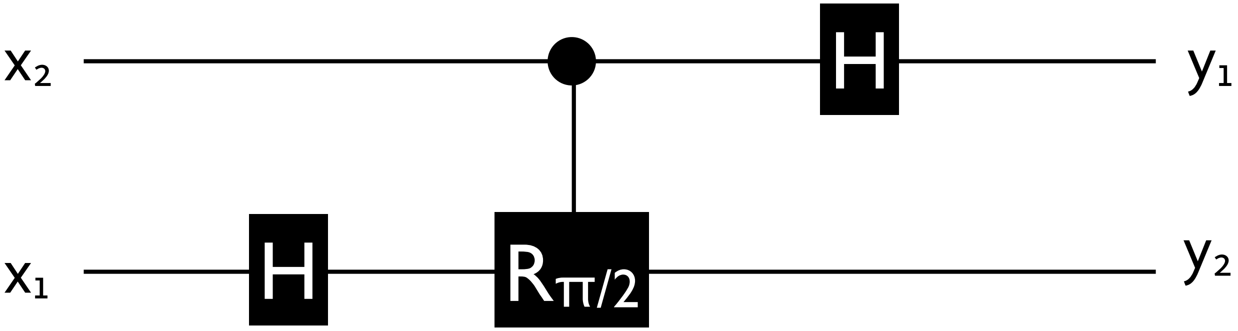

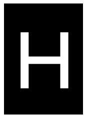

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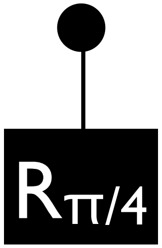

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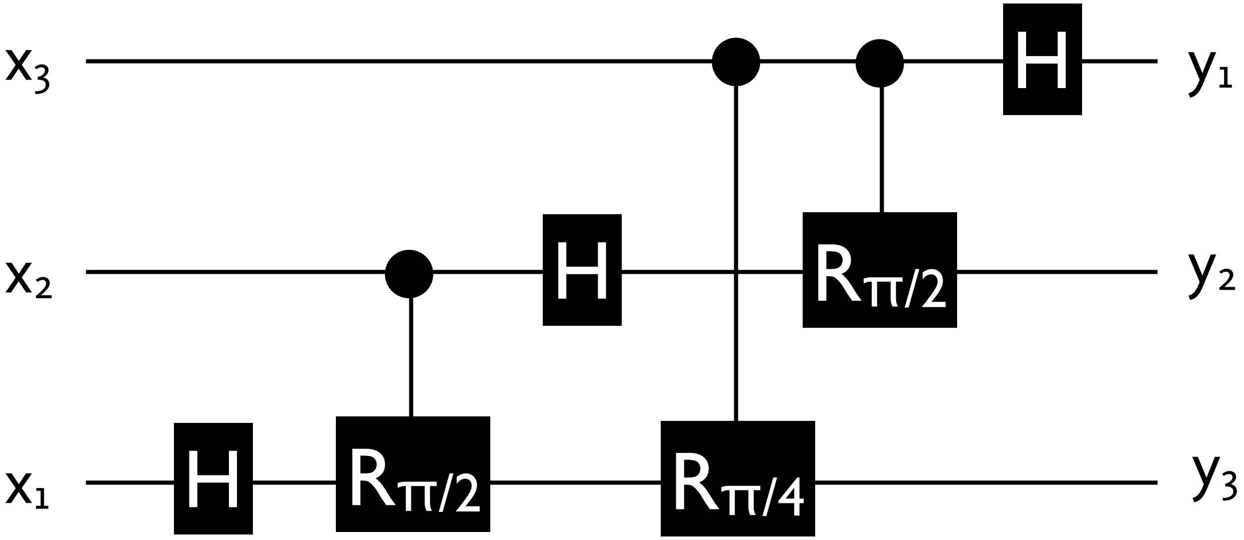
The “score” for the n=3 Fourier transform:



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.

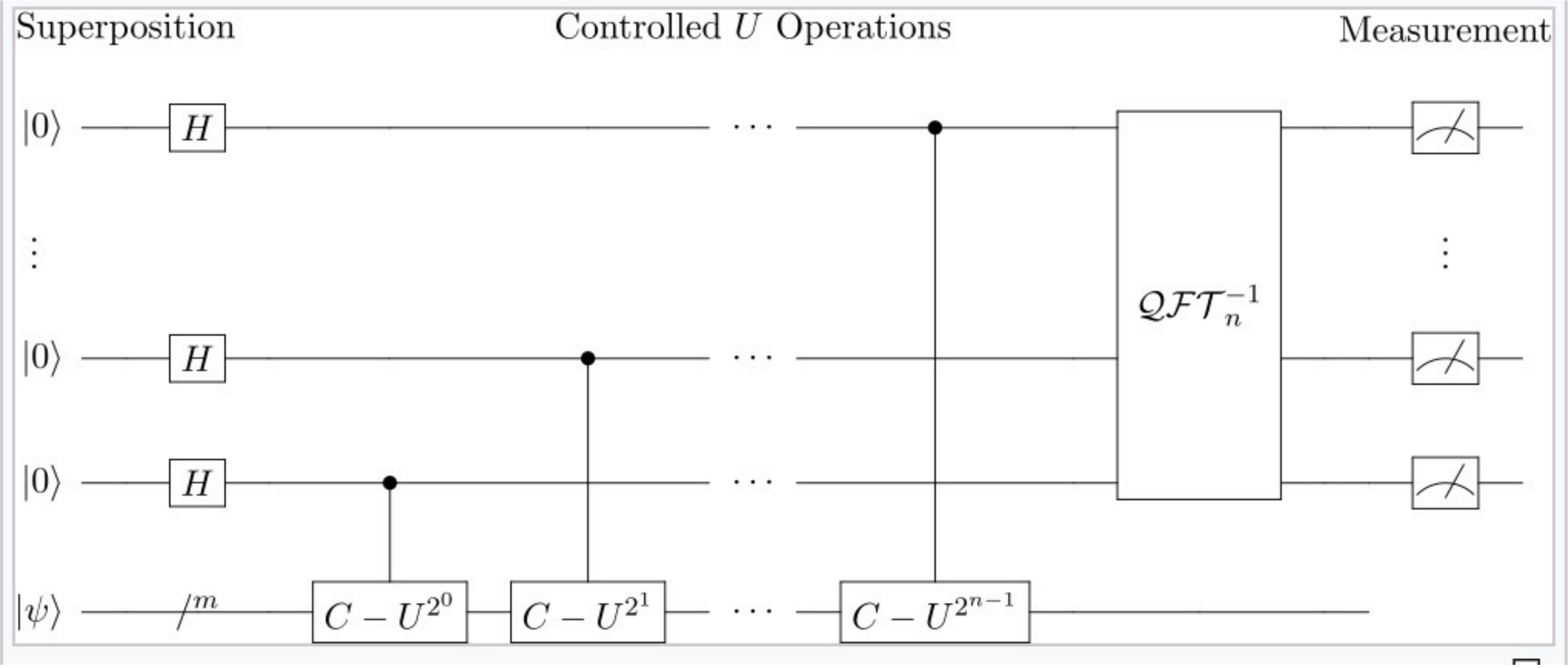
How can you use this for physics?

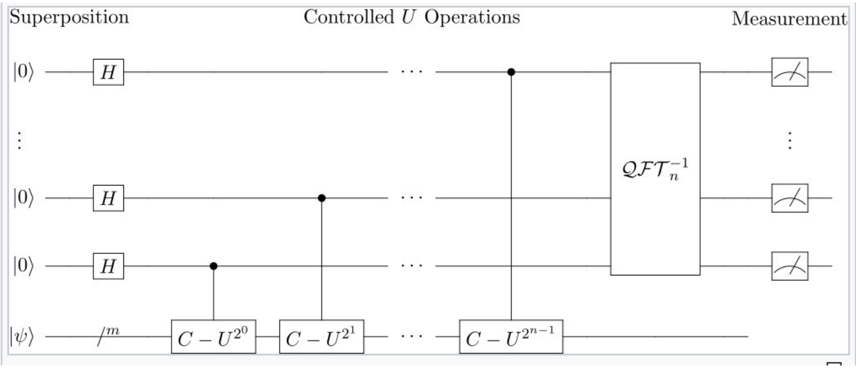
Example: phase estimation algorithm

Suppose |ψ> 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 $|y\rangle$

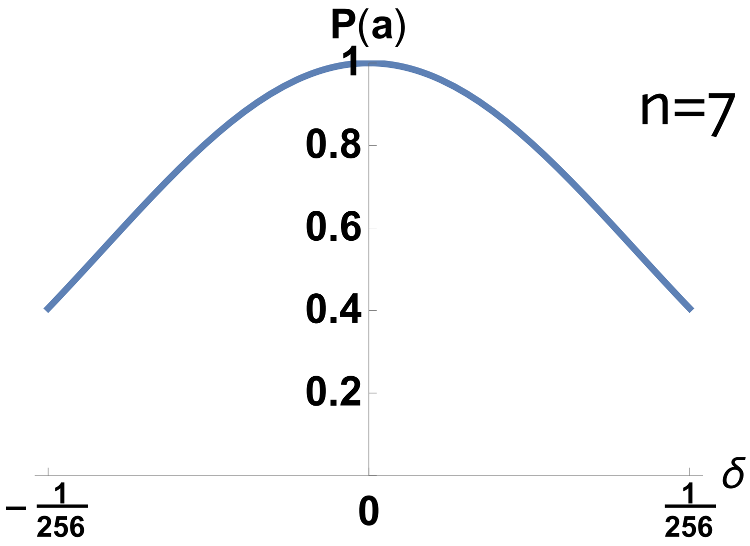
Measuring $|y\rangle$ yields the exact answer for a:

