Quantum computing: a physicist's point of view

Presented at the

INT, University of Washington

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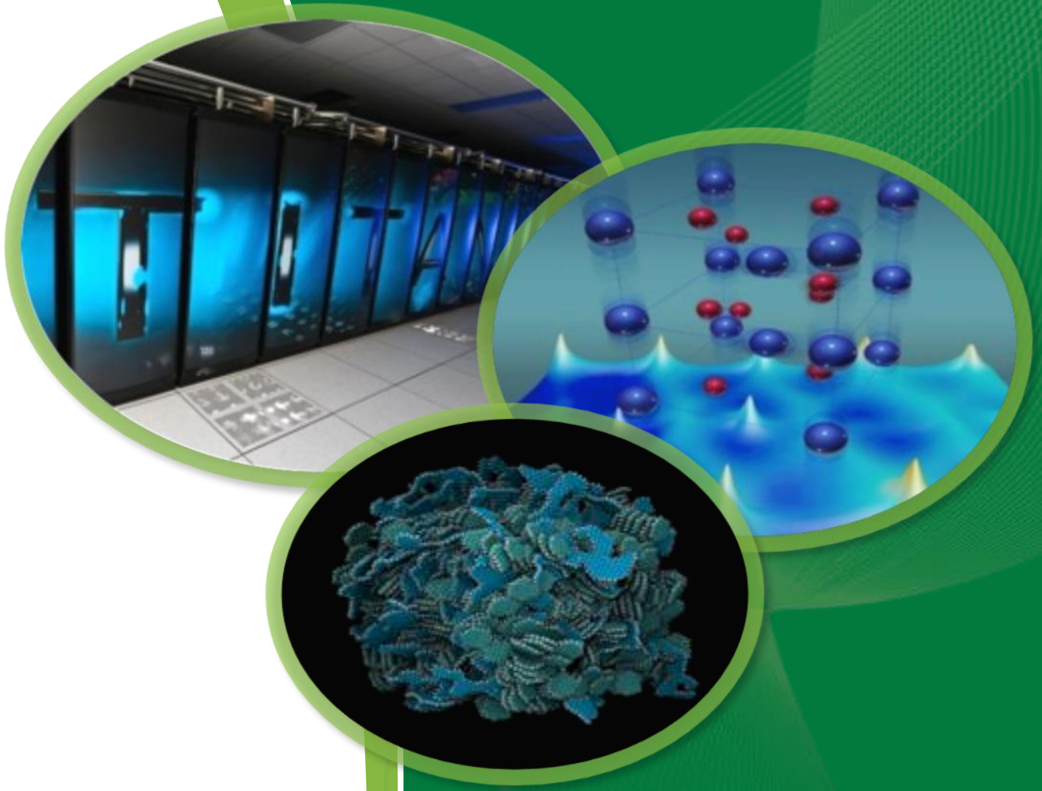
Seattle
November 14, 2017



OAK RIDGE
National Laboratory

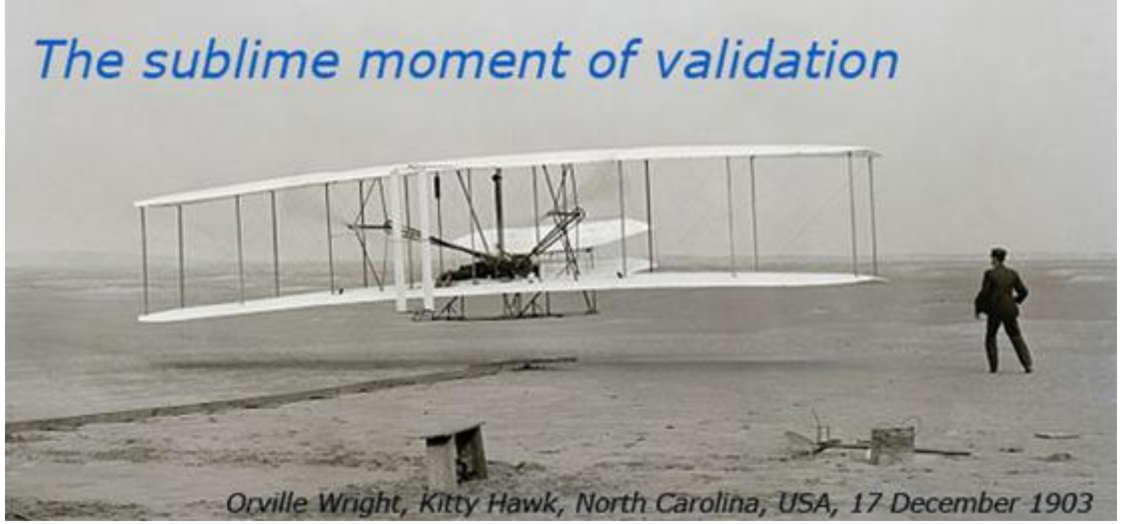
Outline

- Why do we compute?
- Trends in High Performance Computing: Bits
- Beyond exascale: Quantum Bits
  - What they could do
  - Some history
  - Why they are different
- The nuclear quantum many-body problem

Why, how and purpose of computing

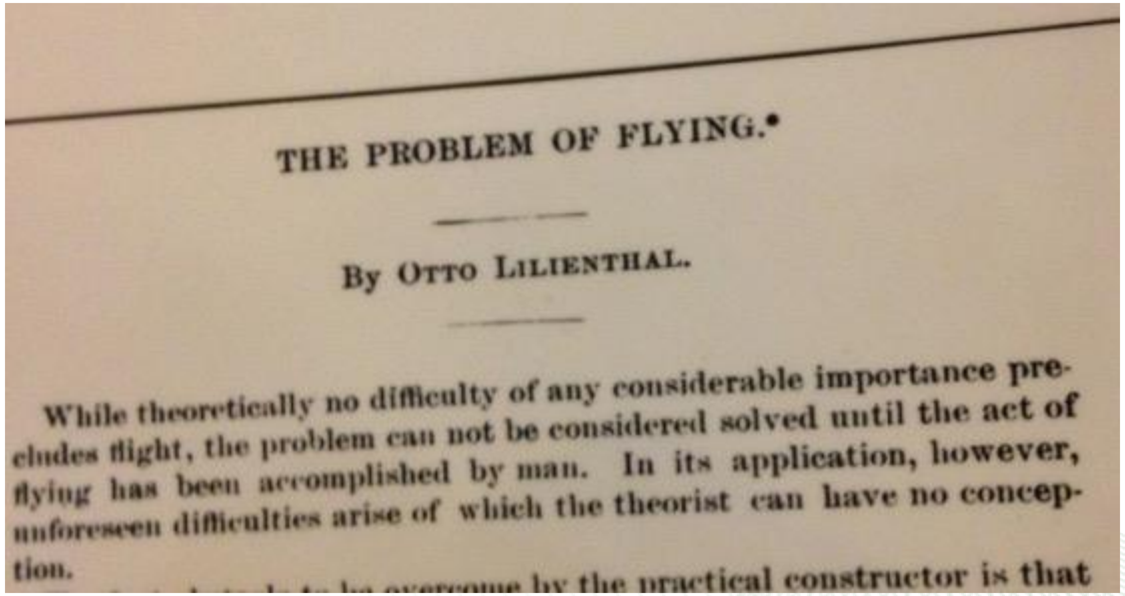
- Why
  - Very few instances of analytical, closed form, real life solutions exist.
  - Nonlinearity and emergent behavior exist everywhere
- How
  - We employ methods of Validation and Verification (V&V)
    - Doing the problem right (numerically sound approaches)
    - Doing the right problem (physically sound approaches)
- Purpose
  - We compare theory (as codified in equations) to experiment
  - We discover new phenomena
  - We predict the outcomes of experiments to test theory
  - We quantify our uncertainties (UQ)

- We ‘always’ apply liberal amounts of physics intuition



The sublime moment of validation

Orville Wright, Kitty Hawk, North Carolina, USA, 17 December 1903

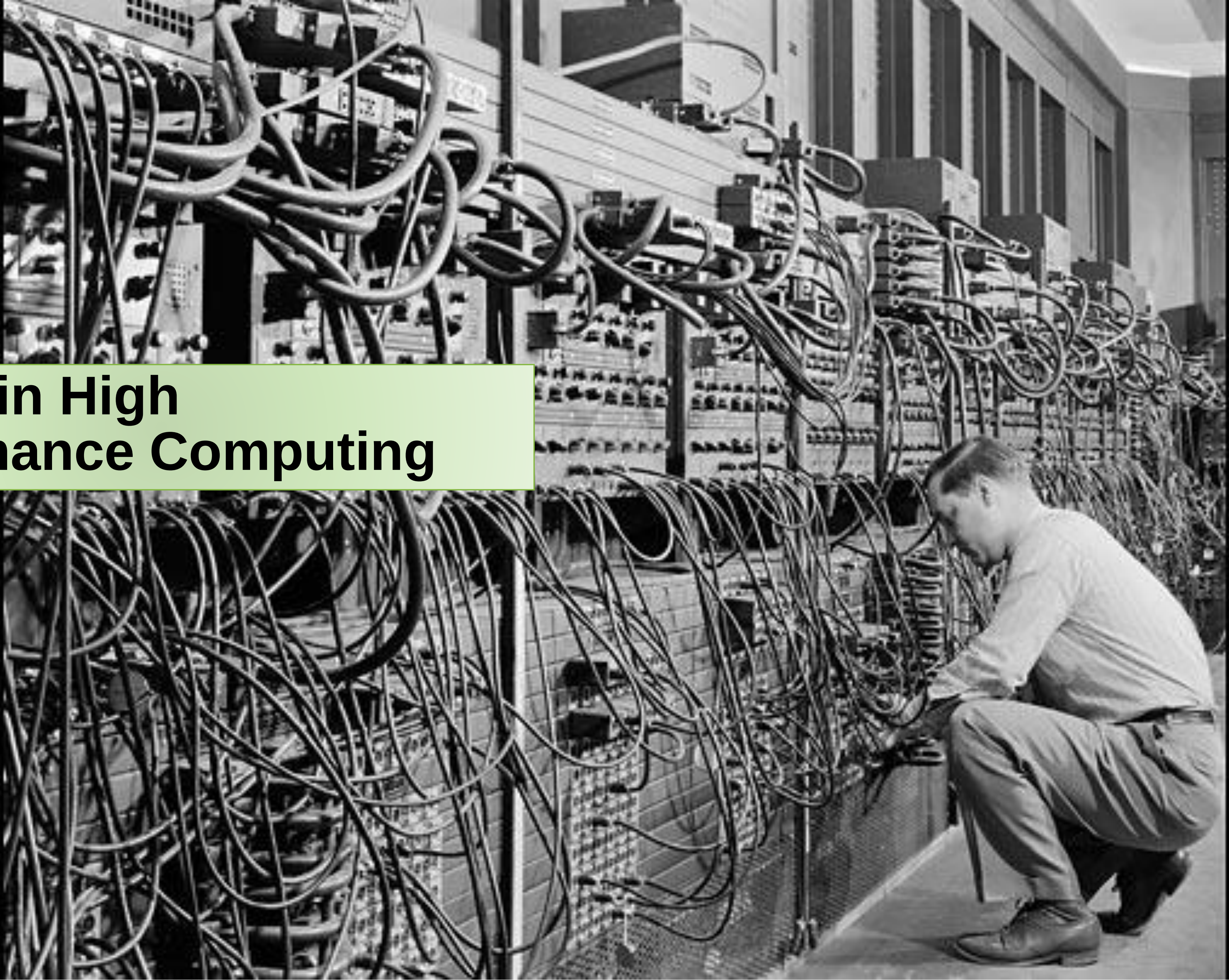


THE PROBLEM OF FLYING.*

By Otto Lilienthal.

