Quantum computing, the Bell inequalities, and qubit entropy

Katharine L. C. Hunt
Department of Chemistry, Michigan State University
Institute for Advanced Studies, Department of Physics and Materials Science, University of Luxembourg

Public Talk, November 16, 2023

INSTITUTE FOR ADVANCED STUDIES (IAS)

Qubits: The Basic Units of Quantum Computers

In a digital computer, each bit has only one of two values, 0 or 1.

In a quantum computer, each bit has a superposition of values. The representation of the bit is a linear combination,

$$| \Psi \rangle = c_0 | 0 \rangle + c_1 | 1 \rangle$$

Both c_0 and c_1 are complex numbers, with the restriction

$$\langle \Psi | \Psi \rangle = c_0^* c_0 + c_1^* c_1 = 1$$

When a qubit state is measured, the probability that the outcome will be 0 is $c_0^* c_0$ and the probability that the outcome will be 1 is $c_1^* c_1$. But these are only probabilities.

Quantum Logic Gates

Operator	Gate(s)	Matrix
Pauli-X (X)	X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H	$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S	$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T	$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)		$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$

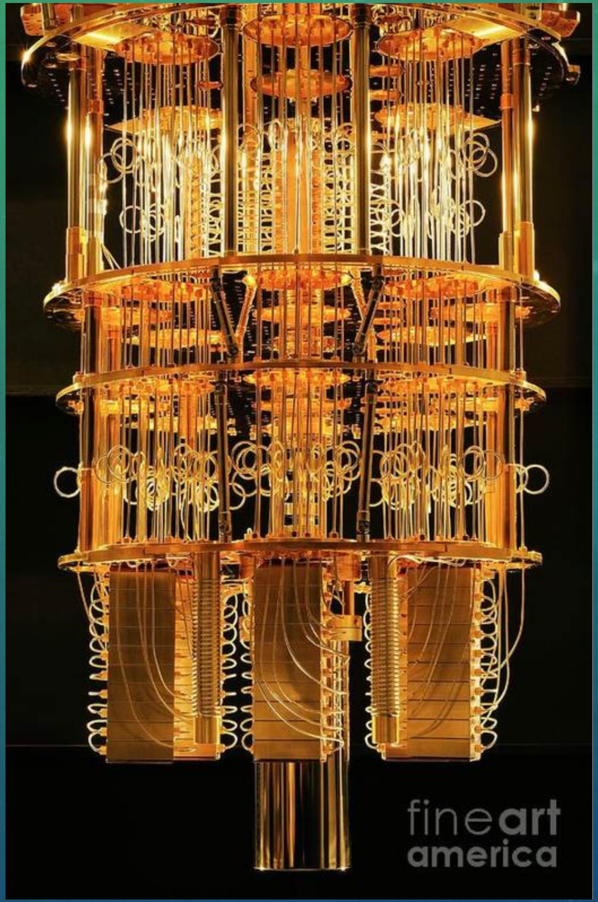
Quantum computers rely on quantum logic gates, which change the states of the qubits in ways that are analogous to digital computer gates. But there is a difference! A "Not" gate on a digital computer changes 0 to 1 and 1 to 0. On a quantum computer, a "Not" gate must be a matrix. It takes the state

$$|\Psi\rangle = c_0 |0\rangle + c_1 |1\rangle$$

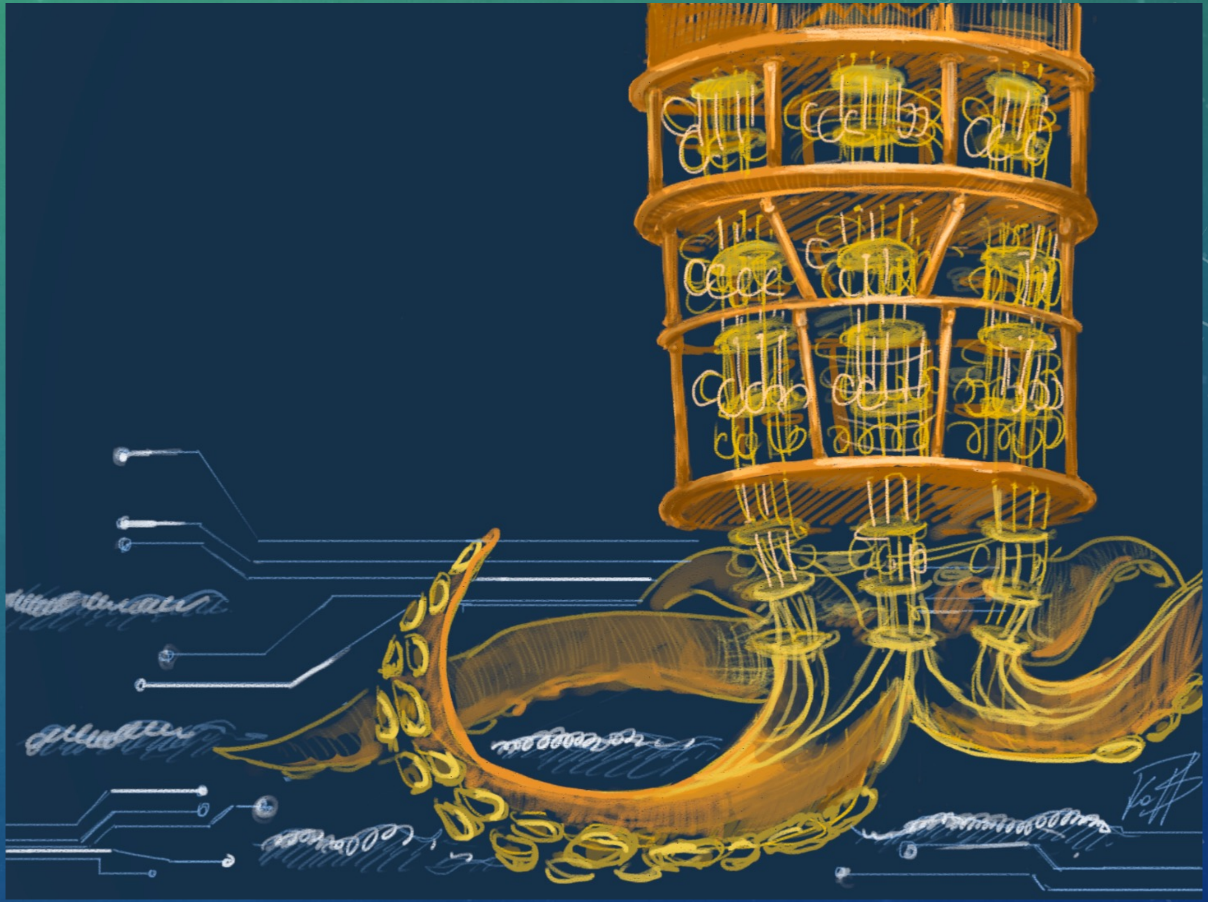
and converts it into the state

$$|\Psi\rangle = c_0 |1\rangle + c_1 |0\rangle$$

A Quantum Computer



IBM Quantum Computer,
photo by fine art america



Artist's representation by Victoria Kozlova,
in *Kinesis Magazine*, February 27, 2020

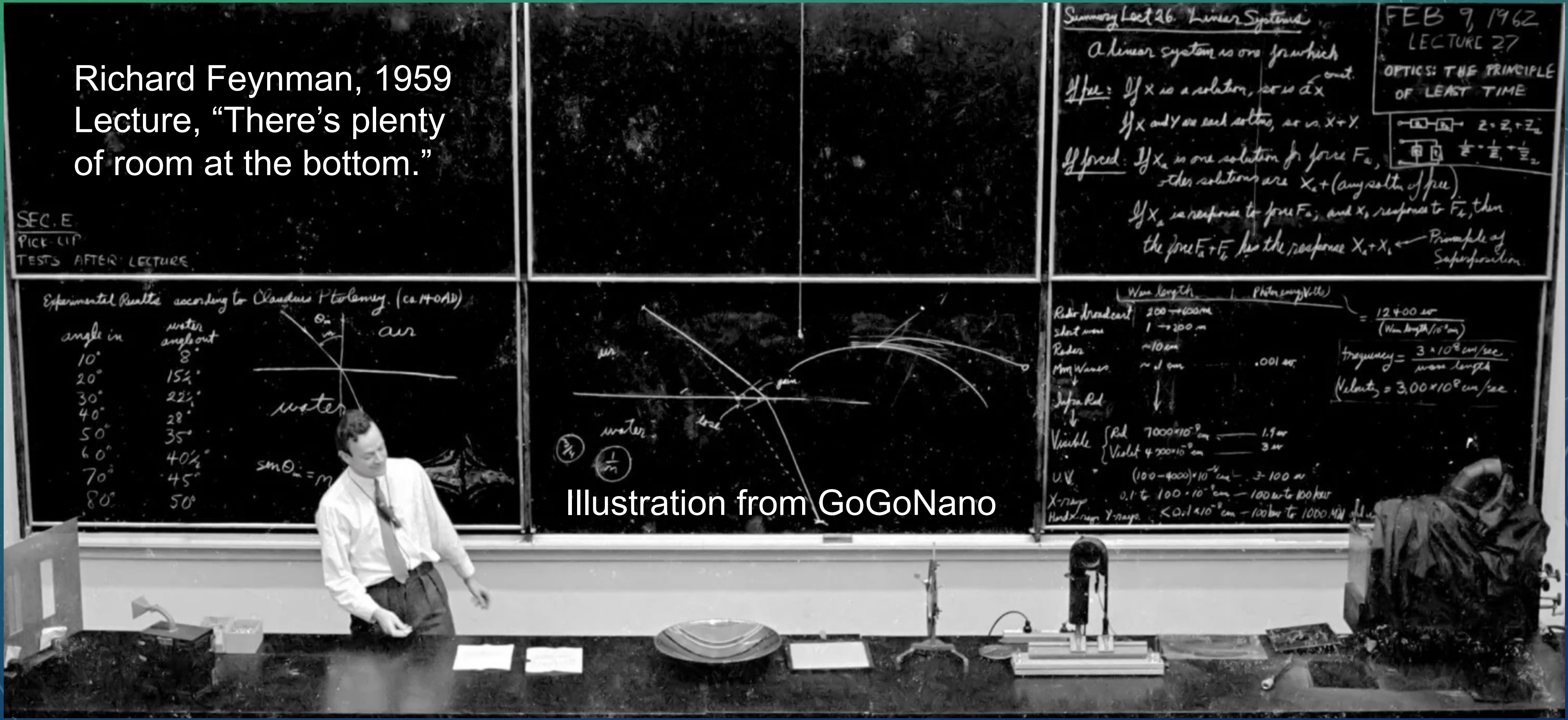
On the Human Scale

Qubits: Aluminum and niobium;
Refrigeration: brass piping plated with gold;
Wiring: copper

Coin Desk/Markets, accompanying an article by Christine Kim

This computer could not run as shown. The operating temperature of IBM's quantum computers is 0.015 K, about 200 times colder than outer space. D-Wave's quantum computer runs at ~0.025 K. Some quantum computers can run at room temperature: e.g., quantum computers based on the polarization state of photons, ion traps, or nitrogen vacancy centers in diamond. High vacuum may be required.