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

all y_i measured to be 0 or 1

If θ = a 2^{-n} + δ 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



$$P(a) = \frac{1}{2^{2n}} \frac{|\sin(\pi 2^n \delta)|^2}{|2\sin\pi\delta|^2}$$

$$\geq \frac{4}{\pi^2} = 0.41 \qquad \text{for} \qquad |\delta| \leq 2^{-(n+1)}$$

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

$$|\psi> = \alpha\ |\theta= a2^{-n}> + \beta\ |\theta= b2^{-n}>$$

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

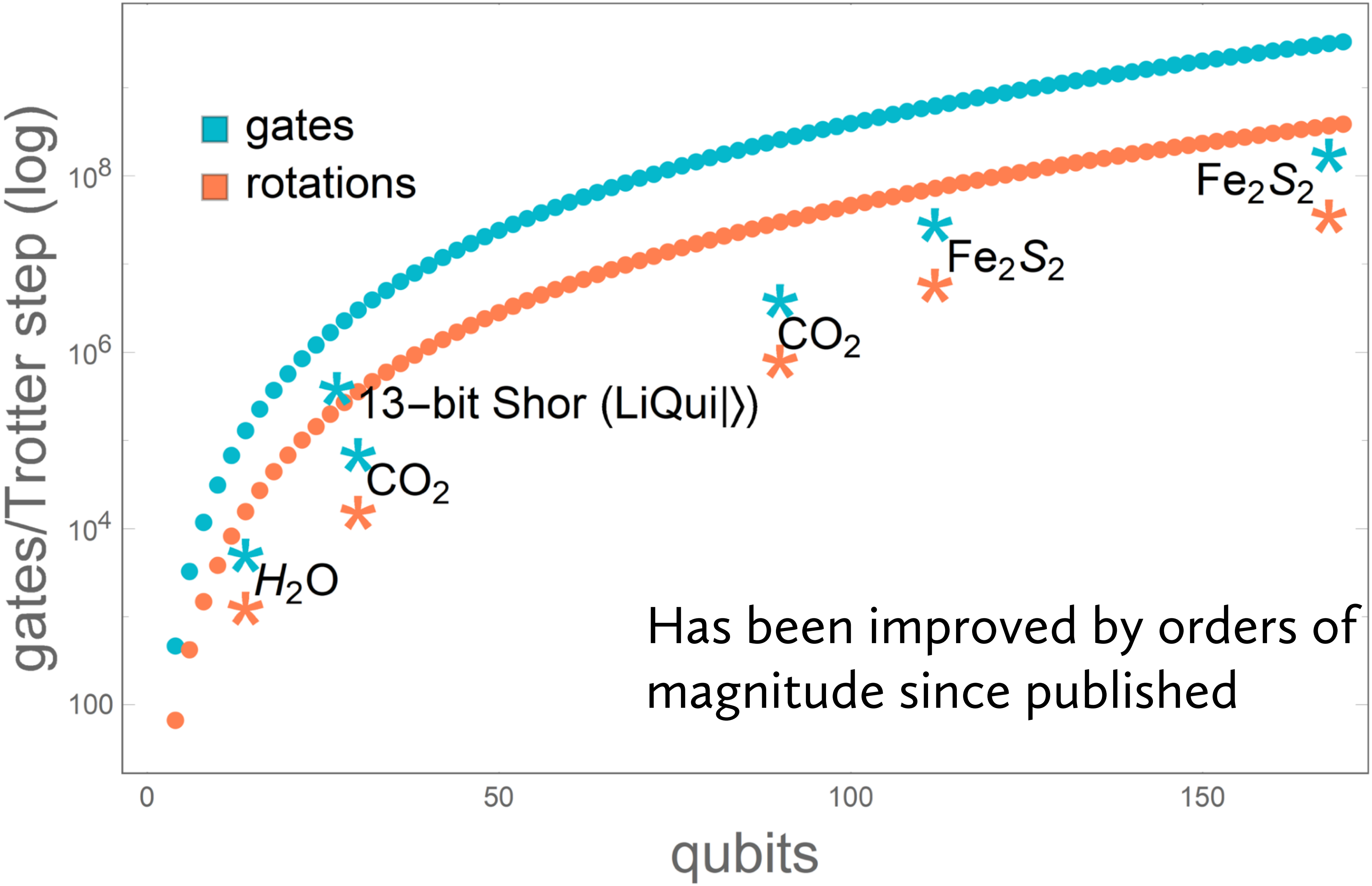
- yield a with probability $|\alpha|^2$ or b with probability $|\beta|^2$
- after measurement, $|\psi>$ collapses to eigenstate

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

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 $|\psi_i>$
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 product of short time evolution operators (Trotterization)
    - Express these in terms of gate operations
3. Measurements at end of QPE will give the spectrum of Et, weighted by overlap of $|<E|\psi_i>|^2$
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

Lots of gates and qubits needed!



Has been improved by orders of magnitude since published

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

Lattice Yang Mills? Start with Hamiltonian formulation

- Fix A₀=0 gauge
- $H = \frac{1}{2}\left(g^2 \vec{E}_a \vec{E}_a + \frac{1}{g^2}\vec{B}_a \vec{B}_a\right)$, $\left[A_a^i, E_b^j\right] = i\hbar\,\delta^{ij}\,\delta_{ab}$
- Physical states obey Gauss constraint: $D_i E_i |\psi\rangle = 0$

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Kogut-Susskind (lattice) Yang-Mills Hamiltonian:

- Fix U=1 gauge on temporal links, U on spatial links ▸ operators
- $\vec{B}_a \vec{B}_a \to -\mathrm{Re}\,\mathrm{Tr}\,\hat{U}_\Box$ (product of U's around plaquette)
- $\vec{E}_a \vec{E}_a \to \hat{\ell}_a^2 = \hat{r}_a^2$ (Casimir operator)
- $\left[\hat{\ell}_a, \hat{U}\right] = -T_a \hat{U}\ , \qquad \left[\hat{r}_a, \hat{U}\right] = \hat{U} T_a$

The Hilbert space: the link operators are coordinates in the gauge group, the ℓ_a, r_a operators are their conjugates

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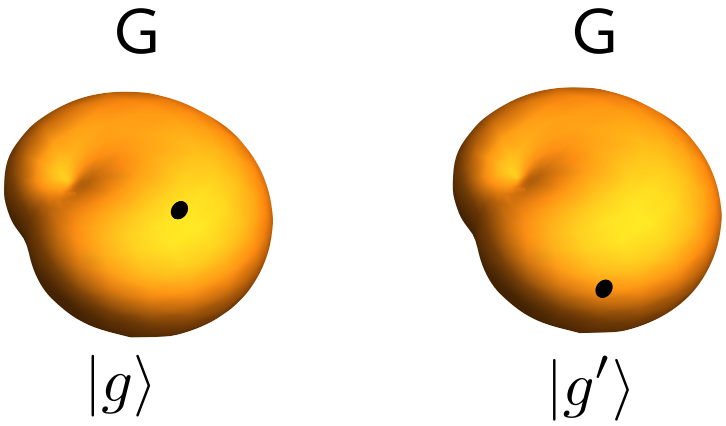
"coordinate" basis:

$$\langle g|g'\rangle = \delta(g-g')\,, \qquad \int dg\,|g\rangle\langle g| = \mathbf{1}$$



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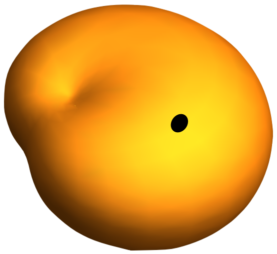
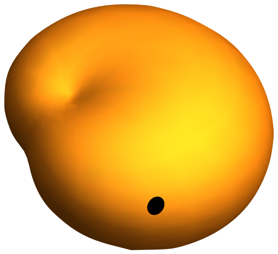
G



$|g\rangle$

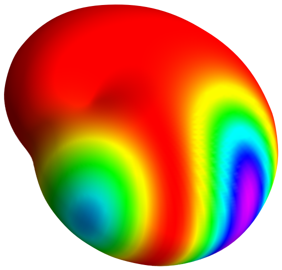
G



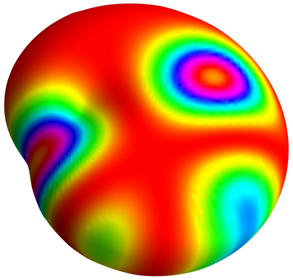
$|g'\rangle$

“momentum” basis:

$$\langle Rab|R'a'b'\rangle = \delta_{RR'}\delta_{aa'}\delta_{bb'}\ , \qquad \sum_{Rab} |Rab\rangle\langle Rab| = \mathbf{1}$$



$|Rab\rangle$



$|R'\,a'\,b'\rangle$

$$\langle Rab|g\rangle \equiv \sqrt{\frac{d_R}{|G|}}\,D^{(R)}_{ab}(g)$$

Irreducible representations of G

The Hilbert space: the link operators are coordinates in the gauge group, the ℓ_a, r_a operators are their conjugates