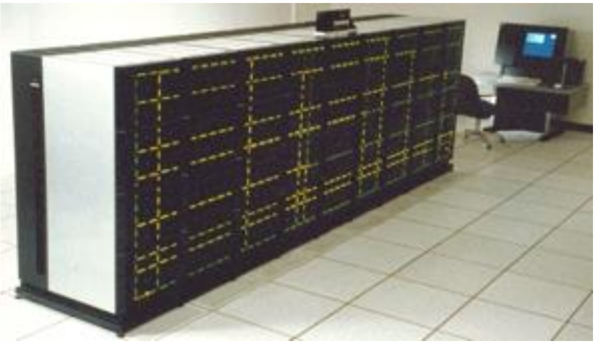
While theoretically no difficulty of any considerable importance precludes flight, the problem can not be considered solved until the act of flying has been accomplished by man. In its application, however, unforeseen difficulties arise of which the theorist can have no conception.

overcome by the practical constructor is that



Trends in High Performance Computing

Some open science computers…

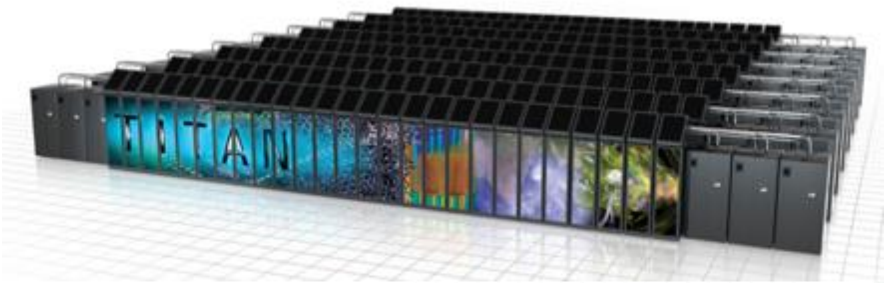


Touchstone Delta – Caltech
June 1993
#8 on Top500
Rpeak=13.9 Gflop/s (#1 = 59.7 GF)

NERSC T3E900
June 1998
#8
321 Gflop/s (#1 = 1,338 GF)

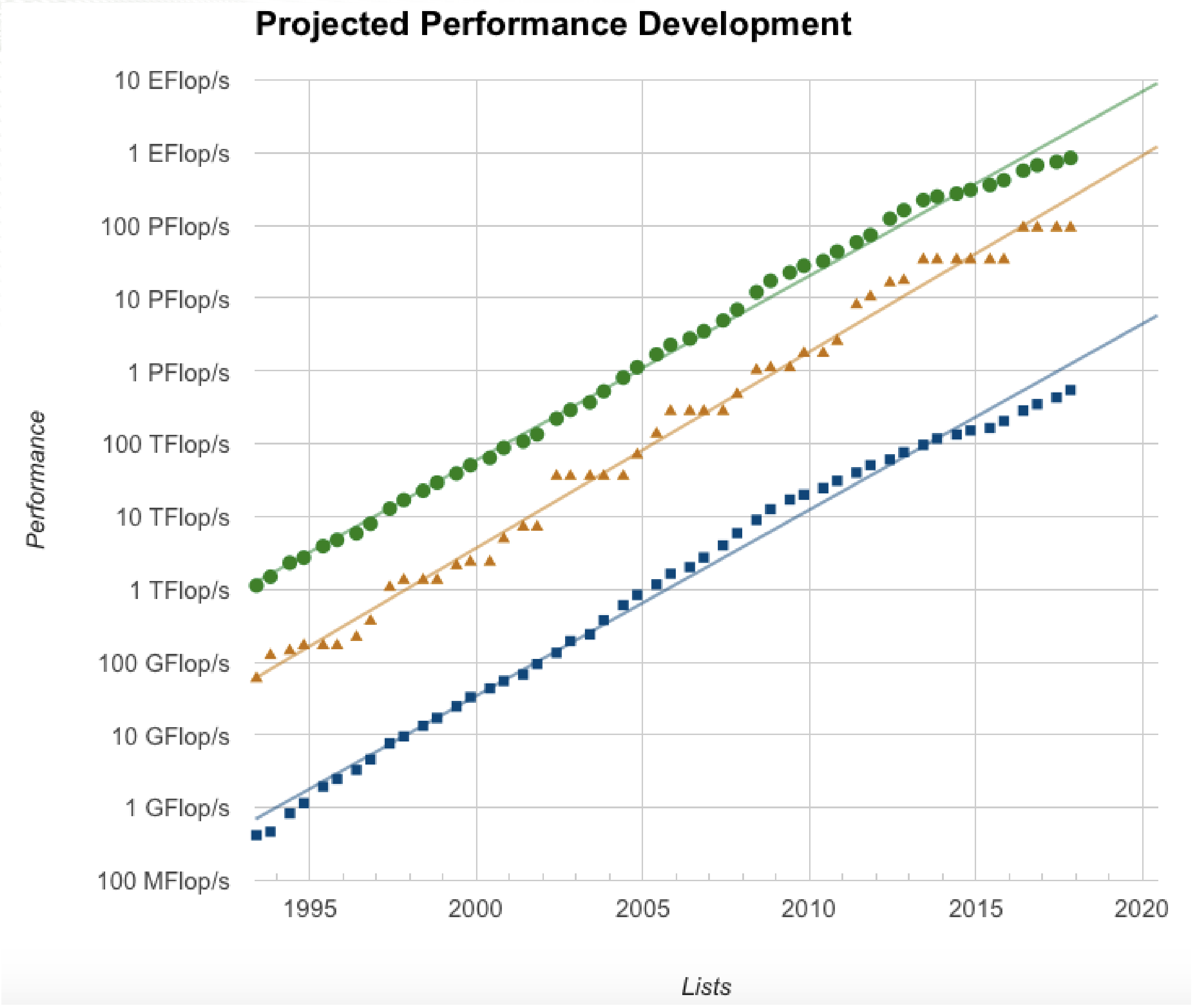
NERSC, IBM SP-3, 16 way
June 2003
#4
7 Tflop/s (#1 = 35.86 TF)

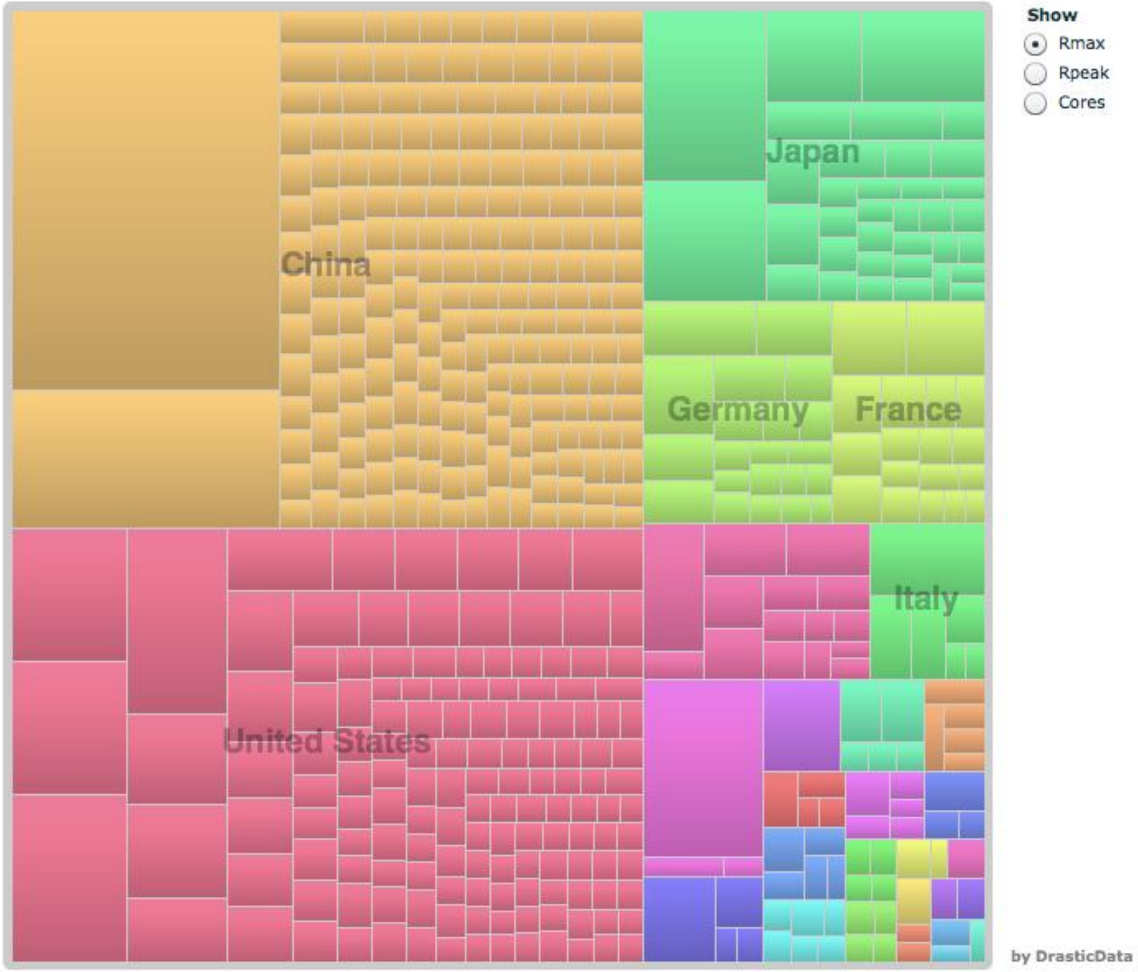
ORNL, Cray XT4 (upgraded components)
June 2008
#6
205 Tflop/s (#1 = 1.026 PF)



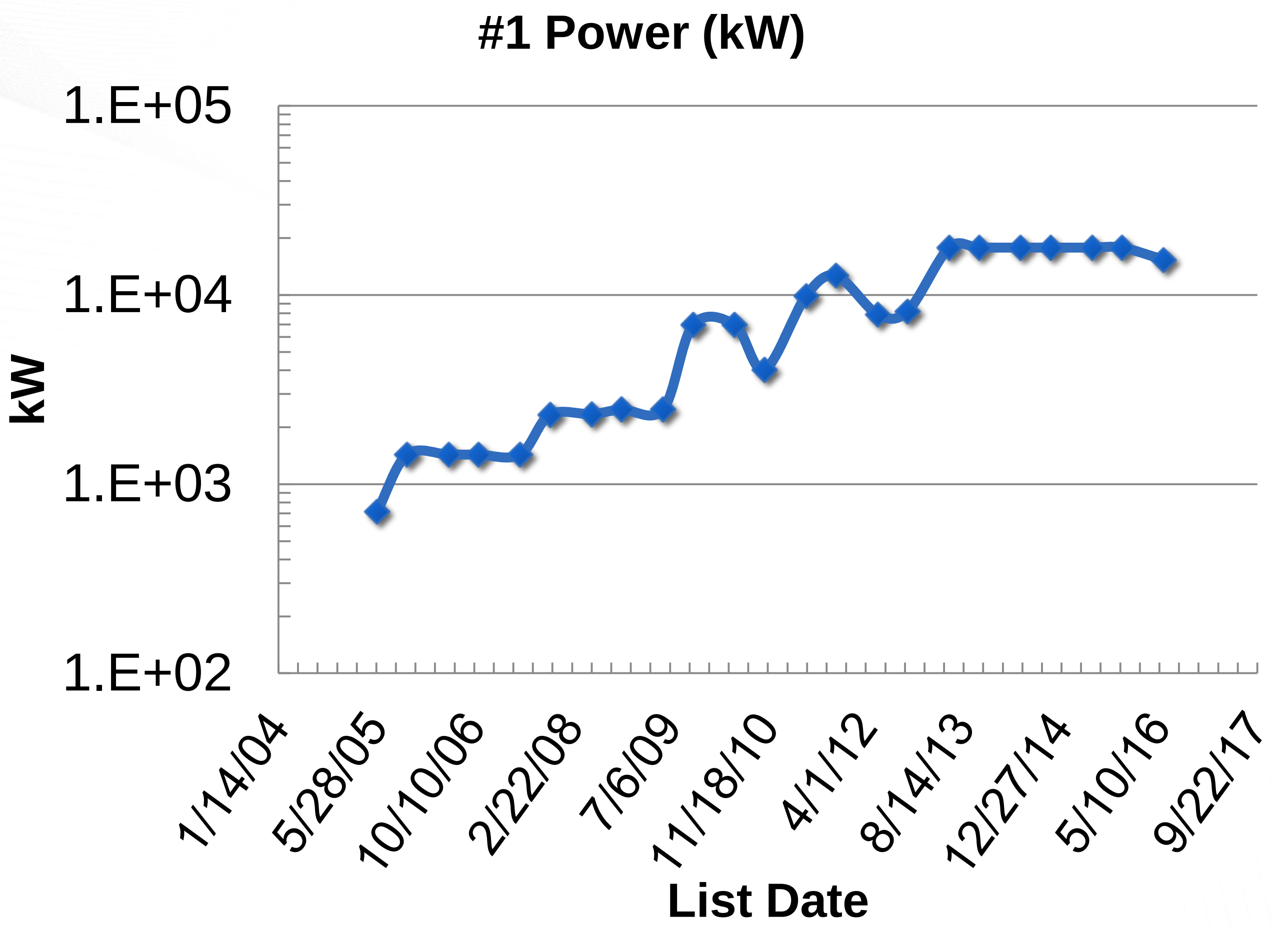
ORNL, Cray XK7
November 2017
#5
17.5 Pflop/s (#1 = 93 Pflop/s)