1981: Richard Feynman, “Nature isn't classical . . . if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”



Richard Feynman, 1959 Lecture, “There’s plenty of room at the bottom.”

Illustration from GoGoNano

The possibility of quantum primacy was first established by David Deutsch and Richard Jozsa in their 1992 paper, "Rapid solution of problems by quantum computation," *Proc. Roy. Soc. London, Ser. A* **439**, 553. Deutsch had discussed quantum computing earlier in *Proc. Roy. Soc. London, Ser A* **400** 97 (1985).

David Deutsch, Photo from the Financial Times, ©Robert Wallis/Corbis/Getty

IBM teleportation group, Photo André Berthiaume

Google's claim to "Quantum Supremacy"


NEWSLETTERS
Sign up to read our regular email newsletters

NewScientist

News Podcasts Video Technology Space Physics Health More Shop Courses Events

It's official: Google has achieved quantum supremacy

PHYSICS 23 October 2019

By Daniel Cossins

Claims and counter-claims

Google: 54-bit quantum computer, random sampling calculation took 3 minutes, 20 seconds

Google claimed that this would take 10,000 years on a classical computer

IBM: No, this can be done on a classical computer in 2.5 days

Google: 2020 in *Science*, Hartree-Fock calculations on 12 hydrogen atoms,12 qubits; also cis-trans isomerization of diazene, N_2H_2

Many quantum chemists: A laptop can do that.

Google: 2022 in *Nature*, quantum Monte Carlo calculations on N_2 and C_2

Quantum supremacy? Quantum Advantage? Quantum Primacy?

Can a quantum computer solve a problem that no classical digital computer can solve, in any realistic amount of time?

The requirements are not very stringent, though.
The quantum computer need not perform any useful task!
The quantum computer need not have high-quality error correction!

Why the concern about a quantum computer? Why the tentacles?
Much computer encryption relies on large composite numbers that are difficult to factorize. Shor's algorithm permits factorization.
Potentially at risk: Credit card transactions, bank transactions, security
"Quantum computing could break bitcoin."

Coin Desk/Markets, accompanying an article by Christine Kim

What integers has it been possible to factor so far with quantum computers?

- 15 was factored using Shor's algorithm with seven spin-1/2 qubits manipulated with nuclear magnetic resonance methods at room temperature, by L. M. K. Vandersypen, M. Steffen, G. Breyta, C. S. Yannoni, M. H. Sherwood, and I. L. Chuang, *Nature* **414**, 883 (2001).
- 21 has been *reliably* factored by E. Martín-López, A. Laing, T. Lawson, R. Alvarez, X.-Q. Zhou, and J. L. O'Brien, *Nature Photonics* **6**, 773 (2012).
- M. Amico, Z. H. Saleem, and M. Kumph factored 15, 21, and 35 using the IBM Q Experience, *Phys. Rev. A* **100**, 012305 (2019).
- My students factored 39 using a modified version of Shor's algorithm suggested in IBM's qiskit documentation (2020), on their quantum simulator.

Is there a problem?

RSA-768 232 decimal digits!

RSA-768 = 1230186684530117755130494958384962720772853569595334792197322452151726400507263657518745202199786469389956474942774063845925192557326303453731548268507917026122142913461670429214311602221240479274737794080665351419597459856902143413

= 33478071698956898786044169848212690817704794983713768568912431388982883793878002287614711652531743087737814467999489 × 36746043666799590428244633799627952632279158164343087642676032283815739666511279233373417143396810270092798736308917

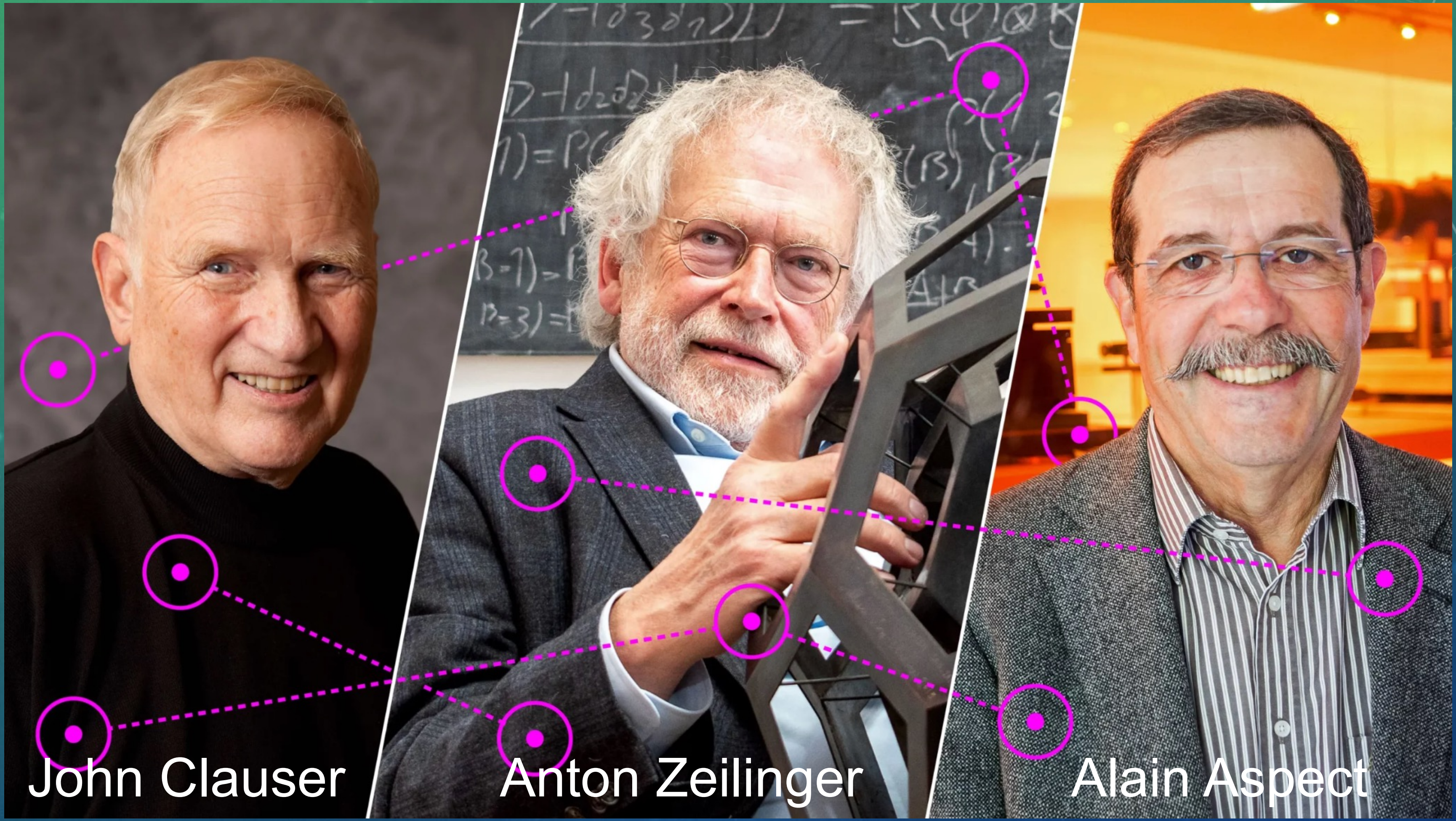
The base a used was

a = 1029031793302493258003488818376905875264575120178567995715921117383374063780955476265714655965556097487715509708453134212472071241551710737667646125017671995537319749739035045343586527599466828935082557618400047627481255809299529939

RSA-768 was factored over a span of 2 years by the 13-person team of Thorsten Kleinjung *et al*. J. A. Smolin, G. Smith, and A. Vargo, *Nature* **499**, 163 (2013) also factored RSA-768 on a classical computer. They observed that the reported factorizations of large numbers on quantum computers required pre-processing on classical computers. “It is not legitimate for the compiler to know the answer to the problem being solved.”

RSA-250 with 250 decimal digits has been factored, but not RSA-260 (Wikipedia).

The 2022 Nobel Prize in Physics



Photos from *Quanta Magazine*, John Clauser, Jacqueline Godany, and Ecole Polytechnique Université Paris-Saclay

The Bell Inequalities

These are inequalities that are obeyed by all classical objects, but not by all quantum mechanical observables

The implications are profound: Violations of the Bell inequalities show that no “hidden variable” theory can be consistent with observations, unless it also allows for transmission of information faster than the speed of light.

J. S. Bell, *Physics, Physique, Fizika* **1**, 195 (1964).

N. Brunner, D. Cavalcanti, S. Pironio, V. Scarani, and S. Wehner, in *Rev. Mod. Phys*. **86**, 419 (2014), have remarked that Bell's theorem "arguably ranks among the most profound scientific discoveries ever made."

Violation of the Bell inequalities was first confirmed experimentally by S. L. Freedman and J. F. Clauser, *Phys. Rev. Lett*. **29**, 938 (1972), in studies of the polarization of entangled photons created in atomic cascades.

The Essence of Entanglement

If two spins are totally paired up/down, designated as α/β, the quantum wave function is

$$| \Psi \rangle = (1/2)^{1/2} [| \alpha(1) \beta(2) \rangle - | \beta(1) \alpha(2) \rangle,$$

They are entangled. The outcomes of spin projection measurements would be opposite, no matter how far apart they are.

The wave function cannot be factored into a product of a wave function for System 1 and a wave function for System 2

Spooky action at a distance?