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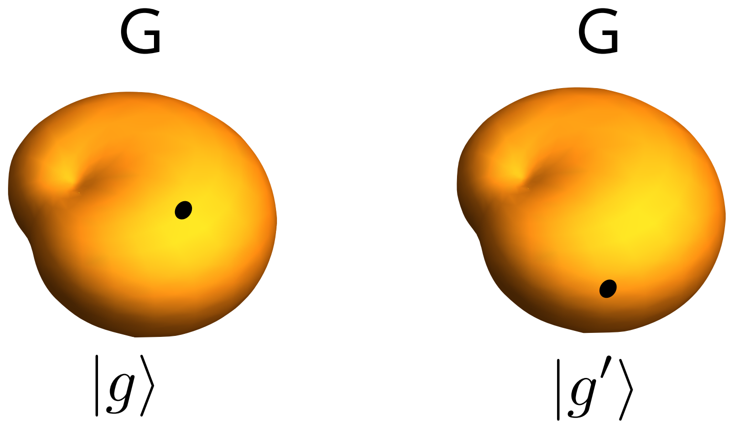

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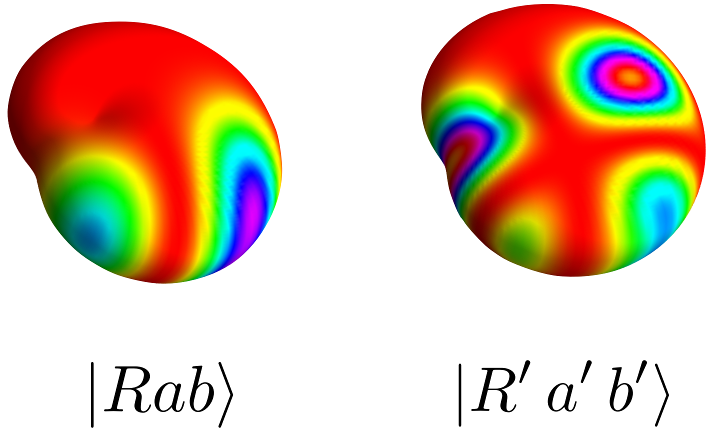

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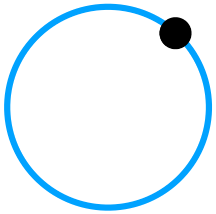
Irreducible representations of G

A Formulation of Lattice Gauge Theories for Quantum Simulations

*Erez Zohar and Michele Burrello, Phys. Rev. D **91**, 054506*

E.g. U(1): particle on a circle



$$|g\rangle \to |\phi\rangle \ , \qquad \phi \in [0, 2\pi)$$

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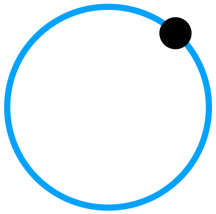

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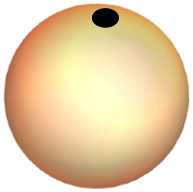
E.g. SU(2): particle on a 3-sphere



$$|g\rangle \to |\vec{\theta}\rangle$$

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(Wigner d-matrices)

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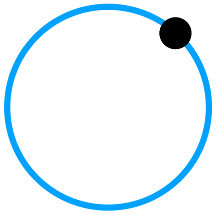

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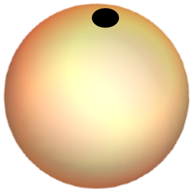

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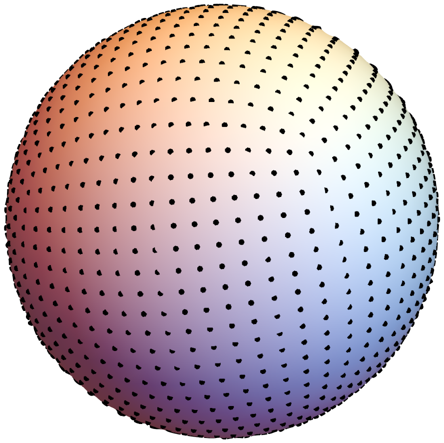
(Wigner d-matrices)

Even with spatial lattice, we have an infinite-dimension Hilbert space:

- The |g> states take continuous values
- The |Rab> states are discrete, but there are ∞ of them

“Latticize” G?



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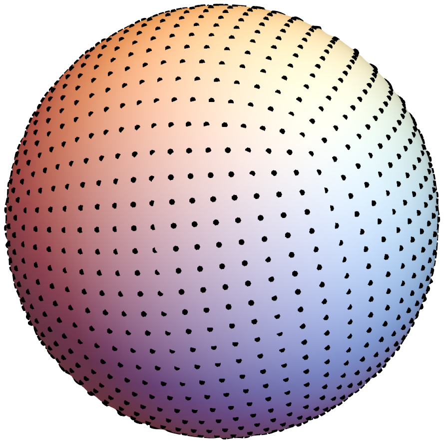

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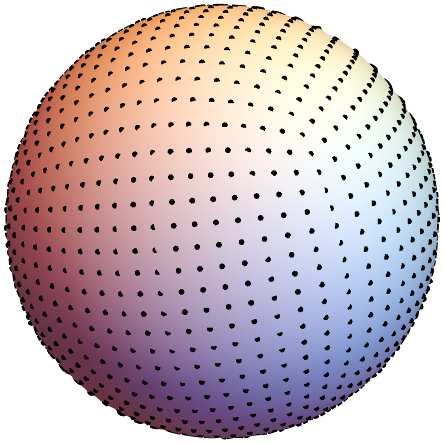

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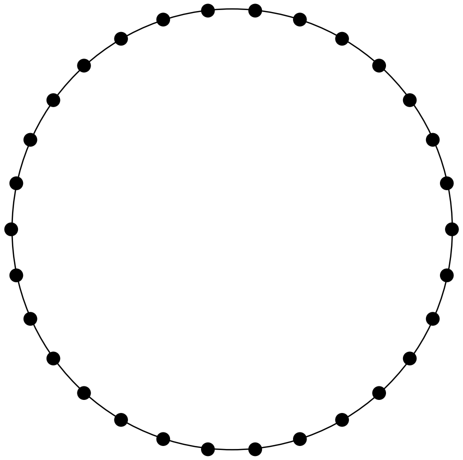
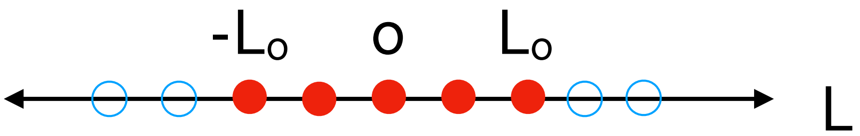


…. except for $Z_N \in U(1)$

Cutoff on |Rab> states (canonical momentum cutoff)?

E.g. U(1), cutoff on L



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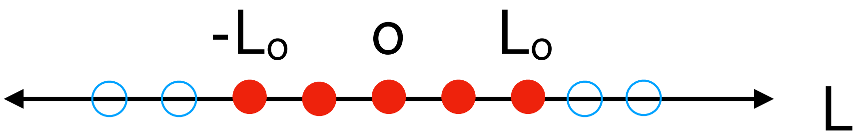
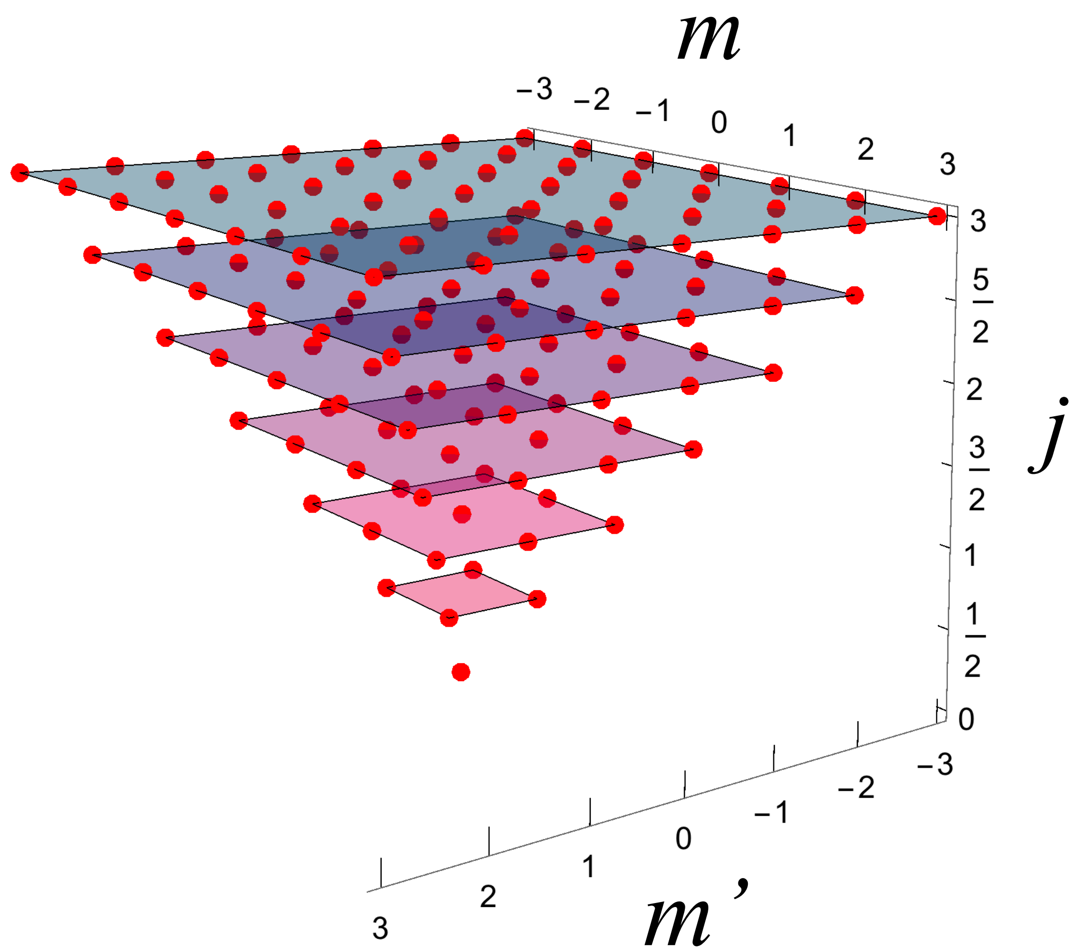