Development with time (top500.org)





A big issue: power



Incremental cost of running RHIC: $550k/week

Incremental cost of running Titan: $140k/week

Incremental cost of running Sunway: $258k/week

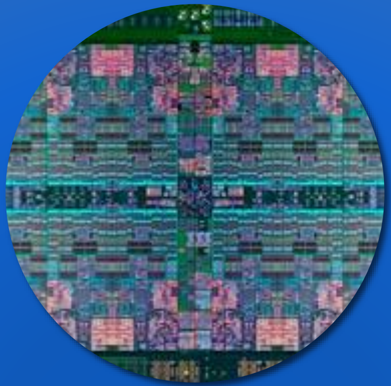
(assume $0.1/kW-h)

June 2005 Tflop/kW = 0.191
Nov. 2017 Tflop/kW = 6.05

32x technology improvement

Beyond exascale landscape

Quantum, Neuromorphic



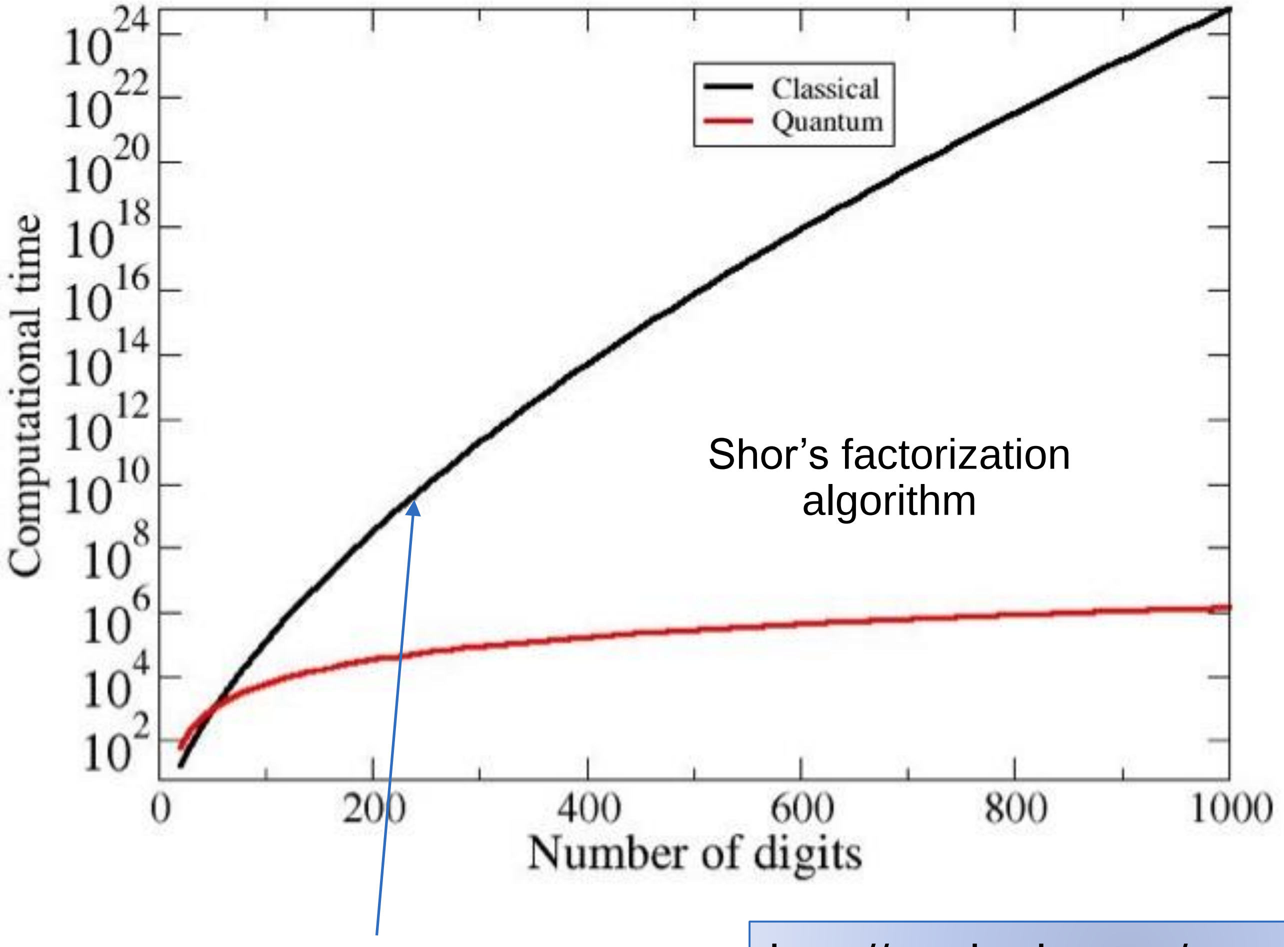
Squeeze out everything one can from CMOS

Beyond CMOS

Materials Science; Device Physics; Software

Quantum computing could crack some really tough problems!

The promise of quantum computing:
Scaling of some of the most difficult algorithms



Shor's factorization algorithm

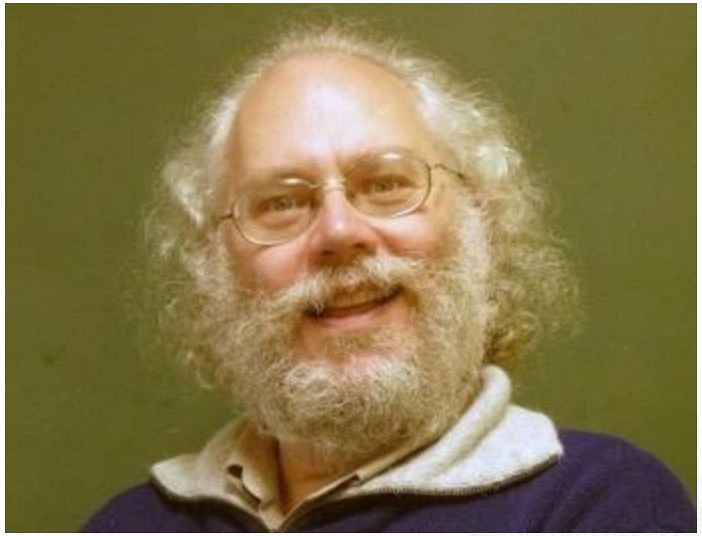
Today AES-256

Quantum

O$((\log N)^2(\log \log N)(\log \log \log N))$

Classical

O$(e^{1.9\ (\log N)^\wedge 1/3\ (\log \log N)^\wedge 2/3})$



http://math.nist.gov/quantum/zoo/

Quantum computing in context

In the sciences

1980s– 1990s

A curious idea; first quantum algorithms

2000s

Proof-of-principle demonstrations
Initial QC hardware

Error correction and control theory

2010s

Focus on practicality and improving quality and control

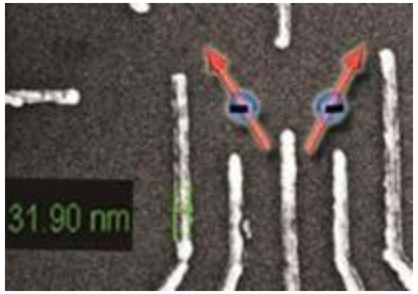
Circuit synthesis

Current status

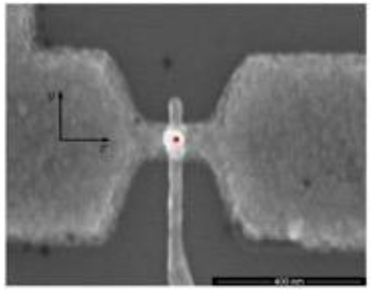
Qubit fragility presents tremendous challenges

Attempt to broaden suite of applications

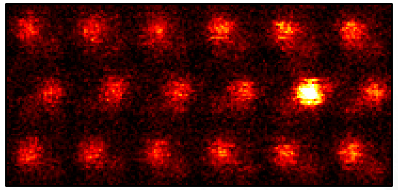
If quantum mechanics hasn't profoundly shocked you, you haven't understood it yet.
– Niels Bohr