A. Einstein, B. Podolsky and N. Rosen, *Phys. Rev*. **47**, 777 (1935). Illustration by David Castelvecchi, *Nature News* 01/16/20

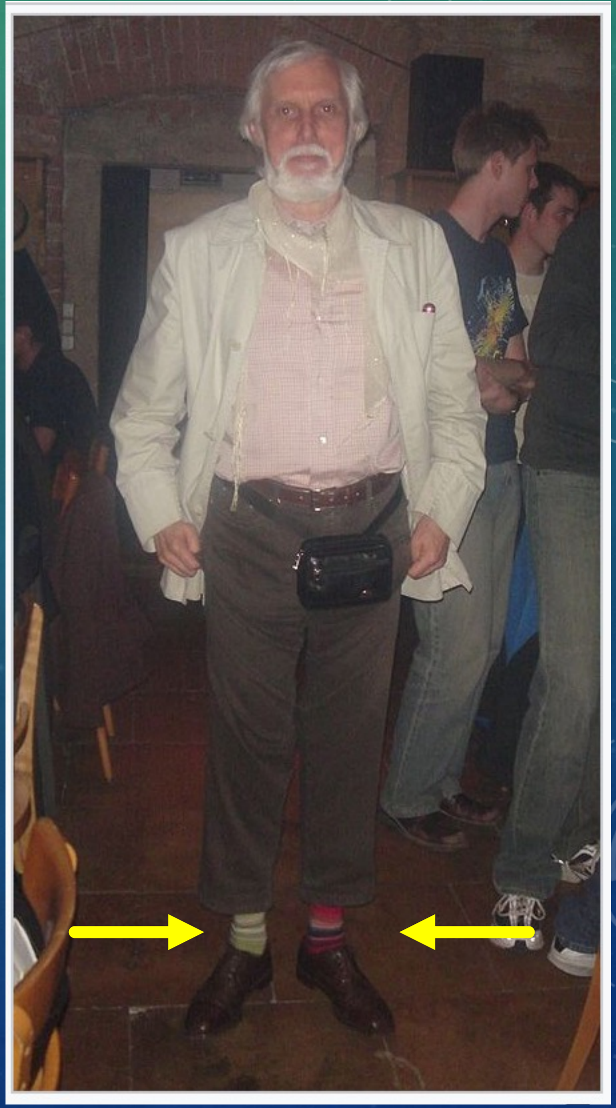
Measure the spin projection of one of the entangled particles along an arbitrary axis. The other will immediately be found to have the same spin projection along that axis, regardless of their separation.

Does the behavior of entangled objects differ from the classical behavior of correlated objects?

Isn't this just like Bertlmann's socks?

They were always mismatched. So, if you saw one of Bertlmann's feet coming in the door, you knew that the other sock was opposite!

J. S. Bell, "Bertlmann's socks and the nature of reality," *J. Phys. Colloq*. **42**, (1981) provides the answer: No, it is not!
Next—how do we see that?



Suppose that we have three axes or three properties, A, B, and C, and each has two possible values. Quantum mechanically, these might be the outcomes of measurements of the spin projections of a spin-1/2 particle, along each axis. The possible outcomes of measurement will be labeled either + or – for each of the axes.

Now, suppose that the objects actually “have” specific values for A, B, and C, and consider pairs of objects.

In that case, we could count the numbers with the characteristics A^+B^+ and call that $N(A^+B^+)$. Then

$$N(A^+B^+) = N(A^+B^+C^+) + N(A^+B^+C^-)$$

$$N(A^+B^+) = N(A^+B^+C^+) + N(A^+B^+C^-)$$

Now add $N(A^+B^-C^+)$ and $N(A^-B^+C^-)$ on the right.
Both of these are greater than or equal to zero.

Therefore,

$$N(A^+B^+) \leq \quad N(A^+B^+C^+) + N(A^+B^-C^+) \quad + \quad N(A^+B^+C^-) + N(A^-B^+C^-)$$

What are these numbers?

$$N(A^+B^+) = N(A^+B^+C^+) + N(A^+B^+C^-)$$

Now add $N(A^+B^-C^+)$ and $N(A^-B^+C^-)$ on the right.
Both of these are greater than or equal to zero.

Therefore,

$$N(A^+B^+) \leq \boxed{N(A^+B^+C^+) + N(A^+B^-C^+)} + \boxed{N(A^+B^+C^-) + N(A^-B^+C^-)}$$

What are these numbers?

$$N(A^+B^+) = N(A^+B^+C^+) + N(A^+B^+C^-)$$

Now add $N(A^+B^-C^+)$ and $N(A^-B^+C^-)$ on the right.
Both of these are greater than or equal to zero.

Therefore,

$$N(A^+B^+) \leq \boxed{N(A^+B^+C^+) + N(A^+B^-C^+)} + \boxed{N(A^+B^+C^-) + N(A^-B^+C^-)}$$

What are these numbers?

$$N(A^+B^+C^+) + N(A^+B^-C^+) = N(A^+C^+)$$

$$N(A^+B^+C^-) + N(A^-B^+C^-) = N(B^+C^-)$$

So

$$N(A^+B^+) \leq N(A^+C^+) + N(B^+C^-)$$

Violations of the Bell inequalities are well known

Over time, various experimental loopholes have been closed in work with spin-paired photons.

- Non-coincidence loophole
- Loss of paired objects loophole
- Lack of randomness loophole
- Unknown means of photon communication loophole*
- Clumsiness loophole!

Clever experimental test: A. Aspect, J. Dalibard, and G. Roger, *Phys. Rev. Lett*. **49**, 1804 (1982).

Experiment with spin-correlated photons

To prevent any possible communication between photons, the orientations of the polarizers are changed while the photons are in flight. No light signal can pass between the photons.

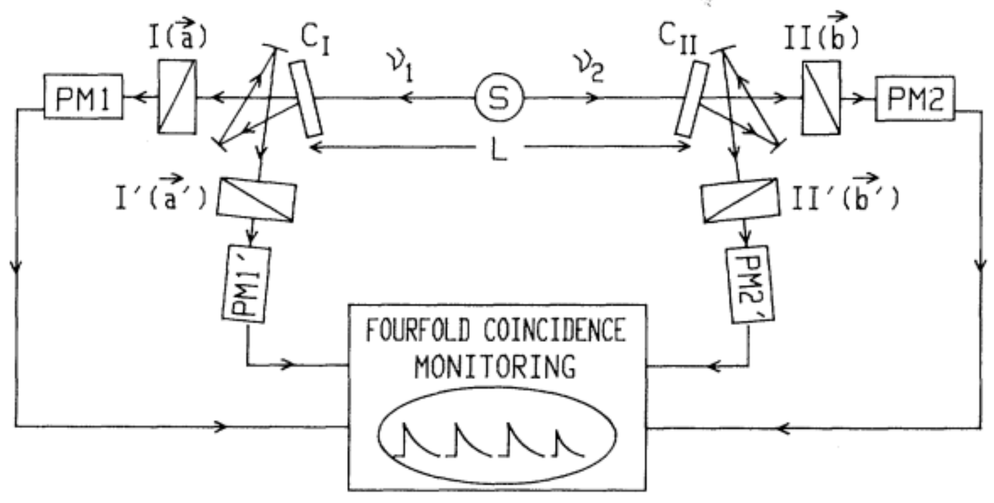


FIG. 2. Timing experiment with optical switches. Each switching device (C_I, C_{II}) is followed by two polarizers in two different orientations. Each combination is equivalent to a polarizer switched fast between two orientations.

Our question: Can violations of the Bell inequalities be seen on Noisy-intermediate scale quantum (NISQ) devices?

Suppose that a qubit really possesses specific spin projections along axes A, B, and C, but there are hidden variables. This was Einstein’s belief.

There is still a problem of measurement! The spin projection of a qubit can only be measured along one axis at a time.

How is it possible to get around this?
Take advantage of entanglement!

It is easy to create the entangled Bell state

$| \Psi \rangle = (1/2)^{1/2} [\, | \alpha(1)\, \alpha(2) \rangle + | \beta(1)\, \beta(2) \rangle$

Use the short quantum computer code:

```
h q[0];
cx q[0], q[1];
```

We need the probabilities

$p(A^+B^+)$, $p(A^+C^+)$, and $p(B^+C^-)$

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

Start with the state

$$| \Psi \rangle = (1/2)^{1/2} [\, | \alpha(1)\, \alpha(2) \rangle + | \beta(1)\, \beta(2) \rangle \,]$$

The qubits remain similarly entangled along any measurement axis.

For an axis rotated by θ in the x, z plane, the possible spin projections are $\hbar/2$ (for state r) or $-\hbar/2$ (for state s) along the new axis. We find

$$| \Psi \rangle = (1/2)^{1/2} [\, | r(1)\, r(2) \rangle + | s(1)\, s(2) \rangle$$

For spin-correlated qubits, measure the spin projection of one qubit along one axis, and measure the spin projection of another along a second axis.

The key observables are probabilities such as $p(A^+B^+)$, $p(A^+C^+)$, and $p(B^+C^-)$

Experience shows that the fault rates for production of qubit state $| 1 \rangle$ are higher than for qubit state $| 0 \rangle$. So, it reduces errors somewhat to look at $p(A^+B^+) + p(A^-B^-)$.

To test the Bell inequalities for spin-coupled qubits, we make spin projections pairwise along two of three coplanar axes A, B, and C, with an angle θ from A to B, θ' from B to C, and $\theta + \theta'$ from A to C.

We define Δ by

$$\Delta(\theta, \theta') = p(A^+B^+) + p(A^-B^-) - [\, p(A^+C^+) + p(A^-C^-) + p(B^+C^-) + p(B^-C^+) \,]$$

But there is a catch: The spin projections can only be measured along z in IBM's publicly accessible quantum computers!

How can we get around this catch?

We use a quantum correspondence relation!

Spin "up" along any axis means that the spin projection is $+\hbar/2$ along that axis.