E.g. SU(2), cutoff on j:



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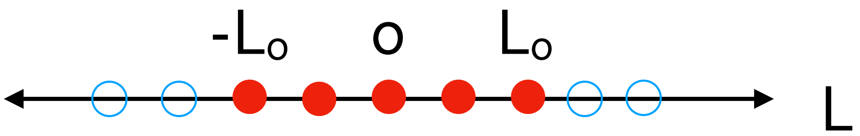

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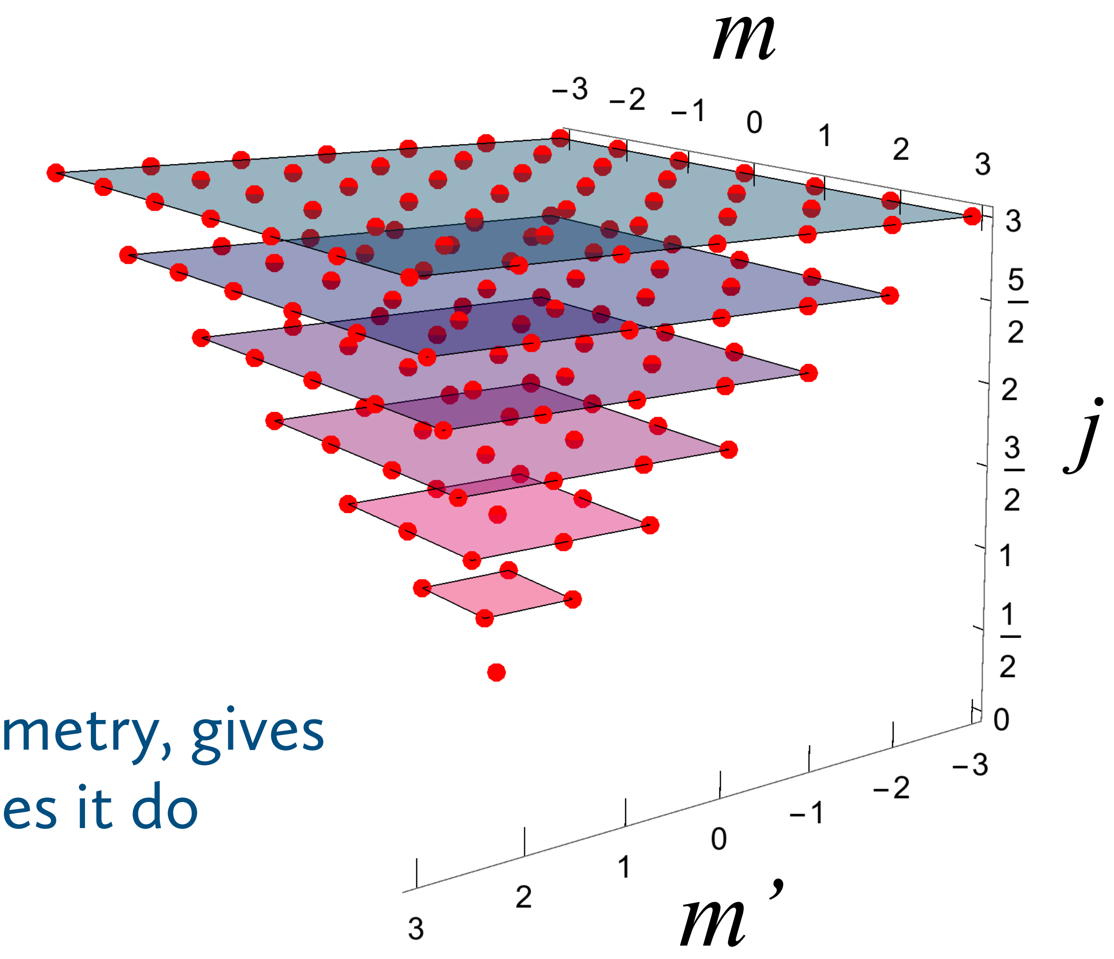

This cutoff maintains gauge symmetry, gives finite Hilbert space, but what does it do to the physics? Open question

Nevertheless, toy models on small lattices with low cutoffs can be interesting in their own right, and perhaps feasible in near-term

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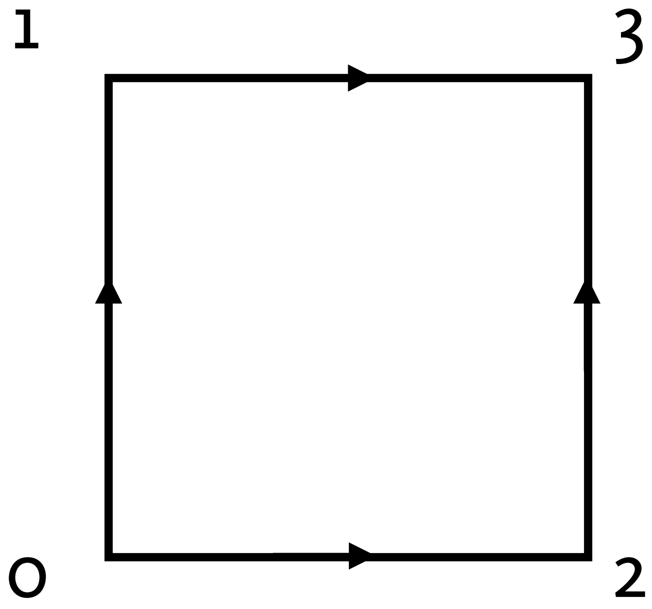
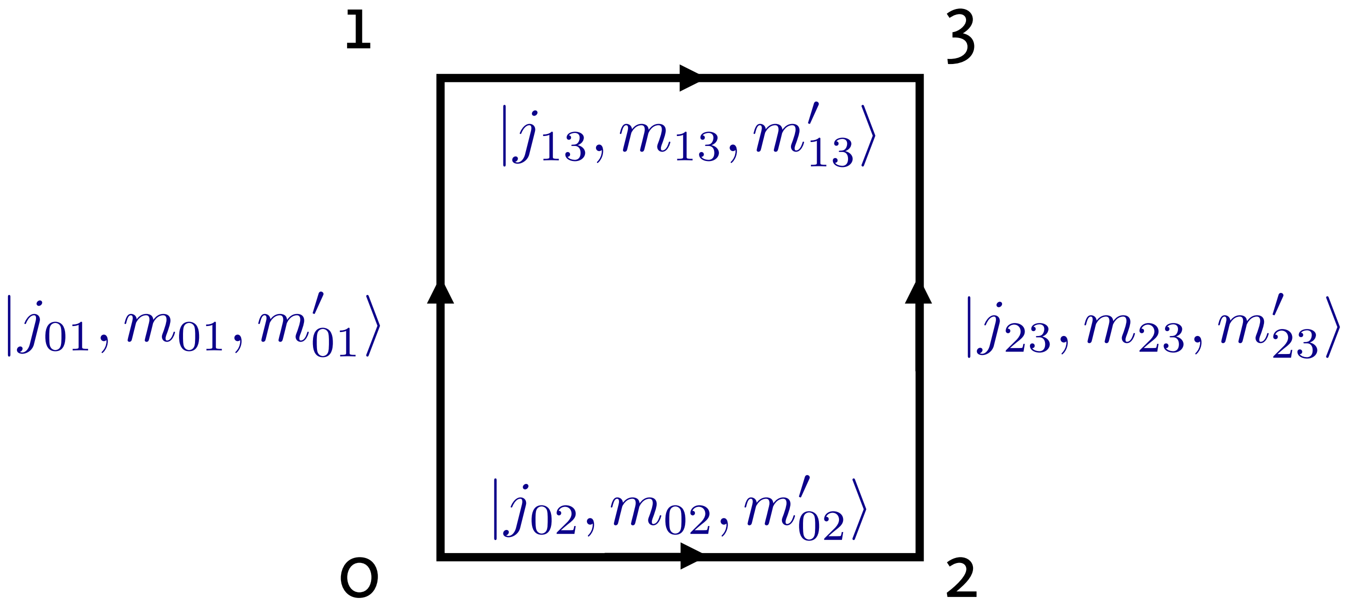
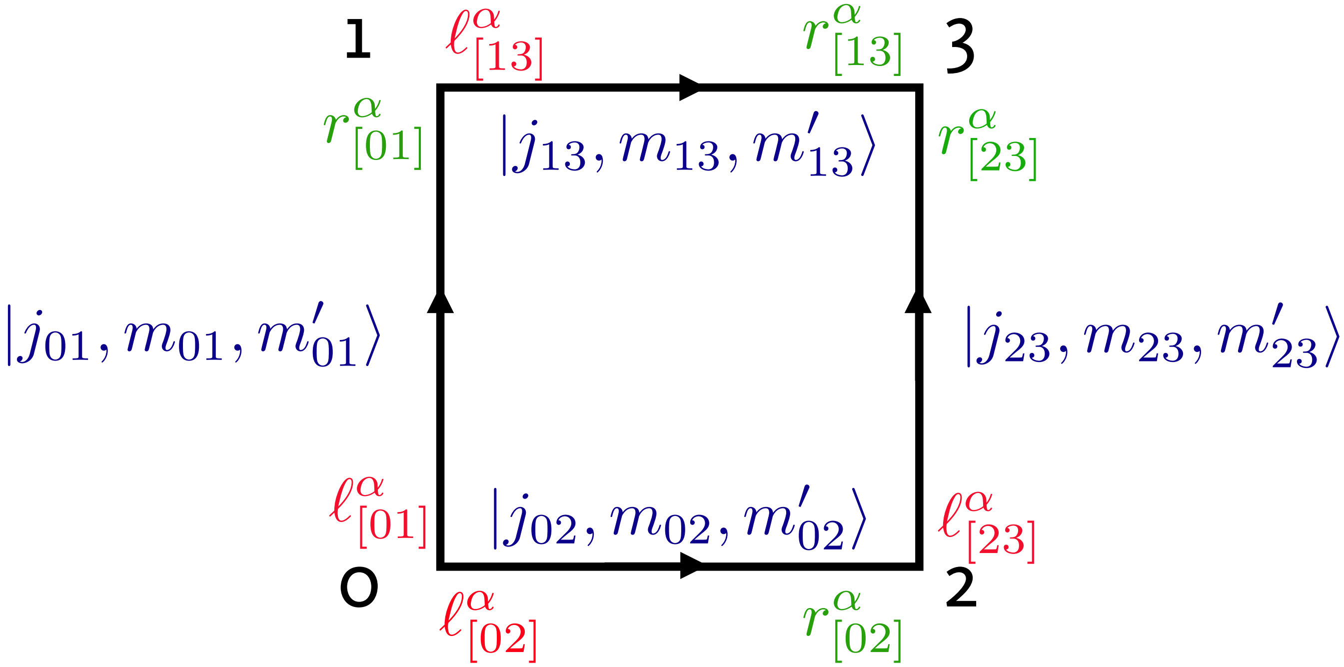
Example: “glueballs” in SU(2), 2+1 dimensions, four lattice sites.