Si Ge qubits
Julich

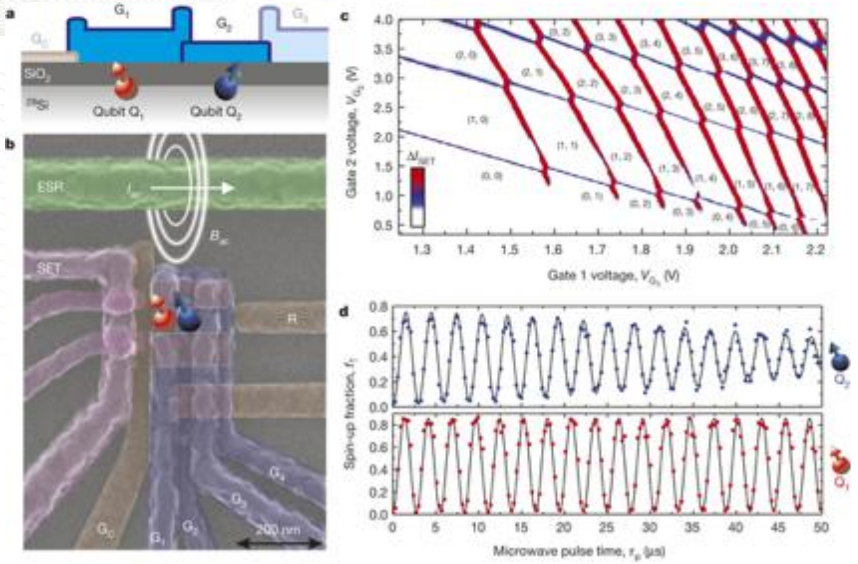


Phosphorous donor
Sydney



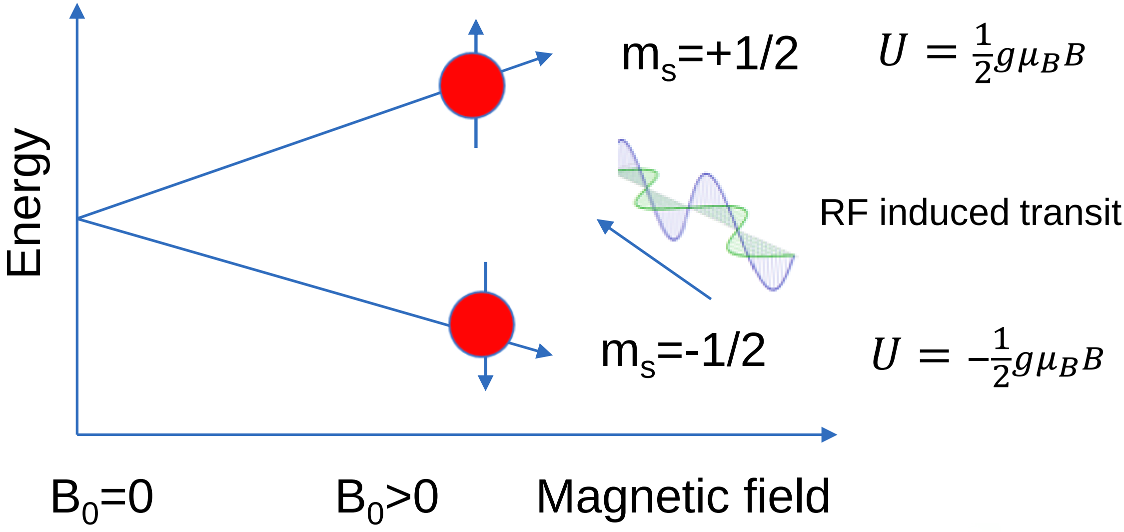
Scientific motivator: "…potential ability to realize full control of large-scale quantum coherent systems…"
BES: Challenges at the frontiers of matter and energy, 2015
Quantum Pathfinder and Quantum Algorithms funding awarded by ASCR (FY17)
BES: Quantum Information Science Round Tables (October, 2017)
HEP funding in FY18 PBR, NP interest – this workshop

How to make a qubit



Veldhorst et al., Nature 526, 410 (2015)

B-field splits the orbital into its projections



Energy

m_s=+1/2 $U = \frac{1}{2} g \mu_B B$

RF induced transition

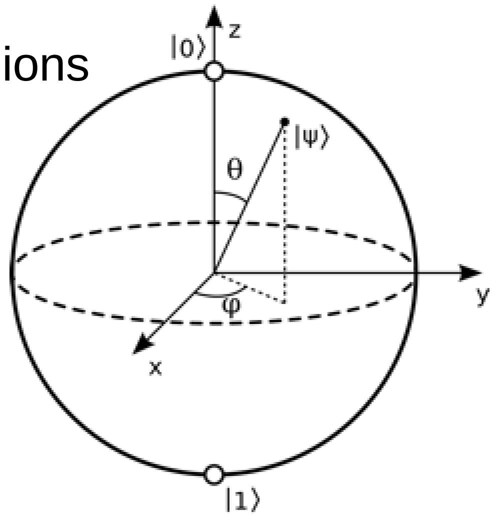
m_s=-1/2 $U = -\frac{1}{2} g \mu_B B$

B_0=0 B_0>0 Magnetic field

Electrons are spin ½ fermions

$$|\Psi> = a|\tfrac{1}{2}> + b|-\tfrac{1}{2}>$$

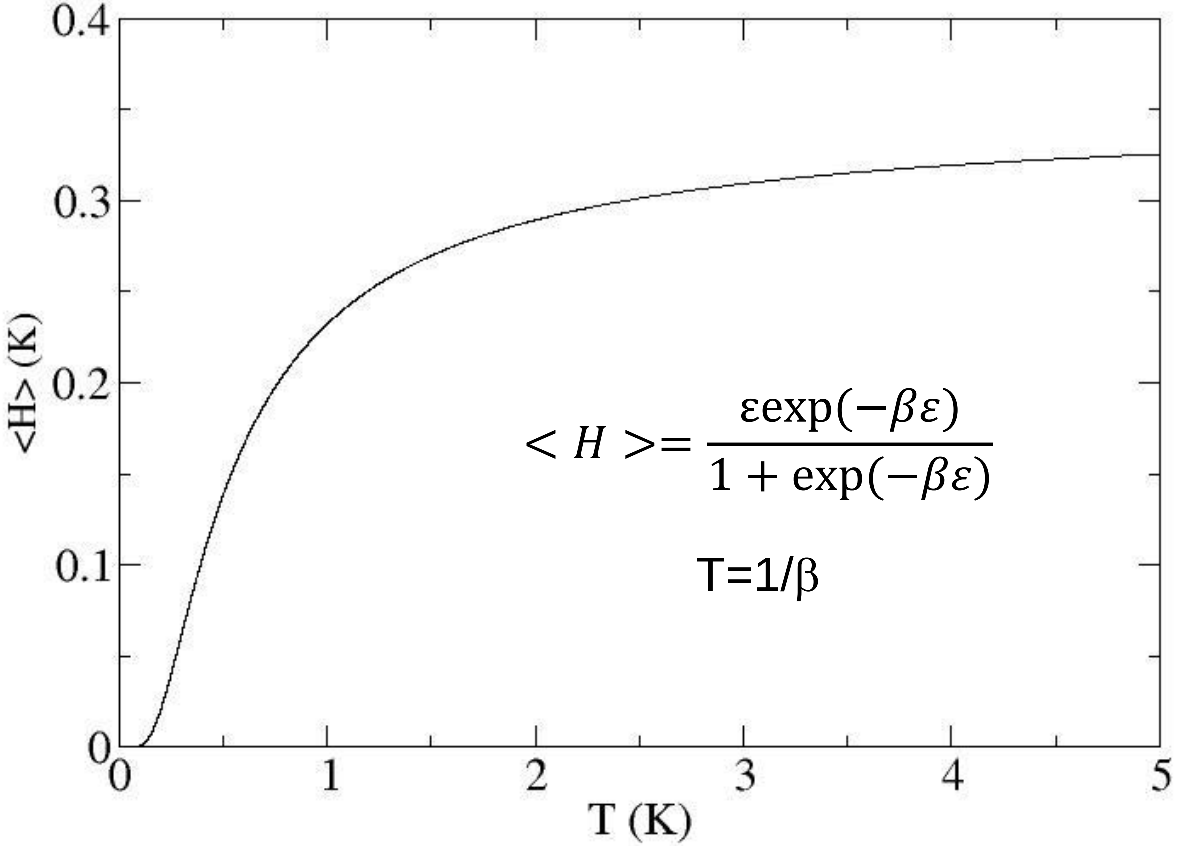
$$|a|^2+|b|^2=1$$



Order of magnitude estimates…
- Landau g factor ~1
- μ_B=5.8x10^{-5} eV/Tesla
- B=1 Tesla
- ε=0.7 K
- 1 K = 20 GHz

Types of decoherence
T_1 – relaxation time
T_2^* – 'dephasing' time

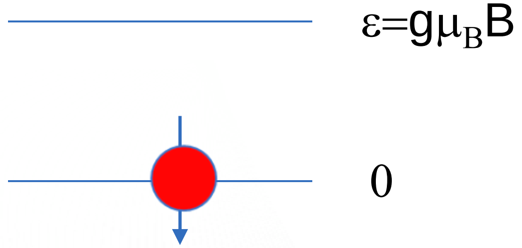
Thermal effects



$$< H >= \frac{\varepsilon \exp(-\beta\varepsilon)}{1+\exp(-\beta\varepsilon)}$$

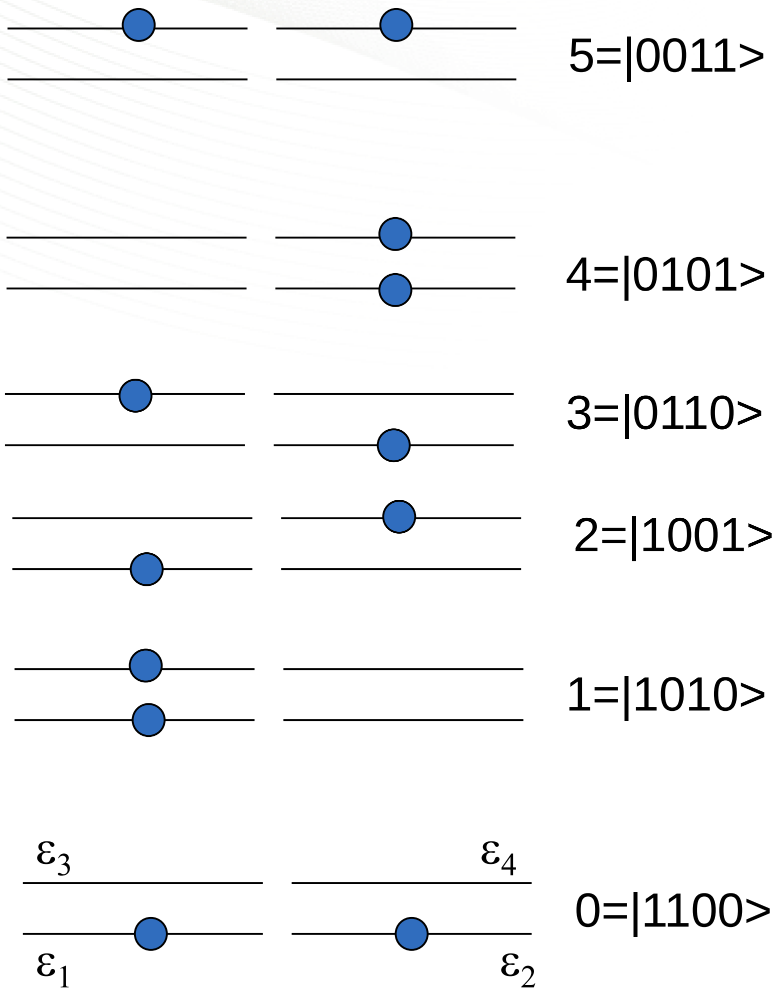
T=1/β

Landau g factor ~1
μ_B=5.8x10^{-5} eV/Tesla
B=1 Tesla
ε=0.7 K
1 K = 20 Ghz



Implies very low temperature operation (mK)

Conceptual quantum mechanics and entanglement



Hamiltonian operator

$$H = \sum_{pq} \langle p|T|q\rangle a_p^{+} a_q + \sum_{pqrs} \langle pq|V|rs\rangle a_p^{+} a_q^{+} a_s a_r$$