The probability that the spin is "up" along z' *if* the spin is up along z

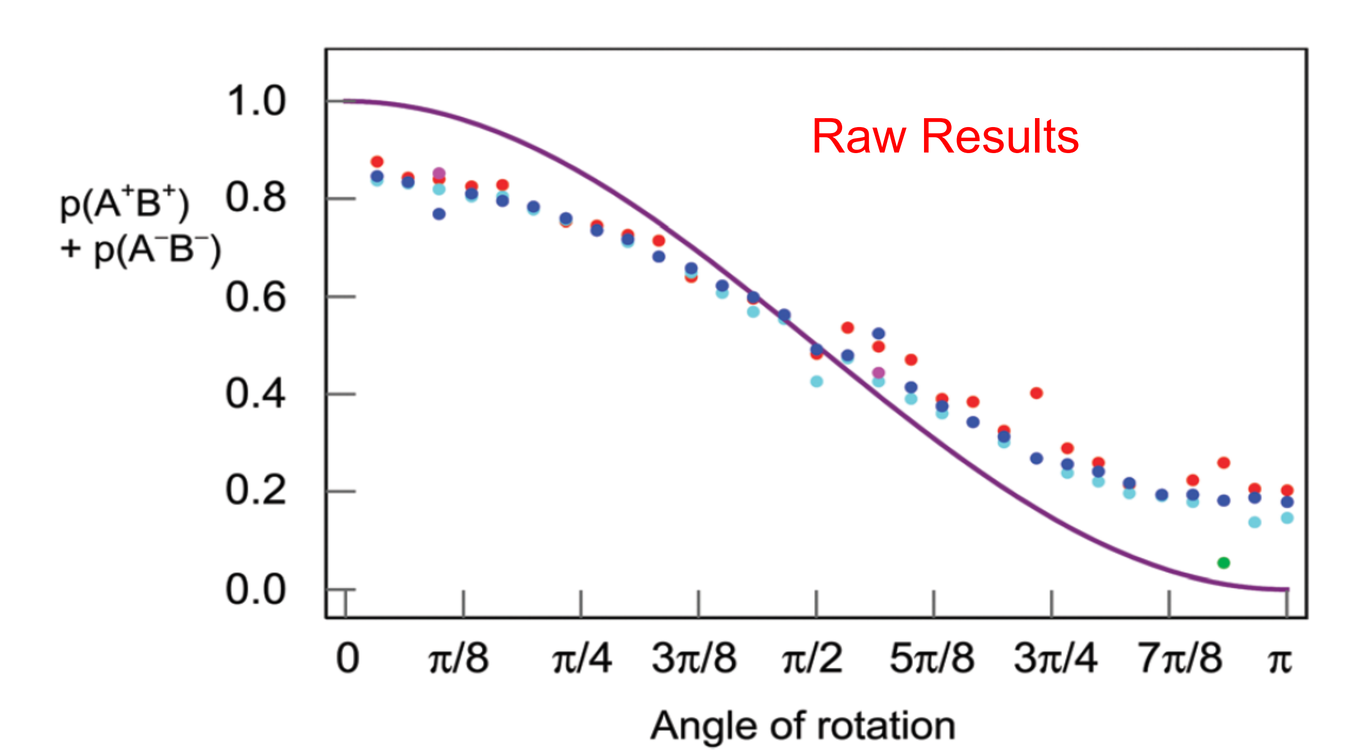
is identical to

the probability that the spin is up along z, *if* it is "up" along z', since

$$\langle \alpha \mid \alpha' \rangle^* \langle \alpha \mid \alpha' \rangle = \langle \alpha' \mid \alpha \rangle^* \langle \alpha' \mid \alpha \rangle$$

So: Rotate one spin vector that is up along z by θ to a new axis z'. That makes it "up" z'. Then measure its spin projection in the z direction. We will need to determine probabilities.

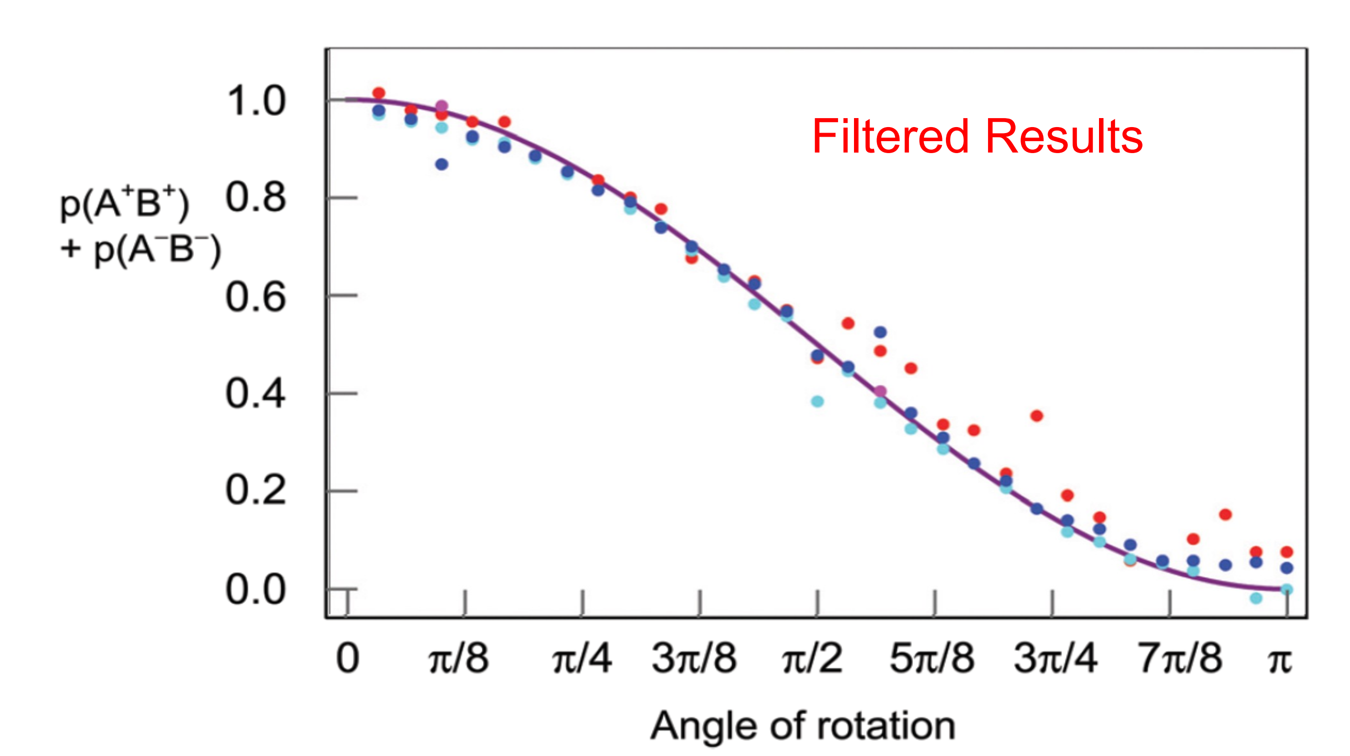
Observations on qubits coupled into Bell states, after rotation of one qubit, on IBM's publicly accessible quantum computers



Values of $p(A^+B^+) + p(A^-B^-)$ plotted as a function of the angle θ between axes A and B. Sets of 10 runs each on IBM's burlington quantum computer with 1024 shots (red), 4196 shots (cyan), and 8192 shots (blue). Where outliers were observed in the initial runs, outcomes of repeat runs are shown in green or magenta. Purple curve: Quantum mechanical prediction

D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and K. L. C. Hunt, *Phys. Chem. Chem. Phys.* **23**, 6370 (2021).

Observations on qubits coupled into Bell states, after rotation of one qubit, on IBM's publicly accessible quantum computers with filtering



D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and K. L. C. Hunt, *Phys. Chem. Chem. Phys.* **23**, 6370 (2021).

Values of $p(A^+B^+) + p(A^-B^-)$ plotted as a function of the angle θ between axes A and B. Sets of 10 runs each on IBM's burlington quantum computer with 1024 shots (red), 4196 shots (cyan), and 8192 shots (blue). Where outliers were observed in the initial runs, outcomes of repeat runs are shown in green or magenta. Purple curve: Quantum mechanical prediction

Filtering by use of mitigation matrices as suggested in qiskit, except that the matrices are determined externally to this program and only once.

Construction of a filtering matrix for error mitigation

Prepare the basis state | 0 0 ⟩, measure and examine the probability of each output | 0 0 ⟩, | 0 1 ⟩, | 1 0 ⟩, and | 1 1 ⟩, based on large numbers of runs, in our case 25 runs with 8192 shots each. Then prepare the basis states and repeat the process. Find the matrix M that connects the vector of prepared states C_{ideal} to the observed state distributions C_{obs}

$$C_{obs} = M\, C_{ideal}$$

Then given any C_{obs}, a good estimate of the ideal vector that would have produced those outcomes is

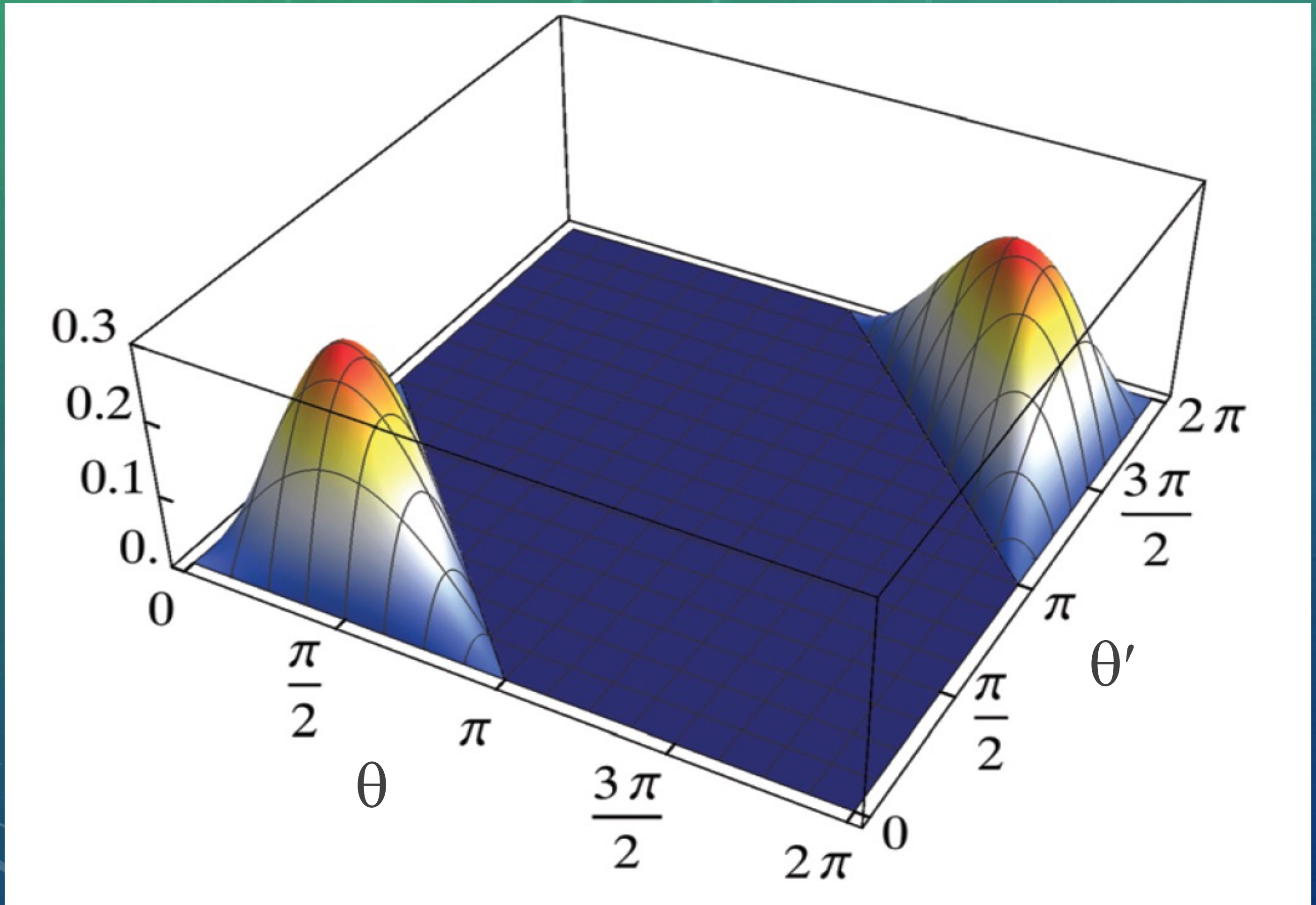
$$C_{est} = M^{-1}\, C_{obs}$$

Interestingly, the filtering matrix changes relatively slowly in time, so it can be determined *outside* of a set of runs, rather than within them. Results are shown for two runs on ibmq_ourense, v1.2.0, five days apart.