minimal:

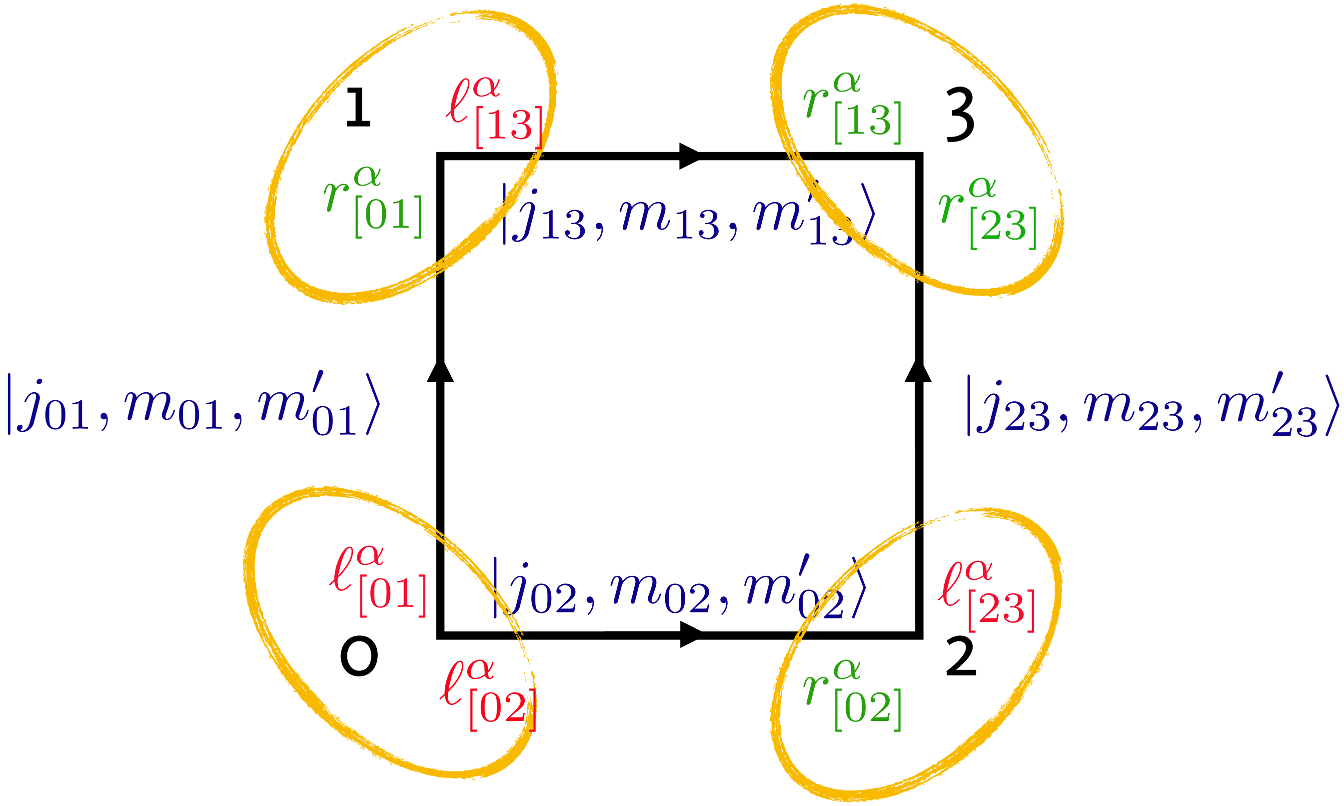
- no glueballs in 1+1 dimensions
- no qlueballs in 2+1 with less than 1 plaquette


1
3
0
2

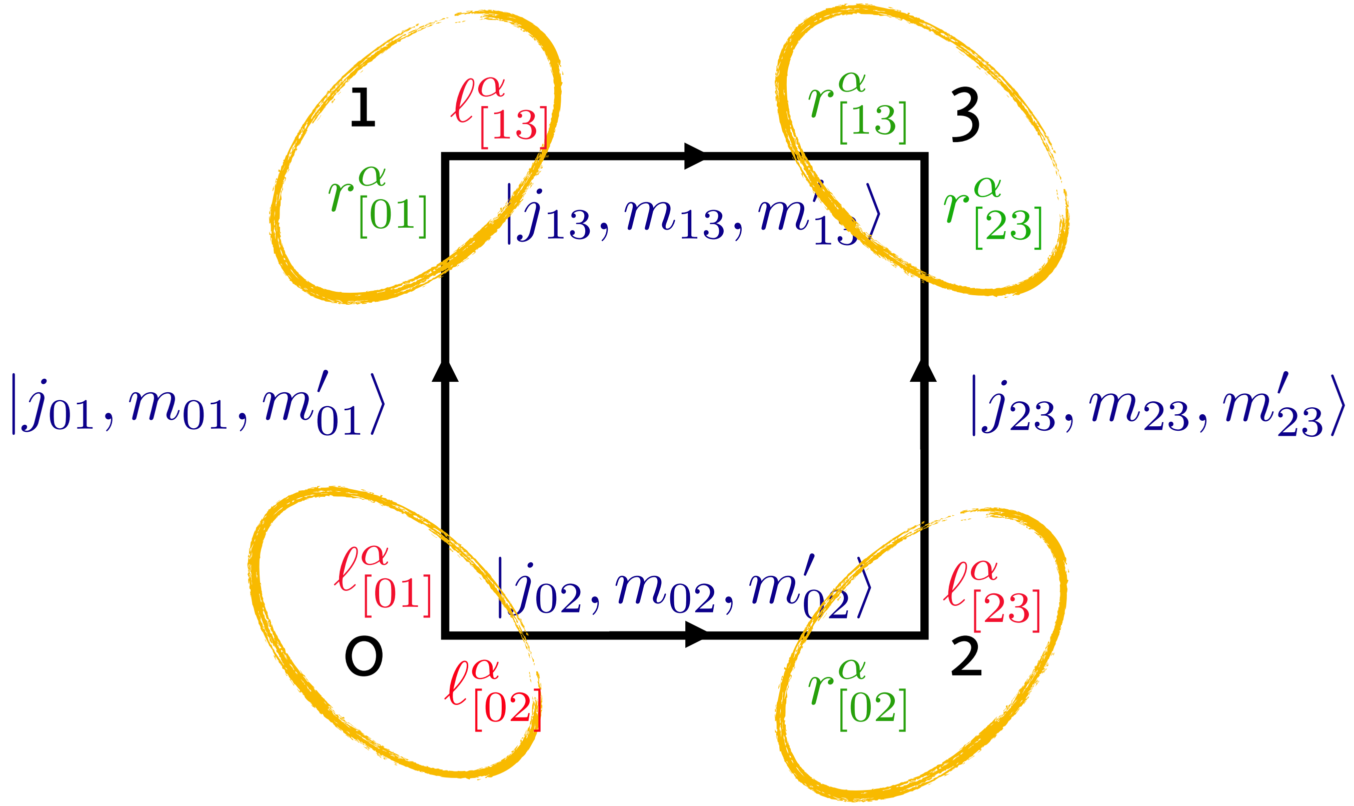

1
3
$|j_{13}, m_{13}, m'_{13}\rangle$
$|j_{01}, m_{01}, m'_{01}\rangle$
$|j_{23}, m_{23}, m'_{23}\rangle$
$|j_{02}, m_{02}, m'_{02}\rangle$
0
2