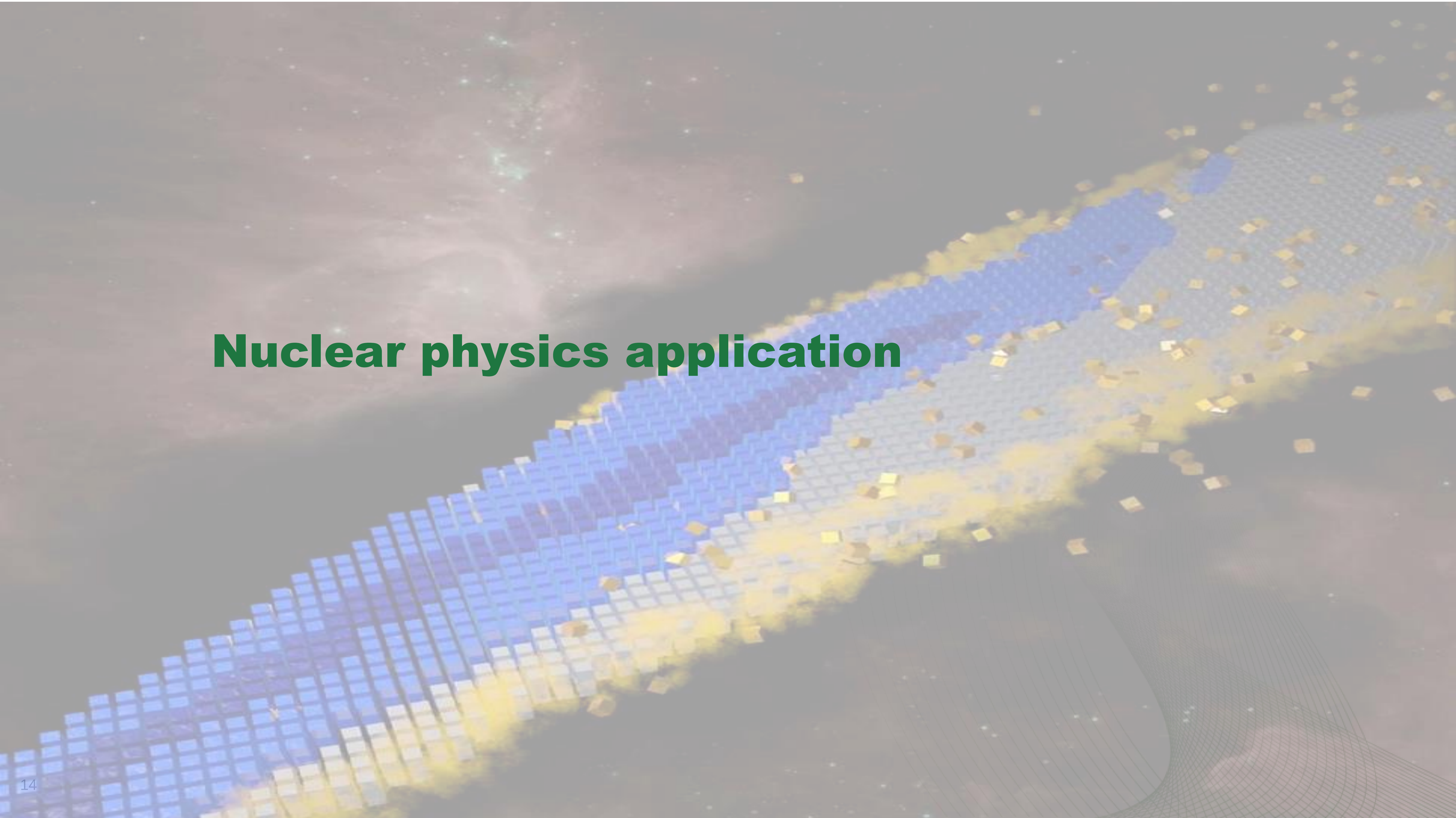
Kinetic energy

Potential energy describes interactions between particles (Coulomb, spin-spin)

$$H =$$

$$\begin{pmatrix}
\varepsilon_1+\varepsilon_2+\frac{1}{2}V_{1212} & \frac{1}{4}V_{1213} & & & & \frac{1}{4}V_{1234} \\
\frac{1}{4}V_{1312} & \varepsilon_1+\varepsilon_3+\frac{1}{2}V_{1313} & & & & \\
 & & \varepsilon_1+\varepsilon_4+\frac{1}{2}V_{1414} & \frac{1}{4}V_{2134} & & \\
 & & \frac{1}{4}V_{2314} & \varepsilon_2+\varepsilon_3+\frac{1}{2}V_{2323} & & \\
 & & & & \varepsilon_3+\varepsilon_4+\frac{1}{2}V_{3434} & \\
\frac{1}{4}V_{3412} & & & & & \varepsilon_3+\varepsilon_4+\frac{1}{2}V_{3434}
\end{pmatrix}$$

Diagonalize H to obtain energy and entangled many-body wave function



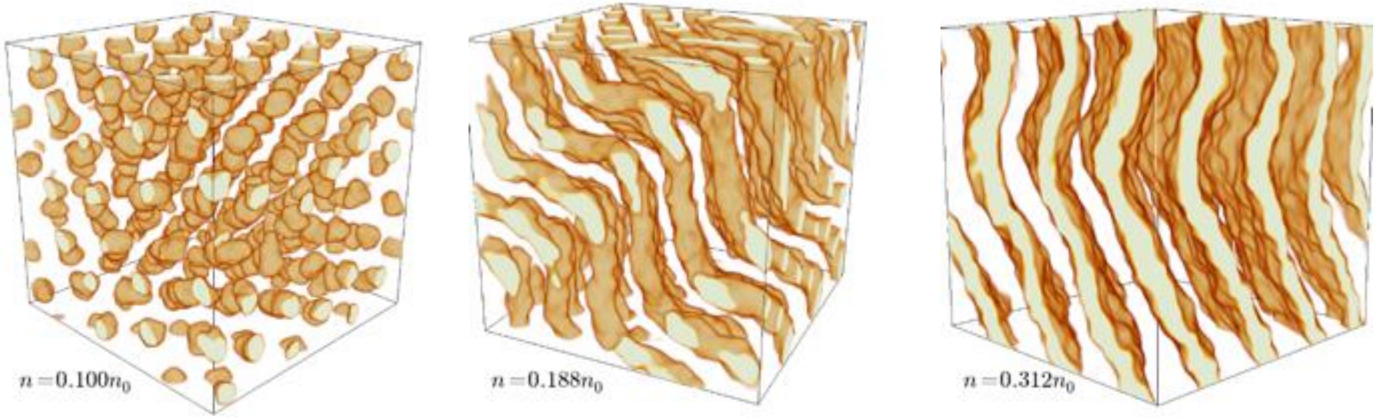
Nuclear physics application

FRIB Science – I

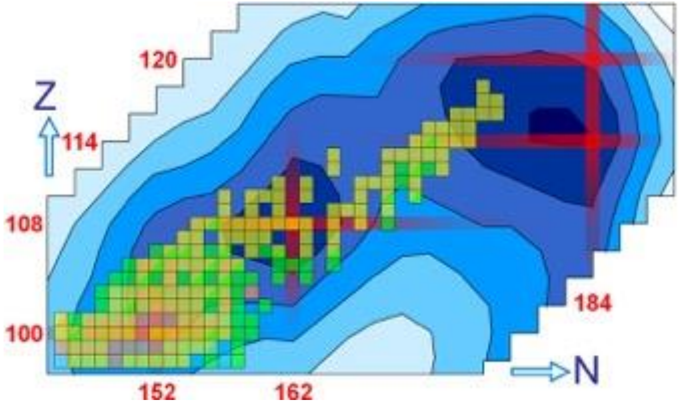
How does subatomic matter self organize and what phenomena emerge?

Many different avenues of research

- Unitary Fermi gases: dilute matter
- Nuclear Equation of State
  - Impacts neutron star properties
- Clustering within nuclei
- Super heavy element discovery

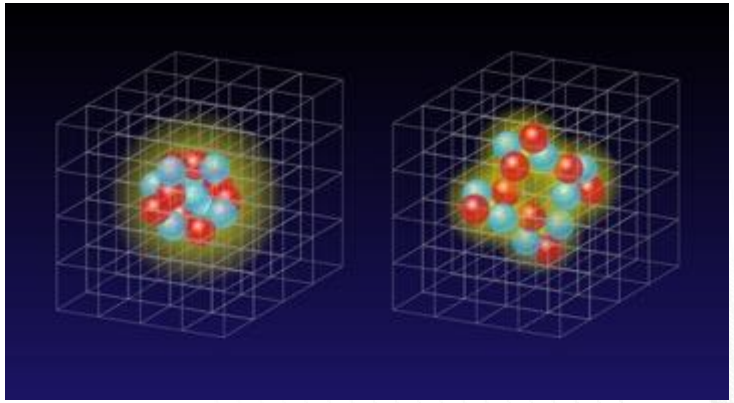


Matt Caplin, PhD thesis, APS/DNP Dissertation Award, 2017



Initial: Phys. Rev. Lett. **104**, 142502 (2010)
Confirmed: Phys. Rev. Lett. **112**, 172501 (2014)

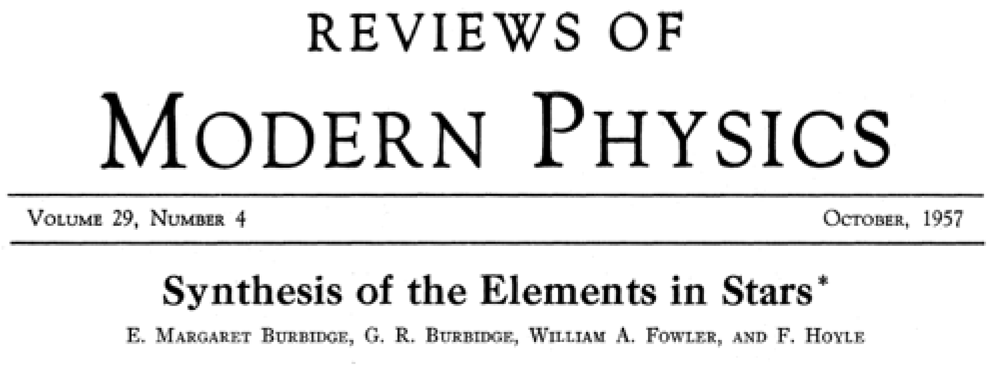
^{249}Bk + ^{48}Ca = ^{294}Ts



Clustering on a lattice, PRL 117, 132501 (2016)

FRIB Science – II

How did visible matter come into being and how did it evolve?



REVIEWS OF

MODERN PHYSICS

VOLUME 29, NUMBER 4 OCTOBER, 1957

Synthesis of the Elements in Stars*

E. MARGARET BURBIDGE, G. R. BURBIDGE, WILLIAM A. FOWLER, AND F. HOYLE

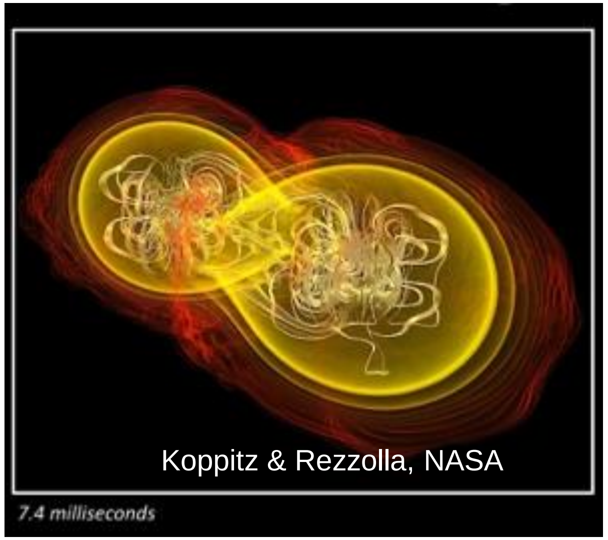
One example:

R-process: rapid neutron capture responsible for ½ of the heavy elements

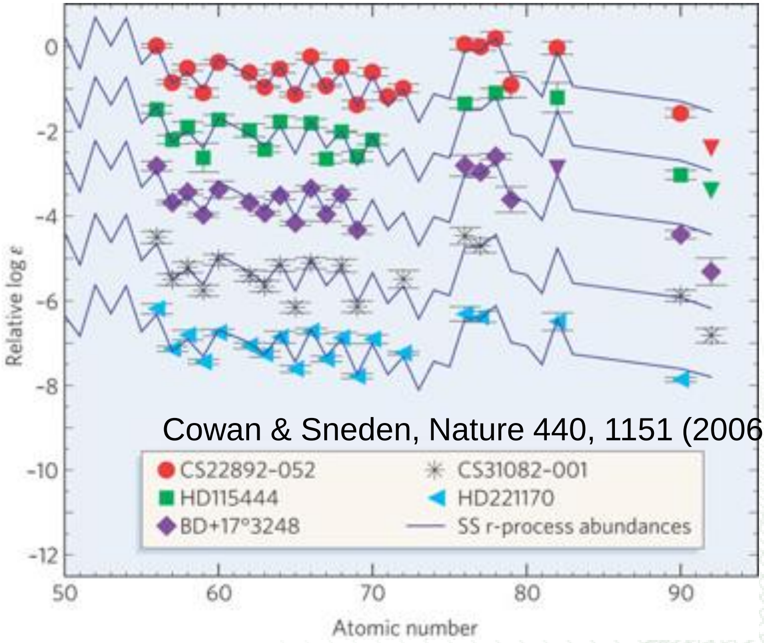
Requires:

- Neutron density: $10^{20\text{-}28}$ n/cm^3
- Fast time scale (seconds)
- Evidence that the process occurs in neutron star mergers: LIGO

HST, 2011



Koppitz & Rezzolla, NASA



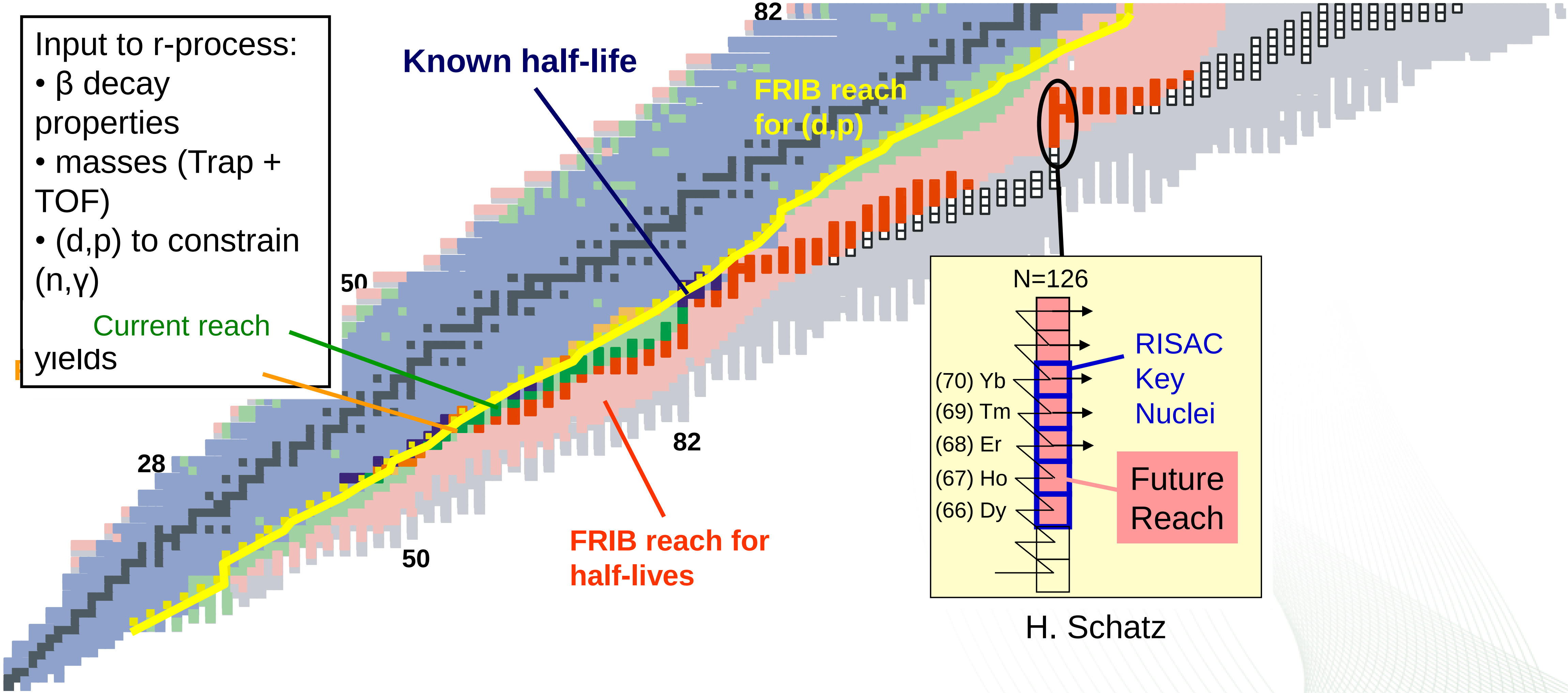
Cowan & Sneden, Nature 440, 1151 (2006)

FRIB Science – II

How did visible matter come into being and how did it evolve?

Input to r-process:
- β decay properties
- masses (Trap + TOF)
- (d,p) to constrain (n,γ)

yields



H. Schatz

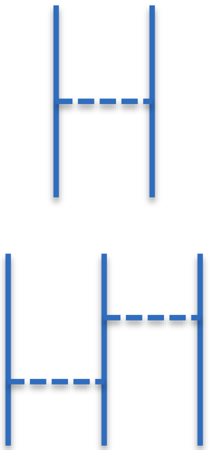
Approaching weakly bound nuclei with coupled cluster theory

A method that captures the physics

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

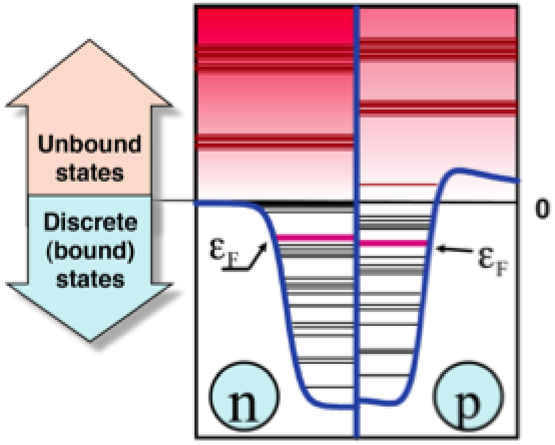
- Coupled cluster theory
- Infinitely summed lower class (1, 2, 3 loop) many-body perturbation theory diagrams
- Amenable to HPC applications

Effective Field Theory for nuclear force (interactions)



- Effective field theory expansion of the nucleon forces that respects symmetries of QCD
- 2-body and 3-body forces

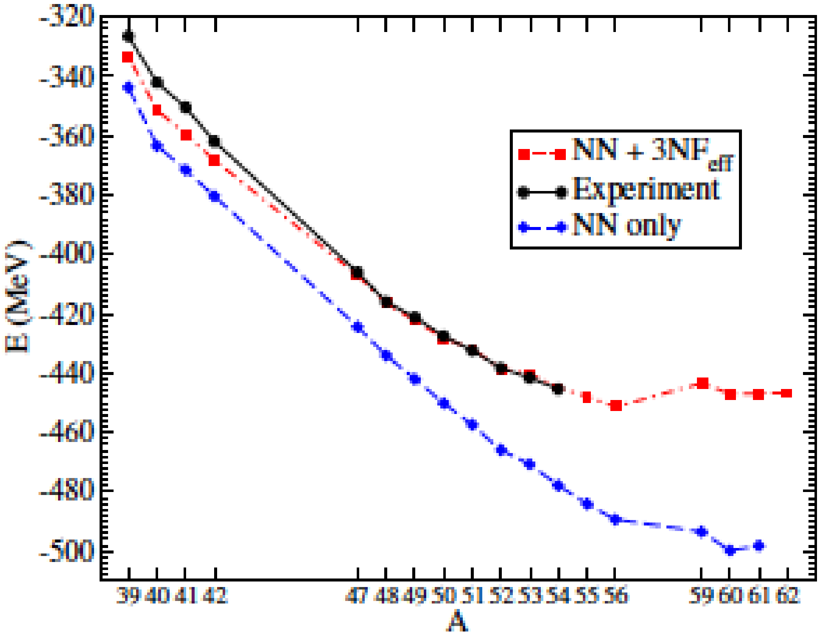
Basis states that incorporate continuum effects

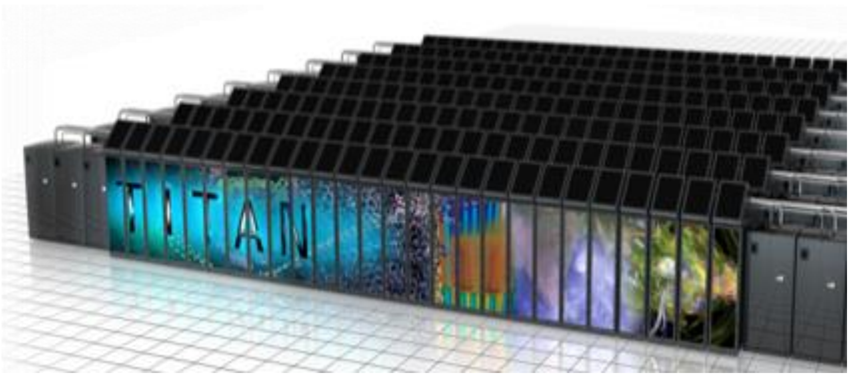


- Basis includes bound, scattering, and continuum states
- Berggren basis

Dean & Hjorth-Jensen, PRC69, 054320 (2004); Kowalski et al., PRL 92, 132501 (2004); Wloch et al., PRL94, 212501 (2005) Gour et al., PRC (2006); Hagen et al, PLB (2006); PRC 2007a, 2007b; Dean, Phys. Today (Nov, 2007)

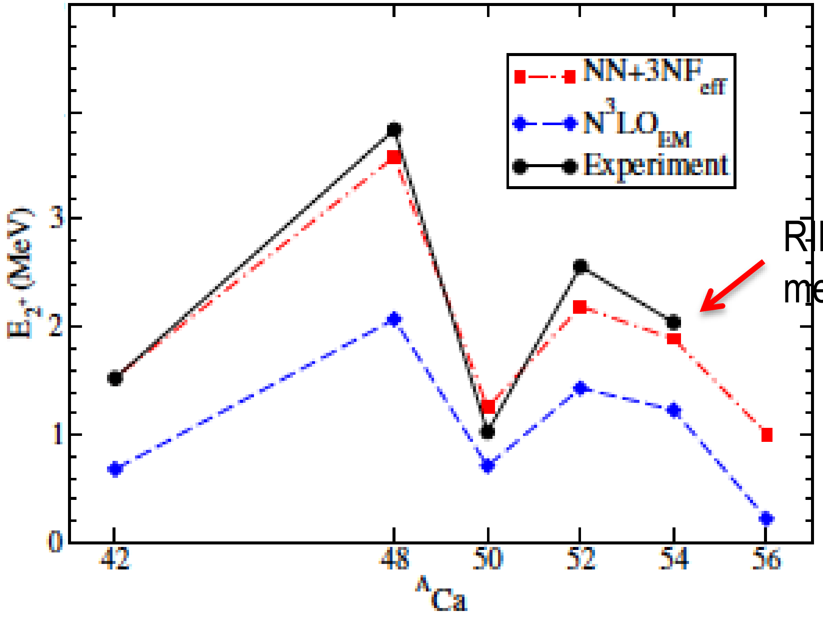
Investigating weakly bound nuclei





How does one approach the drip line (quickly, smoothly, or asymptotically)?

Are there new shell structures beyond our standard nuclear magic numbers?