$$\mathbf{M}^{-1} = \begin{pmatrix} 1.034861 & -0.029335 & -0.034065 & 0.000811 \\ -0.013127 & 1.050248 & 0.000270 & -0.037341 \\ -0.021839 & 0.000571 & 1.047827 & -0.041142 \\ -0.000105 & -0.021485 & -0.014032 & 1.077683 \end{pmatrix}$$

$$\mathbf{M}^{-1} = \begin{pmatrix} 1.032876 & -0.028240 & -0.036447 & 0.000685 \\ -0.012984 & 1.049636 & 0.000263 & -0.042541 \\ -0.020000 & 0.000390 & 1.050376 & -0.029087 \\ -0.000098 & -0.021775 & -0.014192 & 1.070943 \end{pmatrix}$$

Regions of non-classical behavior

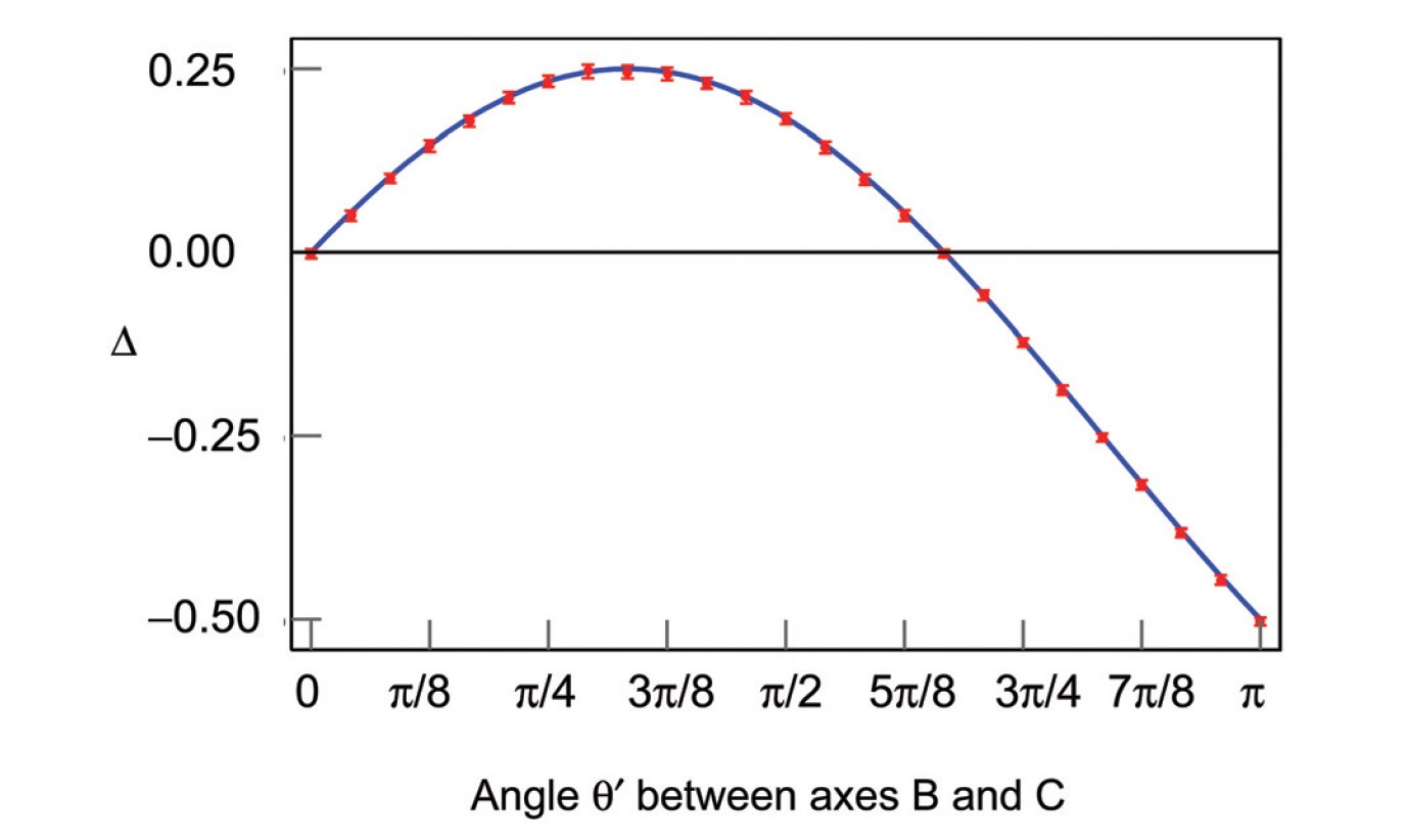


$$\Delta(\theta, \theta') = \cos^2(\theta/2) - \cos^2[(\theta + \theta')/2] - \sin^2(\theta'/2)$$

Positive values of $\Delta(\theta, \theta')$ indicate quantum predictions of violations of the Bell inequalities

Floor in the horizontal plane for $\Delta(\theta, \theta') \leq 0$

Results from IBM's quantum simulator



θ from A to B is fixed at $\pi/3$, while θ' is variable

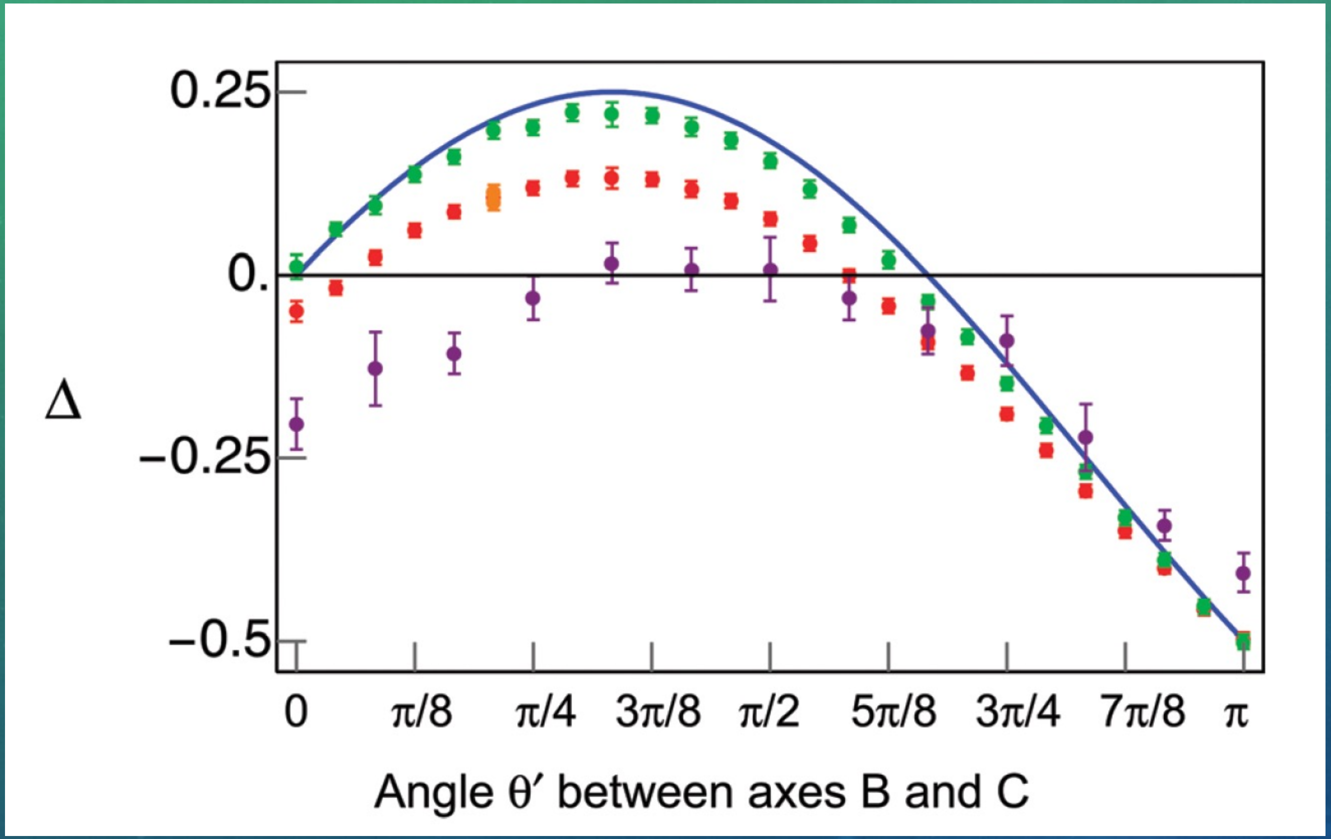
8192 shots per run

10 runs each at fixed angles θ, θ' and $\theta + \theta'$, giving 1000 combinations.

The error bars reach one standard deviation above and below the average values.

D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and K. L. C. Hunt, *Phys. Chem. Chem. Phys*. **23**, 6370 (2021).

With an error matrix for filtering, examine Δ



Fixed angle of $\pi/3$ between axes A and B, variable angle θ' between B and C.

$\Delta \leq 0$ classically.

Some angles show classical behavior.

Others don't!

Red: ibmq_london, v1.1.3

Purple: ibmq_16_melbourne, v2.3.1

$$\Delta = p(A^+B^+) + p(A^-B^-) - [p(A^+C^+) + p(A^-C^-)] - [p(B^+C^-) + p(B^-C^+)]$$

D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and K. L. C. Hunt, *Phys. Chem. Chem. Phys*. **23**, 6370 (2021).