$$\ell^\alpha, r^\alpha \in \mathfrak{su}(2)$$



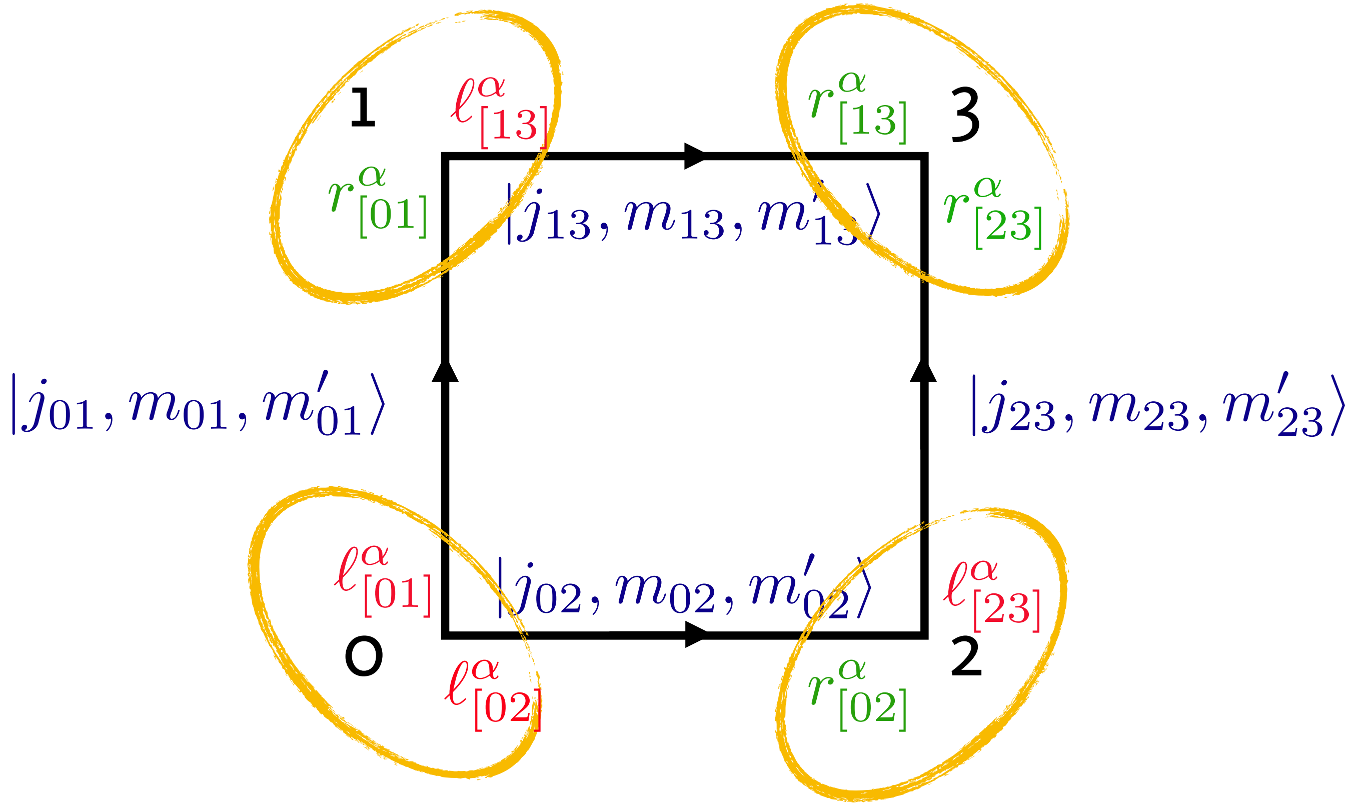
Gauge invariance constraint at each vertex $\ell^{\alpha}, r^{\alpha} \in \mathfrak{su}(2)$



Gauge invariance constraint at each vertex $\ell^\alpha, r^\alpha \in \mathfrak{su}(2)$

general state:

$$|\psi\rangle = |j_{01}, m_{01}, m'_{01}\rangle|j_{13}, m_{13}, m'_{13}\rangle|j_{23}, m_{23}, m'_{23}\rangle|j_{02}, m_{02}, m'_{02}\rangle$$



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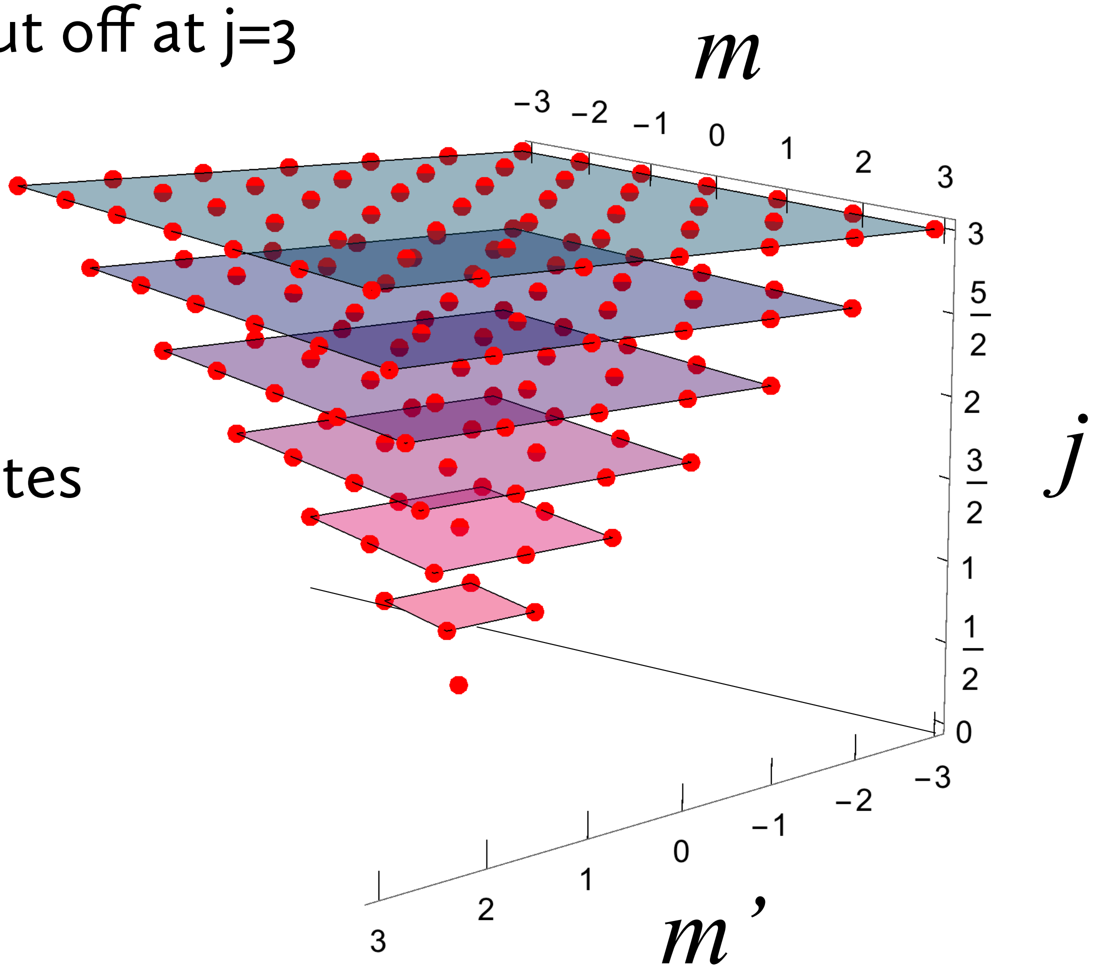
gauge invariant state:

$$|\mathcal{J}\rangle = \frac{1}{(2j+1)^2} \sum_{m_i=-j}^{j} (-1)^{-(m_0+m_3)} |j, m_0, m_1\rangle_{[01]} |j, -m_0, m_2\rangle_{[02]} |j, m_1, m_3\rangle_{[13]} |j, m_2, -m_3\rangle_{[23]}$$

SU(2) Hilbert space for one link, cut off at j=3



140 states

Hilbert space dimension for L links, cutoff J:

$$\left[\sum_{j=0}^{J}(2j+1)^2\right]^L = \left[\frac{(1+J)(1+2J)(3+4J)}{3}\right]^L$$

4-link SU(2) model:

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dimension of Hilbert space with cutoff J:

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gauge invariant state:

Same j on all links; all m's summed

$$|\psi_j\rangle = \frac{1}{(2j+1)^2}\sum_{m_i=-j}^{j}(-1)^{-(m_0+m_3)}|j, m_0, m_1\rangle_{[01]}|j, -m_0, m_2\rangle_{[02]}|j, m_1, m_3\rangle_{[13]}|j, m_2, -m_3\rangle_{[23]}$$