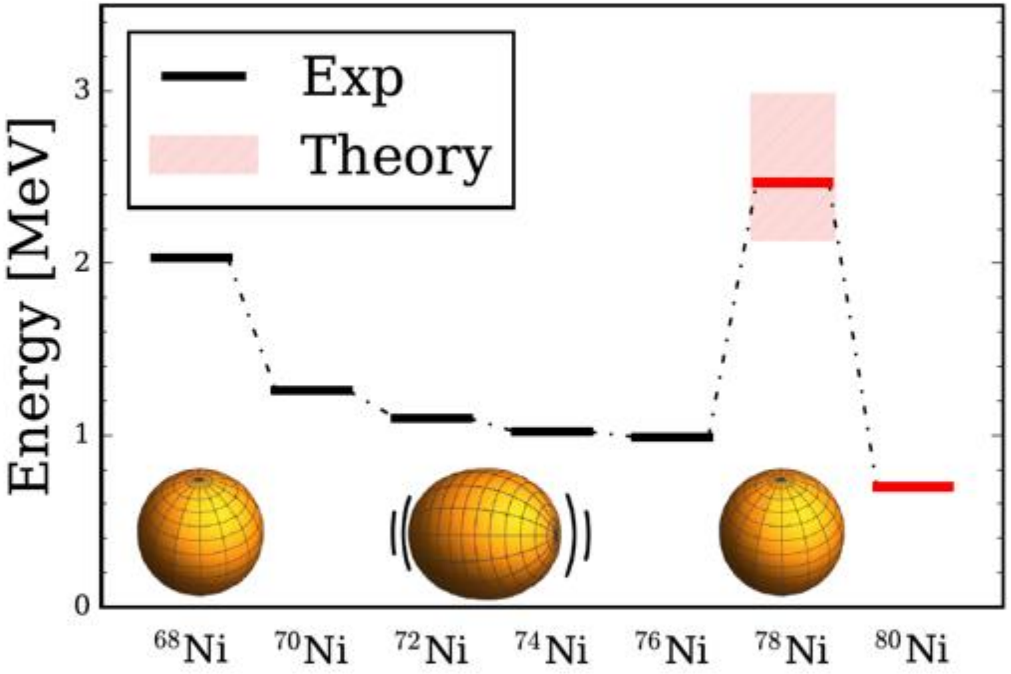
RIKEN measurement

Rep. Prog. Phys. 77, 096302 (2014)

FRIB key nucleus ^{78}Ni

- Supposedly doubly magic nucleus (Z=28, N=50)
- Extreme N/Z ratio magnifies unknown aspects of the nuclear force
- Relevant nucleus for r-process physics / synthesis of heavy elements
- Key nucleus for FRIB and other rare ion beam facilities world wide

- ➢ First results: **FY 2017**
- ➢ Pickup, knockout, and transfer reactions: **FY 2019**
- ➢ Full UQ: **FY 2020**



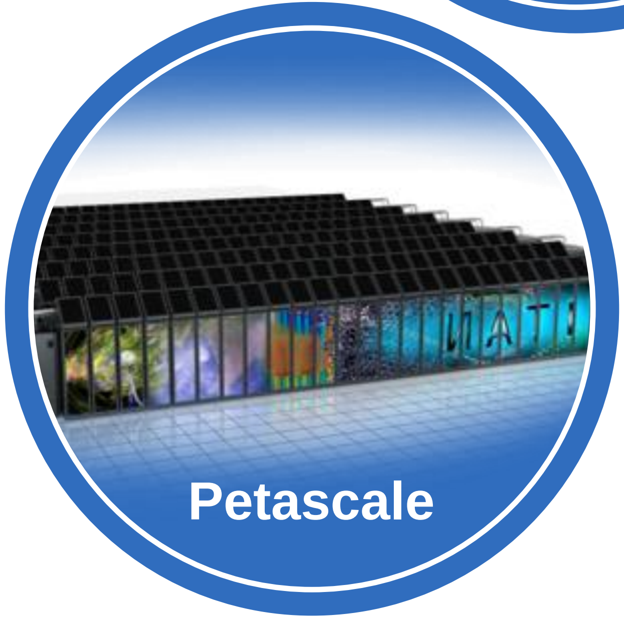
- ▪ We predict that ^{78}Ni is doubly magic due to the relatively high 2^+ excited state
- ▪ We predicted the single-particle structure in ^{79}Ni as basis for shell-model calculations

G. Hagen, G. R. Jansen, and T. Papenbrock, PRL **117**, 172501 (2016)

What the future holds

- Applications on near exascale and exascale machines will provide spectacular physics insights
- The translation of a substantial nuclear physics problem to a quantum computing architecture will be
  - Difficult
  - Worthwhile if the noise from the QC is low
  - QC could offer a unique platform for beyond mean-field scattering/reaction/decay problems (time dependence)
  - Usefulness depends on algorithm development for calculation of many experimental observables (e.g., excited states, beta-decay, LAMC, nuclear-astro reactions, etc…)
- Years of EFT, Coupled Cluster theory and other many-body developments will enable an excellent starting point for a QC application

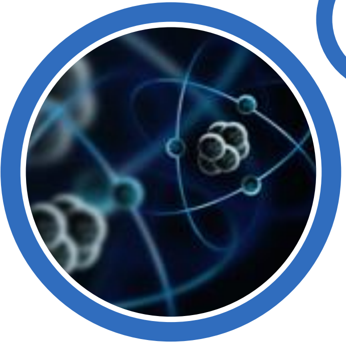
Discussion


Petascale


Pre-exascale


Exascale


Quantum

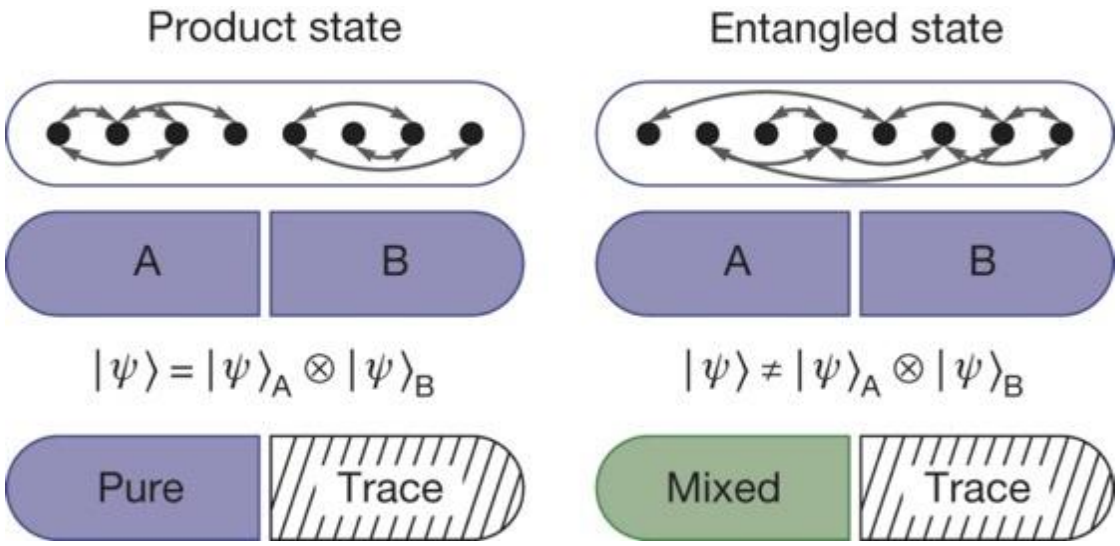


Toward entanglement

The Hamiltonian DRIVES entanglement

For a pure state $\hat{T}r\,r^2 = 1$

For a mixed state $\hat{T}r\,r^2 < 1$



R Islam *et al. Nature* **528,** 78 (2015) doi:10.1038/nature15750

Use a fundamental property of entanglement between two subsystems (bipartite entanglement): ignoring information about one subsystem results in the other becoming a classical mixture of pure quantum states.

$$\hat{T}r\,r_A^2 = \hat{T}r\,r_B^2 = \hat{T}r\,r_{AB}^2 = 1$$

$$\hat{T}r\,r_A^2 = \hat{T}r\,r_B^2 < \hat{T}r\,r_{AB}^2 = 1$$

$$\hat{T}r\,r_A^2 < \hat{T}r\,r_{AB}^2$$

$$\hat{T}r\,r_B^2 < \hat{T}r\,r_{AB}^2$$

If AB is mixed these relations still hold

Entanglement produces ”HUGE” information storage

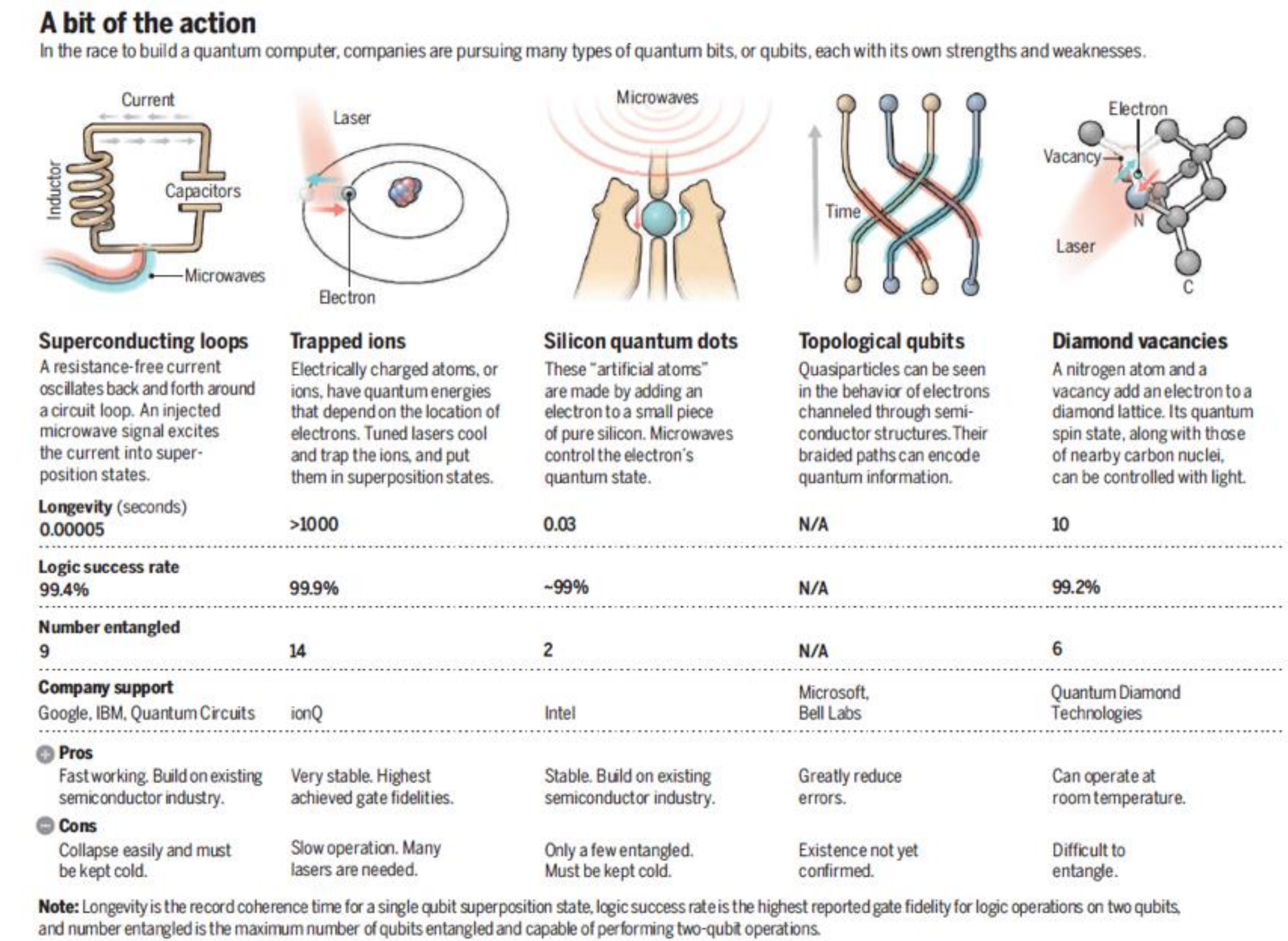
$$2^n$$

$$C(n,r) = \frac{n!}{(n-r)!\,r!}$$

Number of qubits	Classical storage	Non-interacting classical storage	Fully entangled classical storage
1	1	2	2
2	1	4	6
4	1	8	70
8	1	256	12,870
16	1	65,536	601,080,390
64	1	$1.8\text{x}10^{19}$	$2.4\text{x}10^{37}$
100	1	$1.2\text{x}10^{30}$	$9\text{x}10^{58}$ (number of atoms in universe)

- Issues
  - Fidelity of the computation
  - Entanglement across a large number of qubits
  - Lifetime of the information
  - Error

Science 354, 1091 (2016) – 2 December

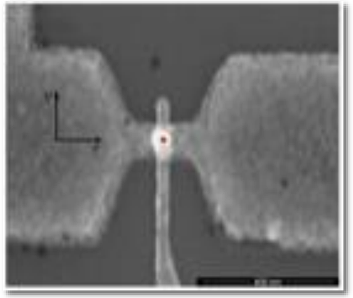


A bit of the action

In the race to build a quantum computer, companies are pursuing many types of quantum bits, or qubits, each with its own strengths and weaknesses.