Clauser-Horne-Shimony-Holt Inequality

This applies to correlation functions of spin projections, rather than probabilities, but the basis of the inequalities is the same. A three-axis version of the CHSH inequality is

$$S = \langle \sigma_A \sigma_B \rangle + \langle \sigma_A \sigma_C \rangle + \langle \sigma_B \sigma_B \rangle - \langle \sigma_B \sigma_C \rangle \leq 2$$

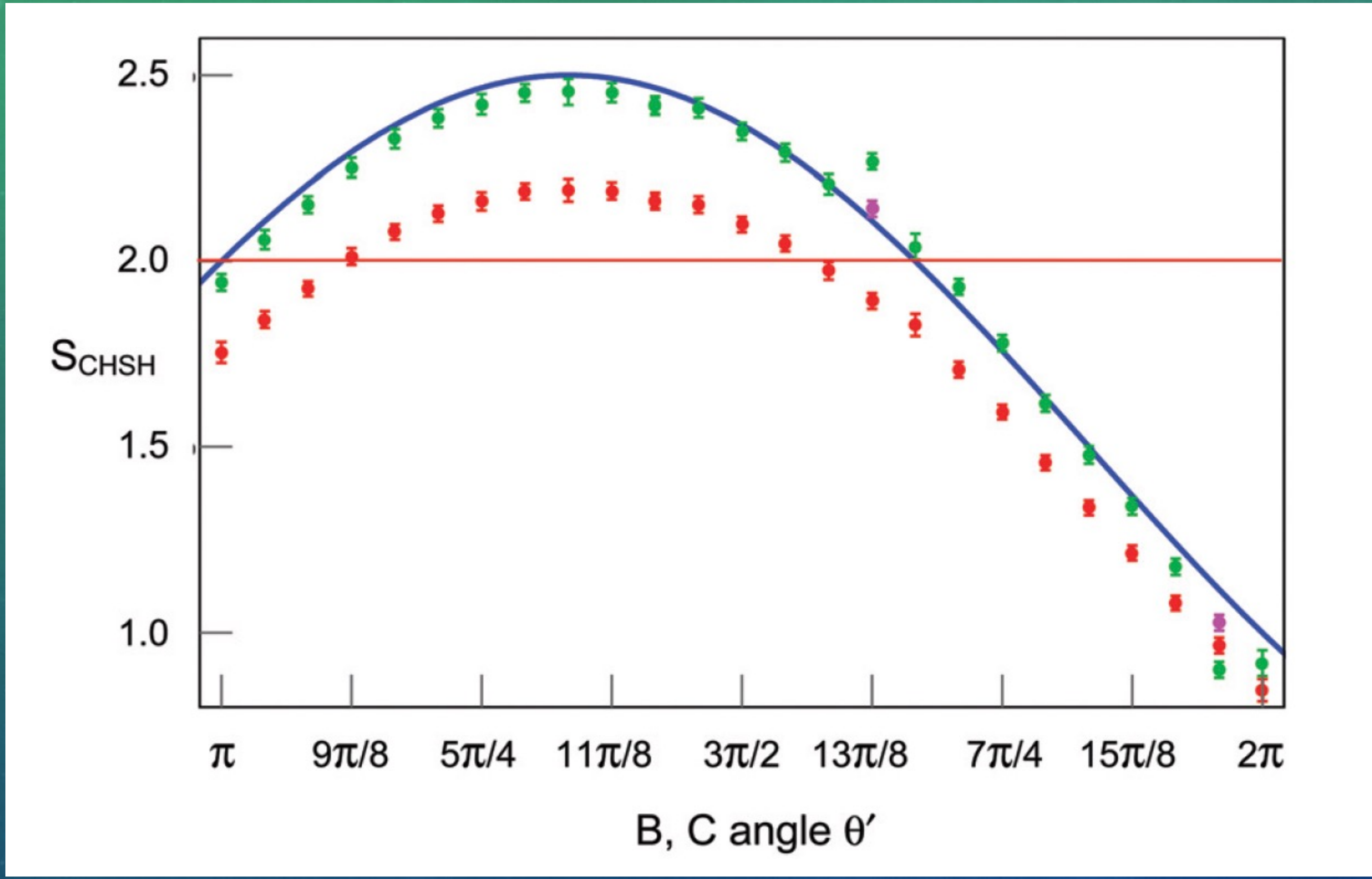
This holds *classically*.

The first spin projection operator refers to particle 1 and the second refers to particle 2.

J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt,
Phys. Rev. Lett. **23**, 880 (1969).

Results on IBM's publicly accessible quantum computers

Standard deviations from 10 runs of 8192 shots, at each angle θ, θ′ and θ + θ′, giving 1000 combinations



Results from ibmq_london v1.1.3

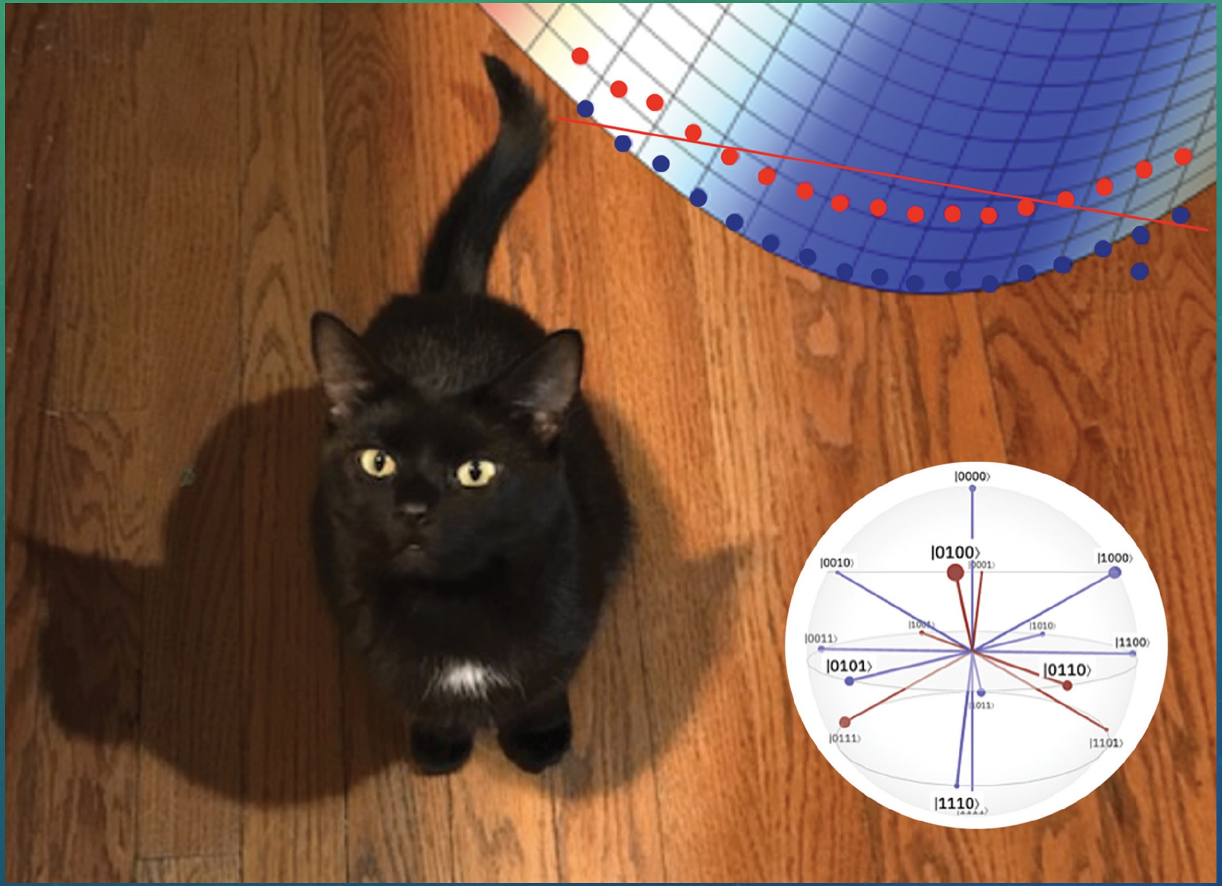
Raw results in red

Error mitigated results in green

Quantum prediction: Blue curve

D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and K. L. C. Hunt, *Phys. Chem. Chem. Phys.* **23**, 6370 (2021).

Schrödinger’s cat states on a quantum computer



D. Z. Wang, A. Q. Gauthier, A. E. Siegmund, and
K. L. C. Hunt, *Phys. Chem. Chem. Phys*. **23**, 6370 (2021).

From the website Seven Good Things

A Schrödinger's cat state

$$| \Psi \rangle = (1/2)^{1/2} \left[| \alpha(1)\, \alpha(2) \ldots \alpha(n) \rangle \right.$$

$$\left. + | \beta(1)\, \beta(2) \ldots \beta(n) \rangle \right]$$

The qubits are all in state 0 or state 1 (α/β), but there is a 50/50 likelihood of each.

A 3-qubit example is the GHZ state of Greenberger, Horne, and Zeilinger.

Construction on a quantum computer at right. Stair-step algorithm (top) and three harpsichord algorithms

D. Greenberger, M. Horne, and A. Zeilinger, *Bell's Theorem, Quantum Theory and Conceptions of the Universe* (Kluwer Academic, Dordrecht, 1989).

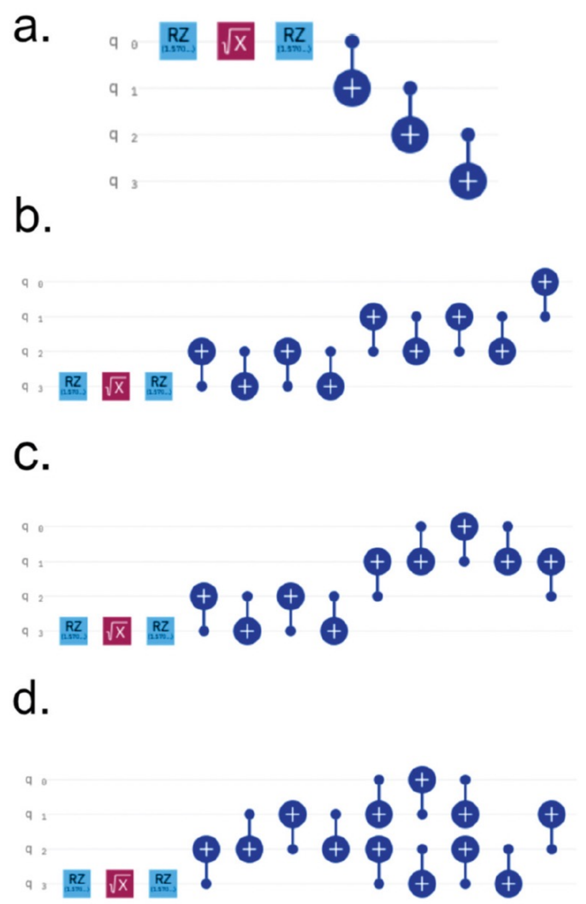


Fig. 3 (a) Transpiled circuits for the stair-step algorithm for 4-qubit cat states, and (b–d) three different transpiled circuits for the harpsichord algorithm for 4-qubit cat states, generated within a single job on manila.