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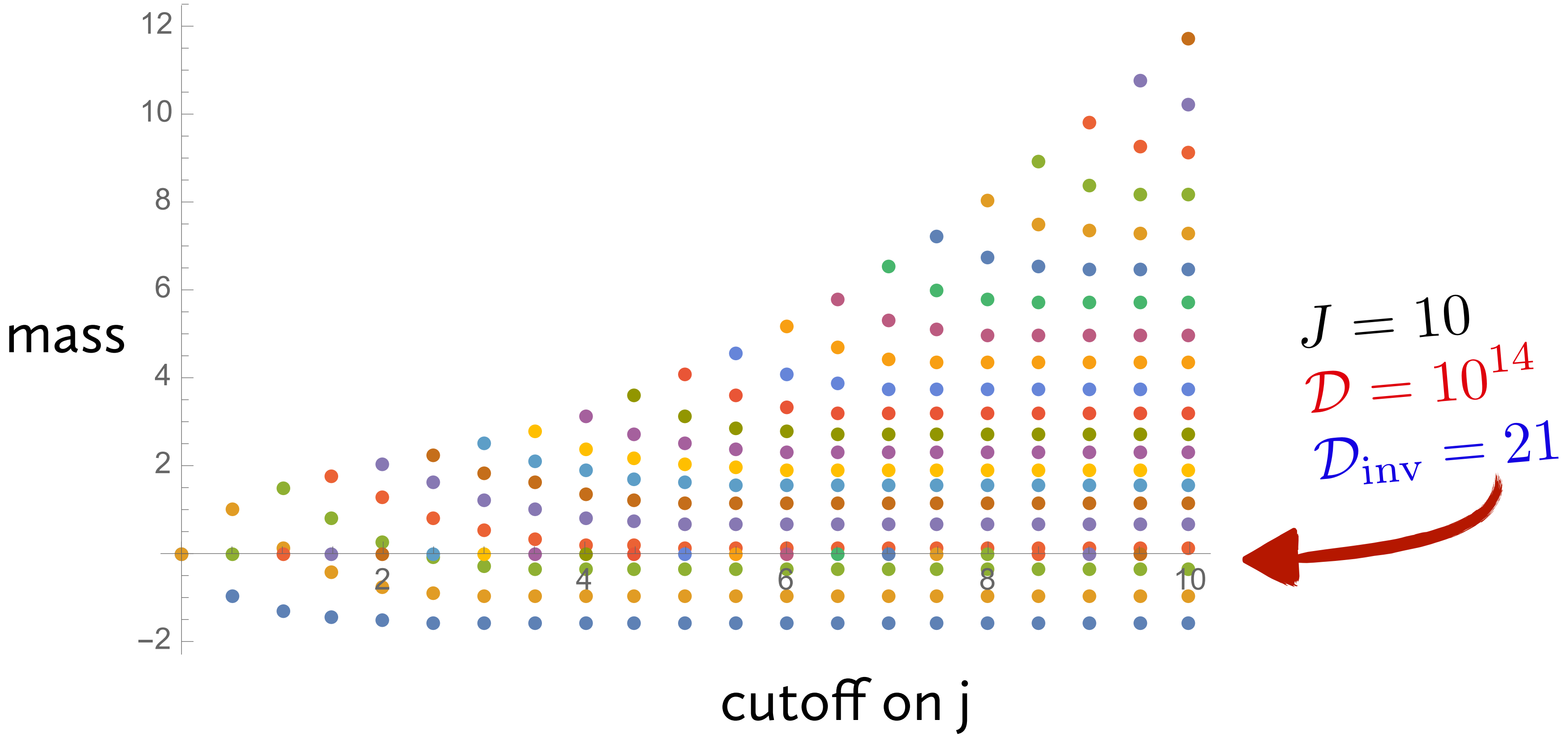
dimension of gauge invariant subspace with cutoff J:

$$\mathcal{D}_{\mathrm{inv}} = 2J+1$$

e.g.: J=3: $\mathcal{D} = 384,160,000$ $\mathcal{D}_{\mathrm{inv}} = 7$

≥ 29 qubits ≥ 3 qubits

The SU(2) glue ball spectrum can be calculated quickly (Mathematica) for this simple system (because gauge invariance can be imposed analytically):



$J = 10$
$\mathcal{D} = 10^{14}$
$\mathcal{D}_{\text{inv}} = 21$

For low cutoff, can this be simulated on an existing quantum computer? Stay tuned.

Major challenges faced in order to do a QCD simulation omg a quantum computer:

Engineering:

Need lots of good qubits, fast gate operations

Qubits will be noisy: need error correction
(~1000 physical qubits for 1 logical qubit?)

Physics:

★ Need a good way to input initial state with overlap with ground state!

.... and lots of other theoretical and algorithmic advances.

Quantum Adiabatic Algorithm:

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

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

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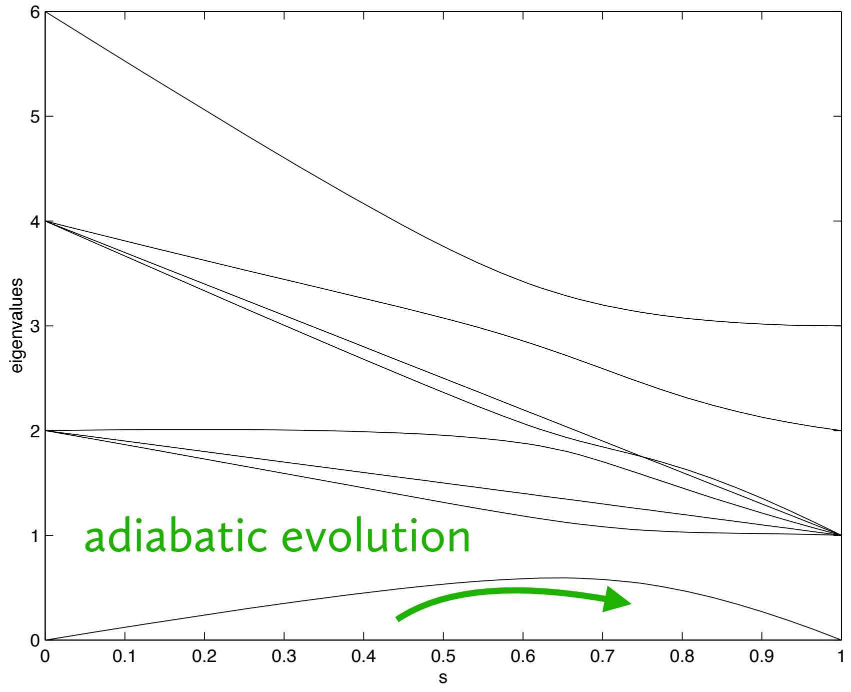
interesting Hamiltonian

- 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

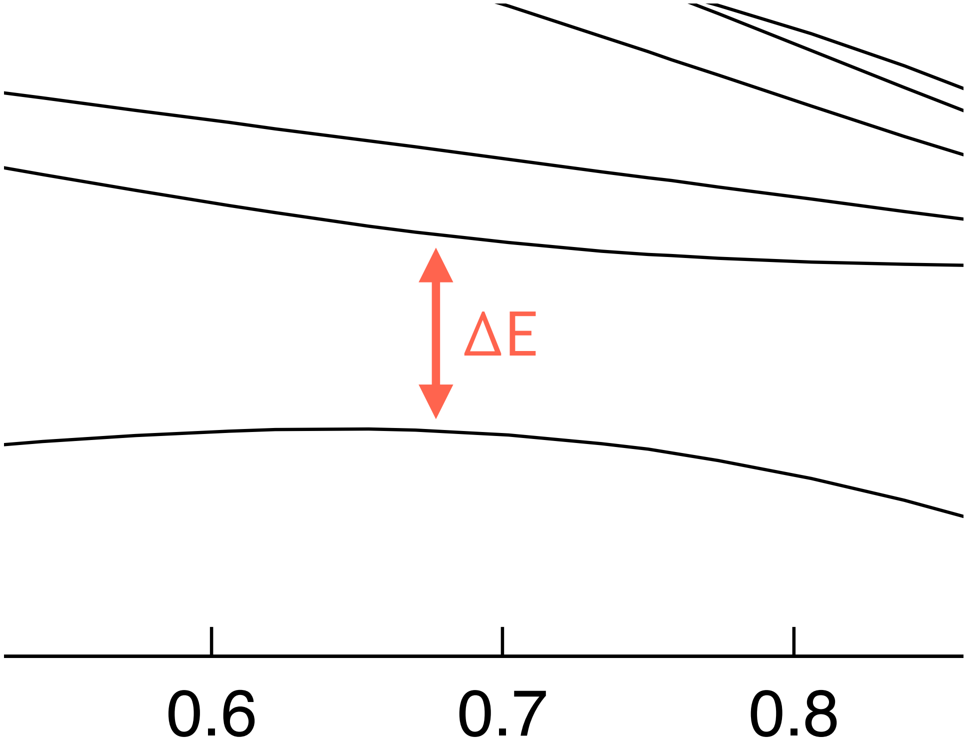


Edward Farhi, Jeffrey Goldstone, Sam Gutmann, Michael **arXiv:quant-ph/0001106**

Drawback of the Quantum Adiabatic Algorithm:

Adiabatic theorem requires evolution time scales as

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



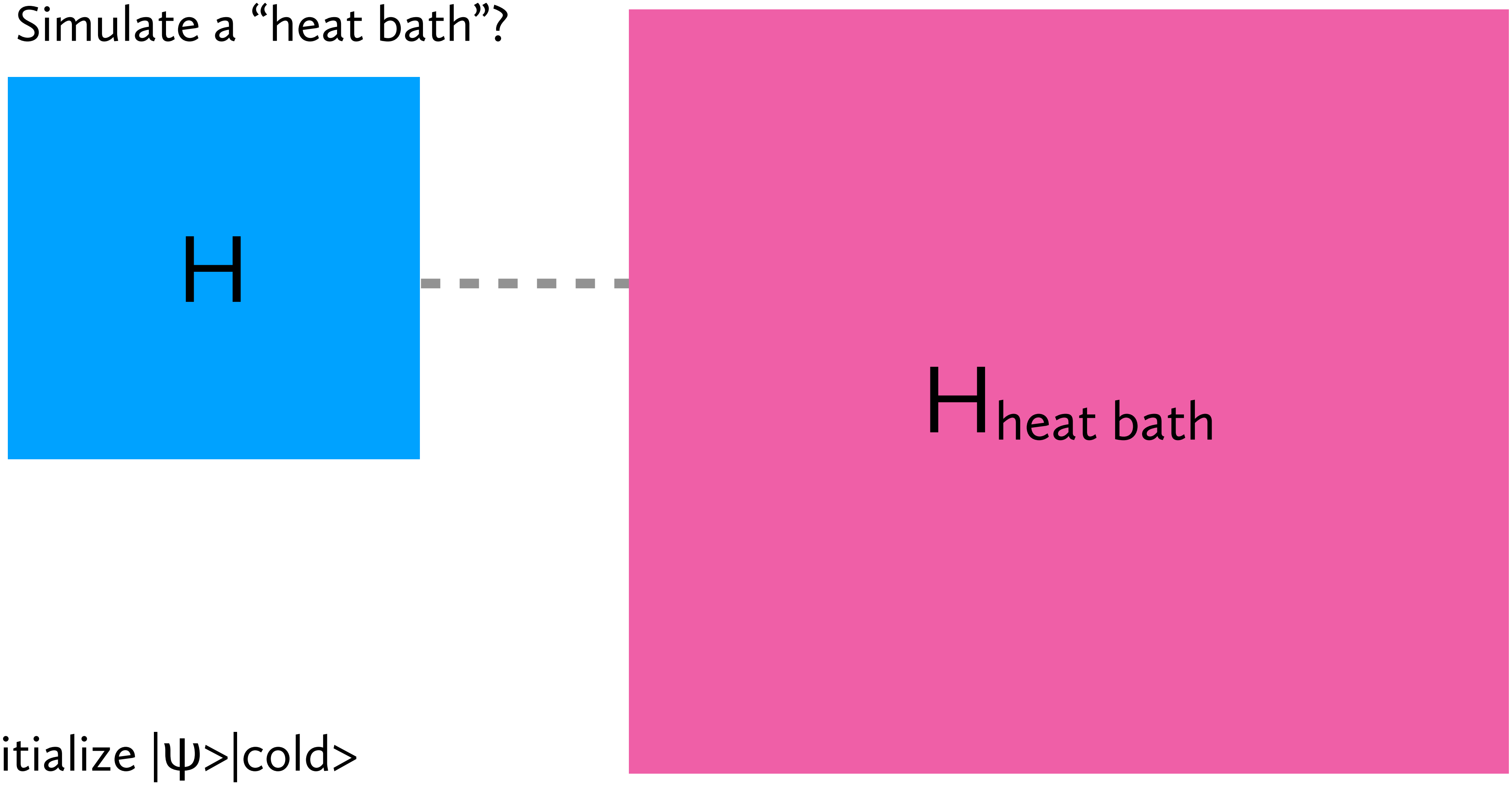
Exponentially slow if there exists exponentially small gap (e.g. in 1st order phase transition)

Maybe OK to start with strong coupling vacuum of LQCD and evolve to weak?

Another possible algorithm: “Spectral Combing”

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

Simulate a “heat bath”?

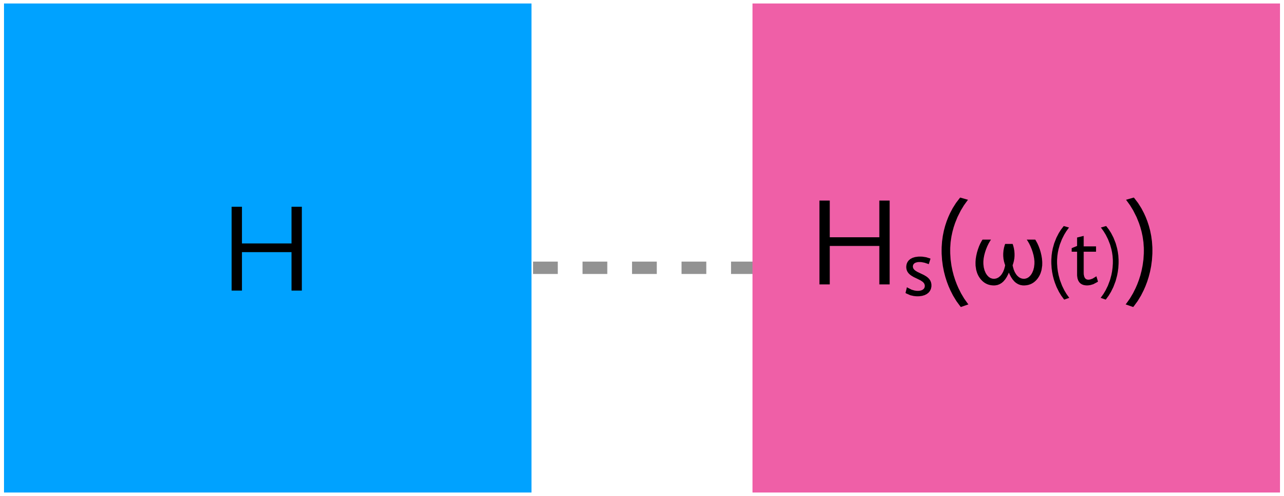


Initialize $|\psi>|\mathrm{cold}>$

Evolves unitarily to entangled state ~ $|\psi_0>|\mathrm{warm}>$

Or, to reduce number of qubits:

Spectral combing:



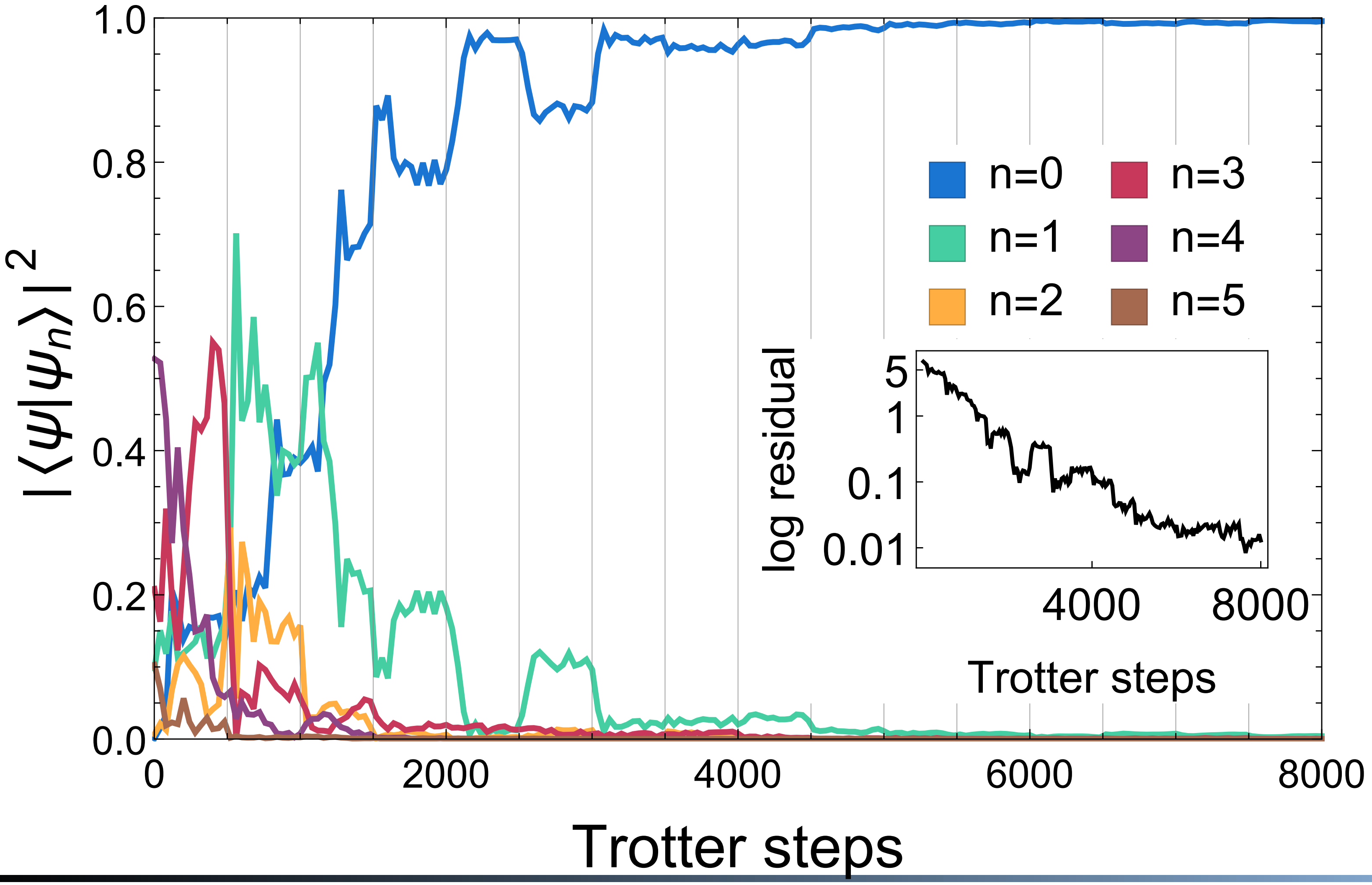
H

$H_s(\omega(t))$

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

Does it work?

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



Conclusions:

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

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In the meantime, lots of fun things for field theorists to think about…