N. Jansen, M. Loucks, S. Gilbert, C. Fleming-Dittenber, J. Egbert, and K. L. C. Hunt, *PCCP* **24**, 7666 (2022).

Shannon entropy of measurement outcomes

$$S = -\sum_j p_j \log_2 p_j$$

where p_j is the probability of outcome j.

Suppose that an n-qubit cat state is produced and measured without faults.

Then measurements should yield

$$0\ 0\ 0\ .\ .\ .\ 0$$

and $\quad 1\ 1\ 1\ .\ .\ .\ 1$

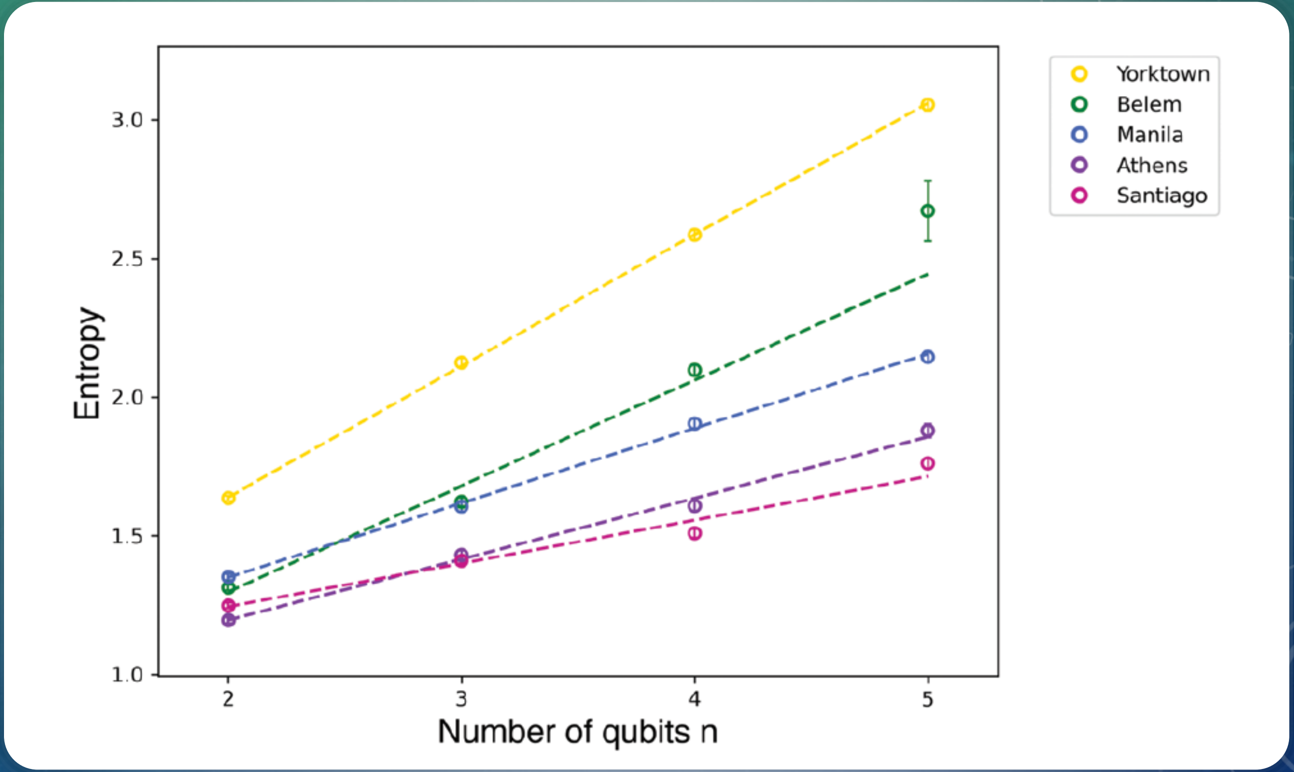
with equal probability.

This gives S = 1, independent of the number of qubits n entangled into the cat state.

Shannon entropy defined by C. E. Shannon, *Bell Syst. Tech. J*. **27**, 379, 623 (1948).

Observed Shannon entropy of measurement outcomes as a function of the number of qubits in the cat state

Stair-step algorithm results from IBM computers Yorktown, Belem, Manila, Athens, and Santiago



N. Jansen, M. Loucks, S. Gilbert, C. Fleming-Dittenber, J. Egbert, and K. L. C. Hunt, *Phys. Chem. Chem. Phys*. **24**, 7666 (2022).

Mathematical model for near-linearity of S

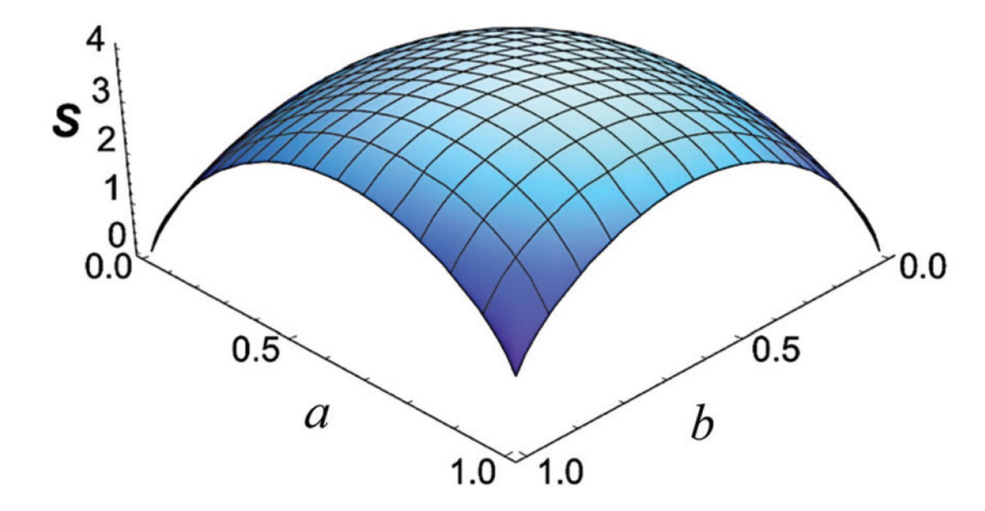
Assume an effective accuracy a for the production and measurement of the state $| 0 \rangle$ and b for the production and measurement of the state $| 1 \rangle$. Then for an n-qubit cat state, the probability p(n, q) to observe q qubits with spin up in a measurement is given by

$$p(n, q) = (1/2)\, C(n, q)\, [\, a^{q} (1 - a)^{n - q} + (1 - b)^{q}\, b^{n - q}\,]$$

Now

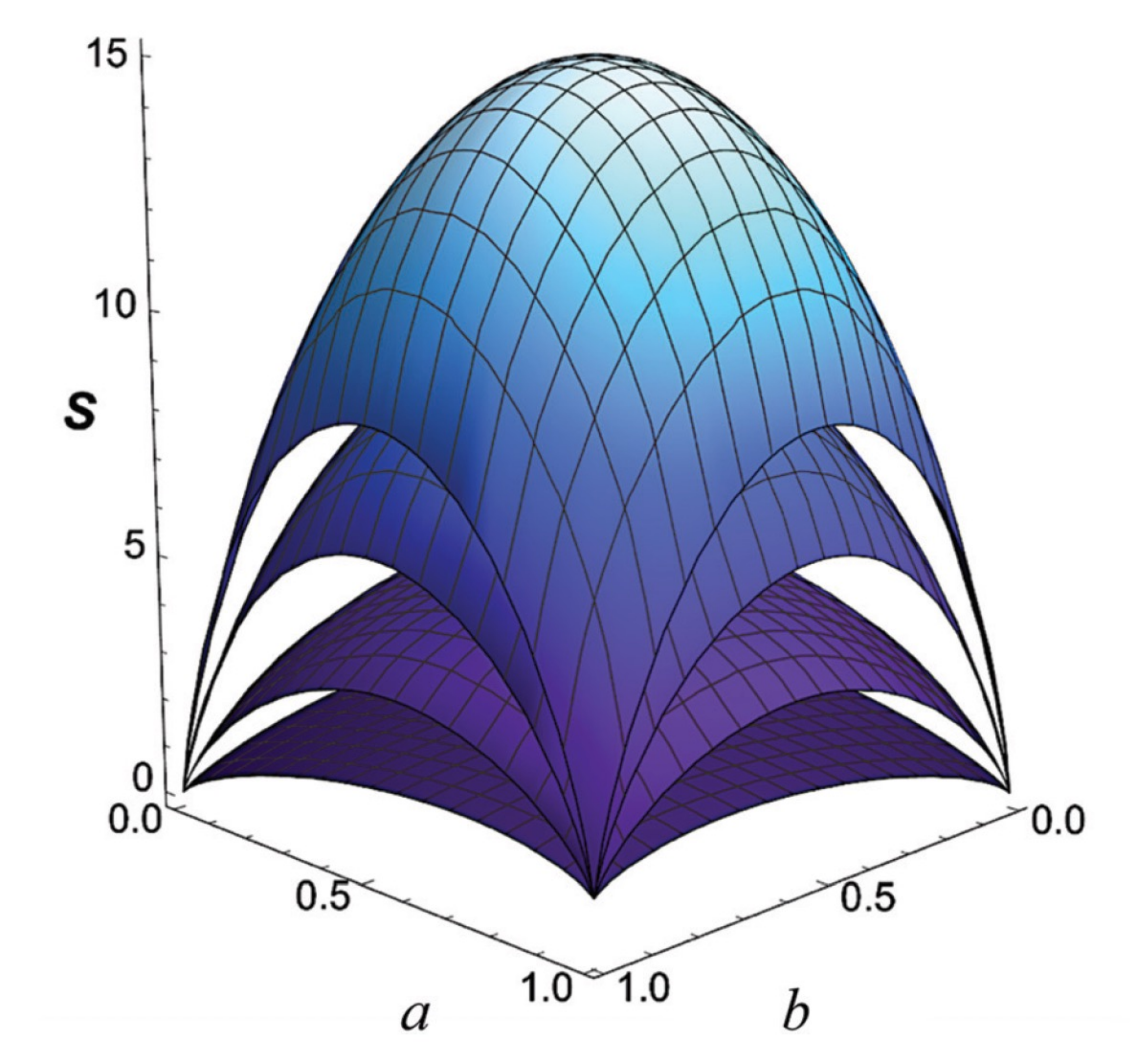
$$S = -\sum_{q = 0}^{n} p(n, q) \log_2 p(n, q)$$

Shape of S in the model

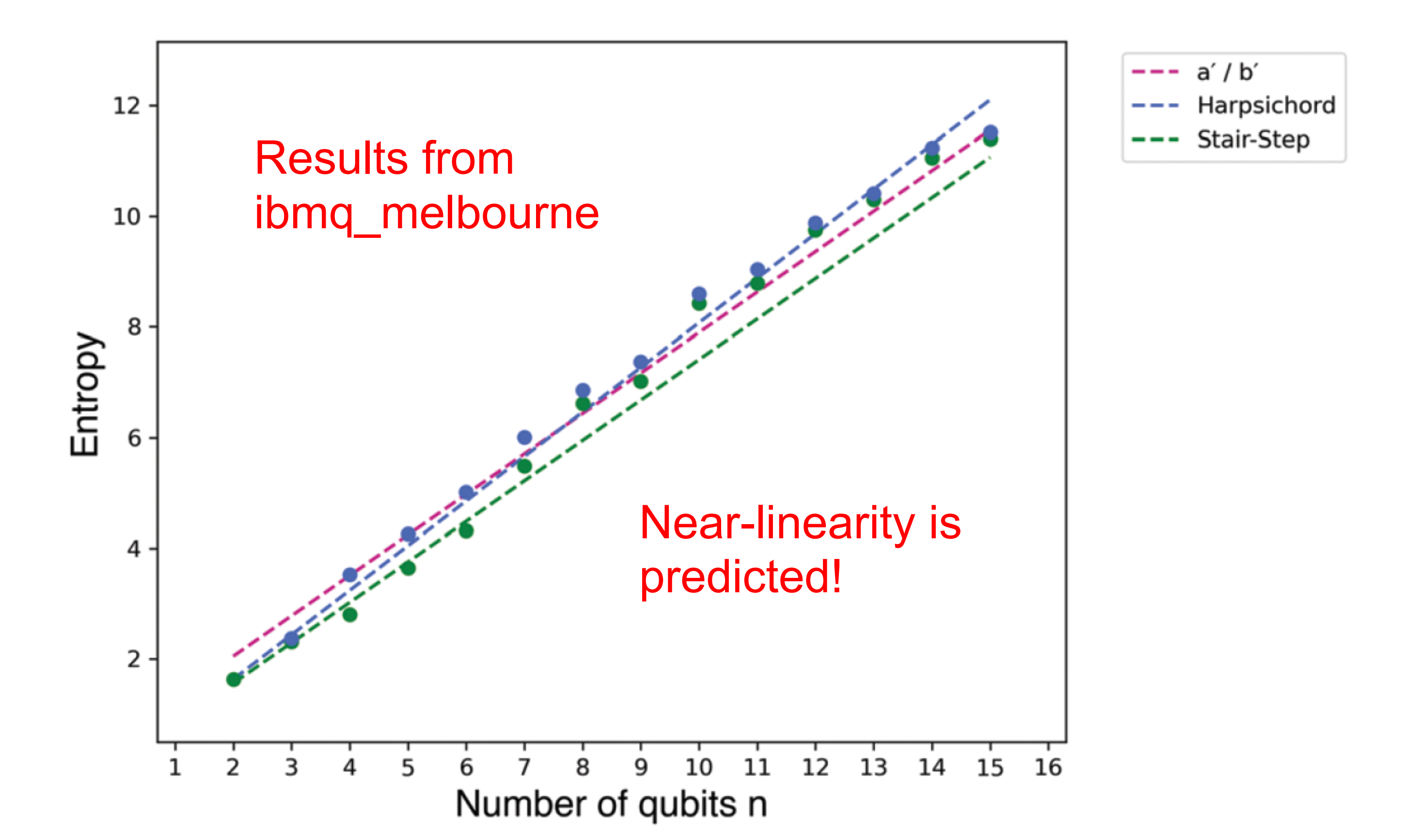


Above: S for 4 qubits

Right: S for 2, 5, 10, and 15 qubits
Maximum when $a = b = 1/2$, S = n



How good is this model?



N. Jansen, M. Loucks, S. Gilbert, C. Fleming-Dittenber, J. Egbert, and K. L. C. Hunt, *Phys. Chem. Chem. Phys*. **24**, 7666 (2022).

Key observation

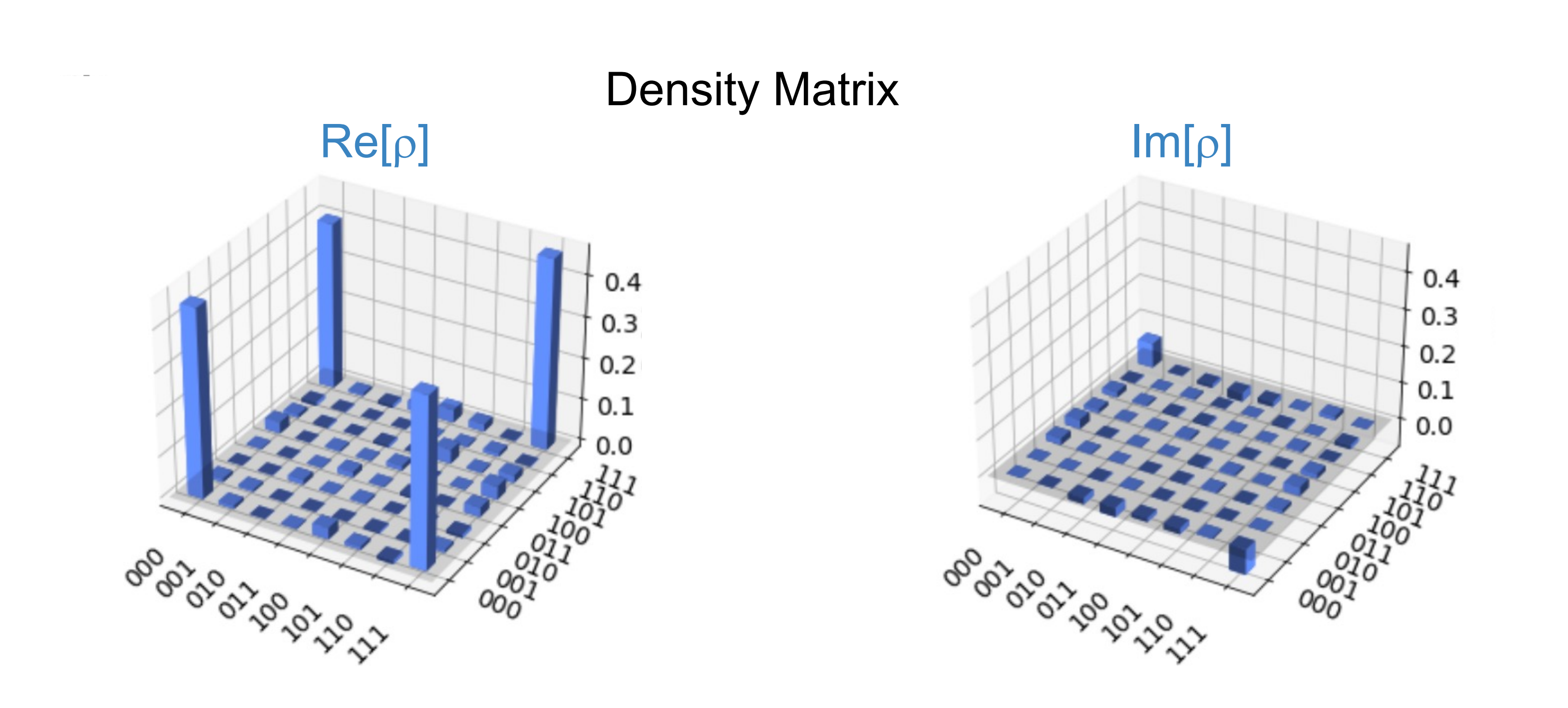
The slope of S(n) vs. n varies among quantum computers with identical quantum volumes! It provides a more sensitive indicator of the quality of an NISQ device.

Computer	dS/dn	V_c	V_g
Melbourne	0.7315	8	8
Yorktown	0.4739	16	8
Belem	0.3823	32	16
Quito	0.3106	32	16
Manila	0.2689	32	32
Athens	0.2204	32	32
Santiago	0.1565	32	32

The von Neumann entropy is obtained from the density matrix ρ, which is determined by quantum state tomography, using qiskit.

$$S_{vN} = -\,\mathrm{Tr}\,[\rho \log_2 \rho]$$

S_{vN} is proportional to the thermodynamic entropy



Nathan Jansen
Chemistry Ph.D.
Student at MSU

David Z. Wang
Summer Intern
2019, 2020

Aidan Q. Gauthier
Summer Intern
2019, 2020

Ashley E. Siegmund
Summer Intern
2019, 2020

Drew Scheffer
Summer Intern
2020

Matthew Loucks
Summer Intern
2020

Scott Gilbert
Summer Intern
2020

Corbin Fleming-
Dittenber
Summer Intern 2020

Jessica Messing
Summer Intern
2020

Garrett Mai
Summer Intern
2020

Acknowledgments: National Science Foundation
Grants CHE-1900399 and CHE-2154028

Herbert H. and Grace A. Dow Foundation

Rollin M. Gerstacker Foundation

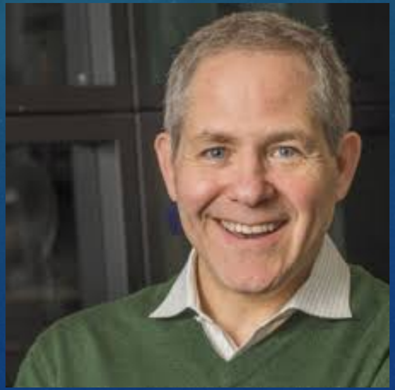
Charles J. Strosacker Foundation

Thanks for Letters of Collaboration from:

Prof. Ben Levine
Stony Brook

Prof. Elad Harel
MSU

Prof. Warren Beck
MSU



Prof. Marcos Dantus
MSU

Prof. Richard Zare
Stanford

I am very grateful to the Institute for Advanced Studies of the University of Luxembourg for a DISTINGUISHED grant, which has made my visit possible, and to Professor Jens Kreisel, Rector of the University of Luxembourg, Professor Catherine Léglu, Vice-Rector for Academic Affairs, Professor Claus Vögele, Head of the Institute for Advanced Studies, Dr. Sylvie Fromentin, Paula Souza, and Manuel Quaino, F. M. and Logistics Officer.

Very special thanks are due to Professor Alexandre Tkatchenko, Head of the Department of Physics and Materials Science, Professor Aurélia Chenu, Professor Susanne Siebentritt, Dr. Dmitry Fedorov, Dr. Ariadni Boziki, Dr. Dahvyd Wing, Dr. Matteo Gori, Dr. Jorge Alfonso Charry Martinez, Dr. Gregory Cordeiro Fonseca, Dr. Szabolcs Góger, Dr. Igor Poltavskyi, Dr. Adil Kabylda, Mirela Puleva, Matyas Nachtigall, and all additional graduate students and postdoctoral researchers in the Tkatchenko research group. I am also very grateful to Dr. Elodie Duriez and Yolande Edjogo!