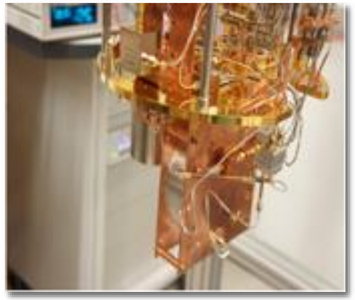
	Superconducting loops	Trapped ions	Silicon quantum dots	Topological qubits	Diamond vacancies
	A resistance-free current oscillates back and forth around a circuit loop. An injected microwave signal excites the current into superposition states.	Electrically charged atoms, or ions, have quantum energies that depend on the location of electrons. Tuned lasers cool and trap the ions, and put them in superposition states.	These "artificial atoms" are made by adding an electron to a small piece of pure silicon. Microwaves control the electron's quantum state.	Quasiparticles can be seen in the behavior of electrons channeled through semiconductor structures. Their braided paths can encode quantum information.	A nitrogen atom and a vacancy add an electron to a diamond lattice. Its quantum spin state, along with those of nearby carbon nuclei, can be controlled with light.
Longevity (seconds)	0.00005	>1000	0.03	N/A	10
Logic success rate	99.4%	99.9%	~99%	N/A	99.2%
Number entangled	9	14	2	N/A	6
Company support	Google, IBM, Quantum Circuits	ionQ	Intel	Microsoft, Bell Labs	Quantum Diamond Technologies
⊕ **Pros**	Fast working. Build on existing semiconductor industry.	Very stable. Highest achieved gate fidelities.	Stable. Build on existing semiconductor industry.	Greatly reduce errors.	Can operate at room temperature.
⊖ **Cons**	Collapse easily and must be kept cold.	Slow operation. Many lasers are needed.	Only a few entangled. Must be kept cold.	Existence not yet confirmed.	Difficult to entangle.

Note: Longevity is the record coherence time for a single qubit superposition state, logic success rate is the highest reported gate fidelity for logic operations on two qubits, and number entangled is the maximum number of qubits entangled and capable of performing two-qubit operations.



characterize

HREM, APT, SPM
Multiscale modeling



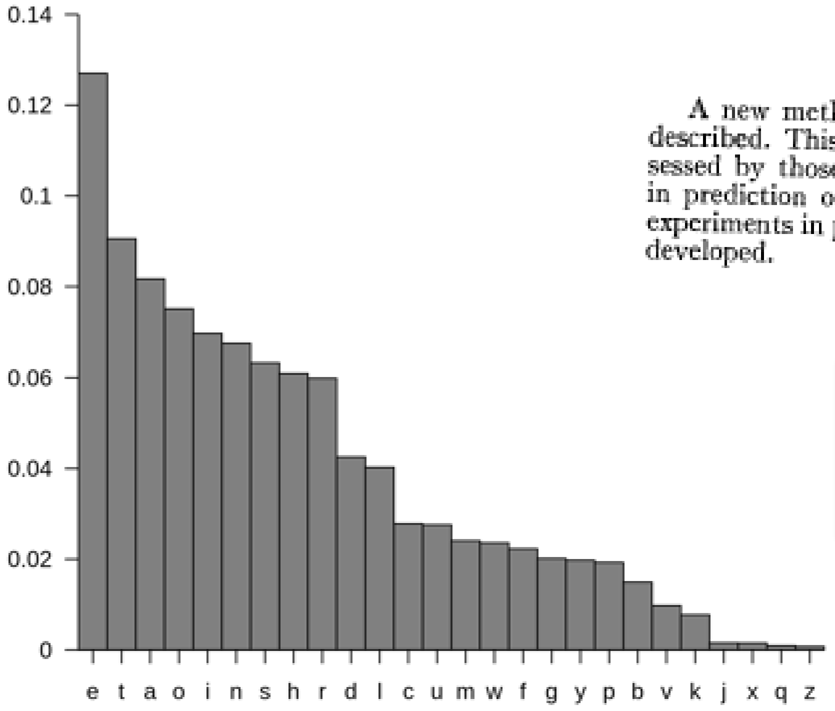
Classical quantum interface

From mK to 300K

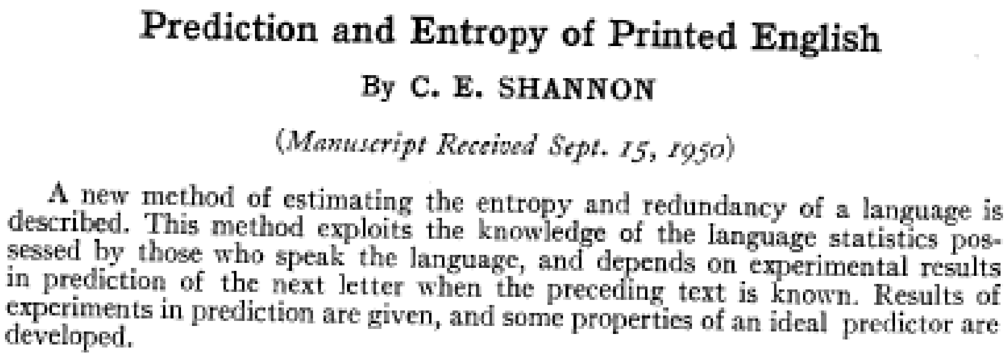
Program Qubits

QIS and other groups

Entropy: how to calculate something



Without correlation: 4.7 bits of entropy
With correlation: English text has between 0.6 and 1.3 bits of entropy for each character of message.



Prediction and Entropy of Printed English

By C. E. SHANNON

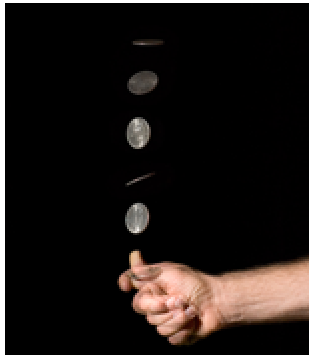
(*Manuscript Received Sept. 15, 1950*)

A new method of estimating the entropy and redundancy of a language is described. This method exploits the knowledge of the language statistics possessed by those who speak the language, and depends on experimental results in prediction of the next letter when the preceding text is known. Results of experiments in prediction are given, and some properties of an ideal predictor are developed.

- Translation to quantum systems?
- What does it mean?
- What is the application?

$$S(E) = \sum_i p_i \log_2 p_i$$

Classical coin tosses and entropy



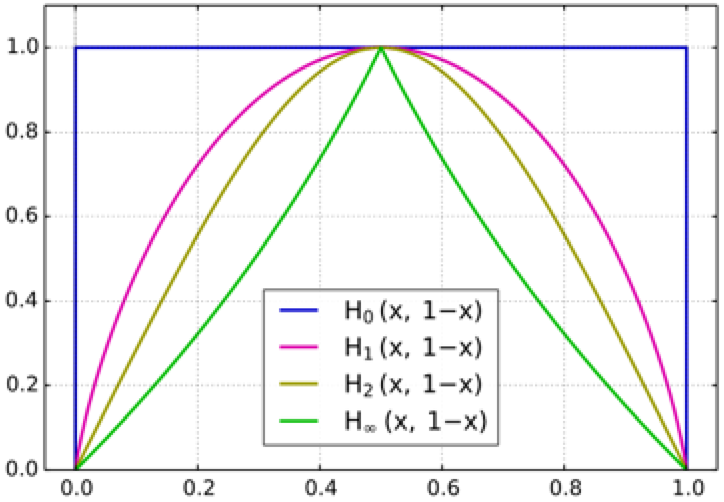
Generalized Re'nyi Entropies

$$H_\alpha(x) = \frac{1}{1-\alpha}\log_2\left(\sum_i p_i^\alpha\right)$$

$$p_i = \Pr(x=i) \text{ for } i = 1, 2, \ldots, n$$

1 Shannon is the information content of an event when the probability of that event occurring is ½)

α=1 is the Shannon entropy



In quantum mechanics, define $\rho = e^{-\beta\hat{H}}$

$$Z = \hat{T}r\,\hat{\rho}$$

$$S_\alpha = \frac{1}{1-\alpha}\log\frac{Z_{\alpha,A}}{Z^\alpha} = \frac{1}{1-\alpha}\log\rho_A^\alpha$$

Entanglement represents the unique correlation property of quantum states, without any classical counterpart, and as such it can play a fundamental role in our understanding of quantum many-body phases from the point of view of non-local correlations. (see e.g., Humeniuk & Roscilde, arXiv:1203.5752)

Tagliacozzo, Evenbly, Vidal, Phys. Rev. B 80, 235127 (2009)

How to calculate Trρ^2

$$Y_{1,N}(\beta) = \frac{Z_N(\beta)}{Z_A(\beta)} = \frac{\hat{T}r\hat{P}_N\hat{U}}{\hat{T}r\hat{P}_A\hat{U}}$$

$$\hat{P}_A = \delta\left(A - \hat{A}\right)$$

$$\hat{P}_N = \delta\left(N_p - \hat{N}_p\right)\delta\left(N_h - \hat{N}_h\right)$$

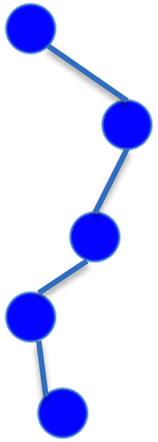
$$A = N_p + N_h$$

$$\sum_{i=0,N} Y_{1,N}(\beta) = 1$$

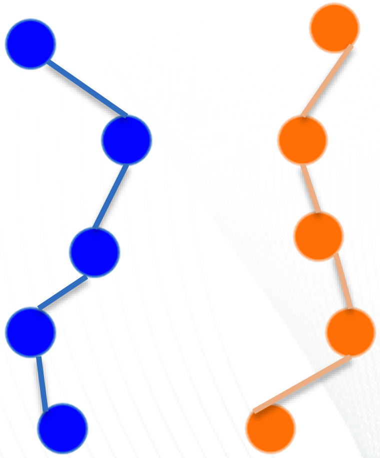
Dean & Koonin, PRC60, 054306 (1999)

$$\rho_N^2(\beta) = \frac{Z_{2,N}(\beta)}{Z_A^2(\beta)} = \frac{\hat{T}r\hat{P}_N\hat{U}\hat{U}}{\hat{T}r\hat{P}_A\hat{U}\,\hat{T}r\hat{P}_A\hat{U}}$$

See e.g., Milko et al., PRB 82, 100409 (2010)
Iaconis et al, PRB 87, 195134 (2013)

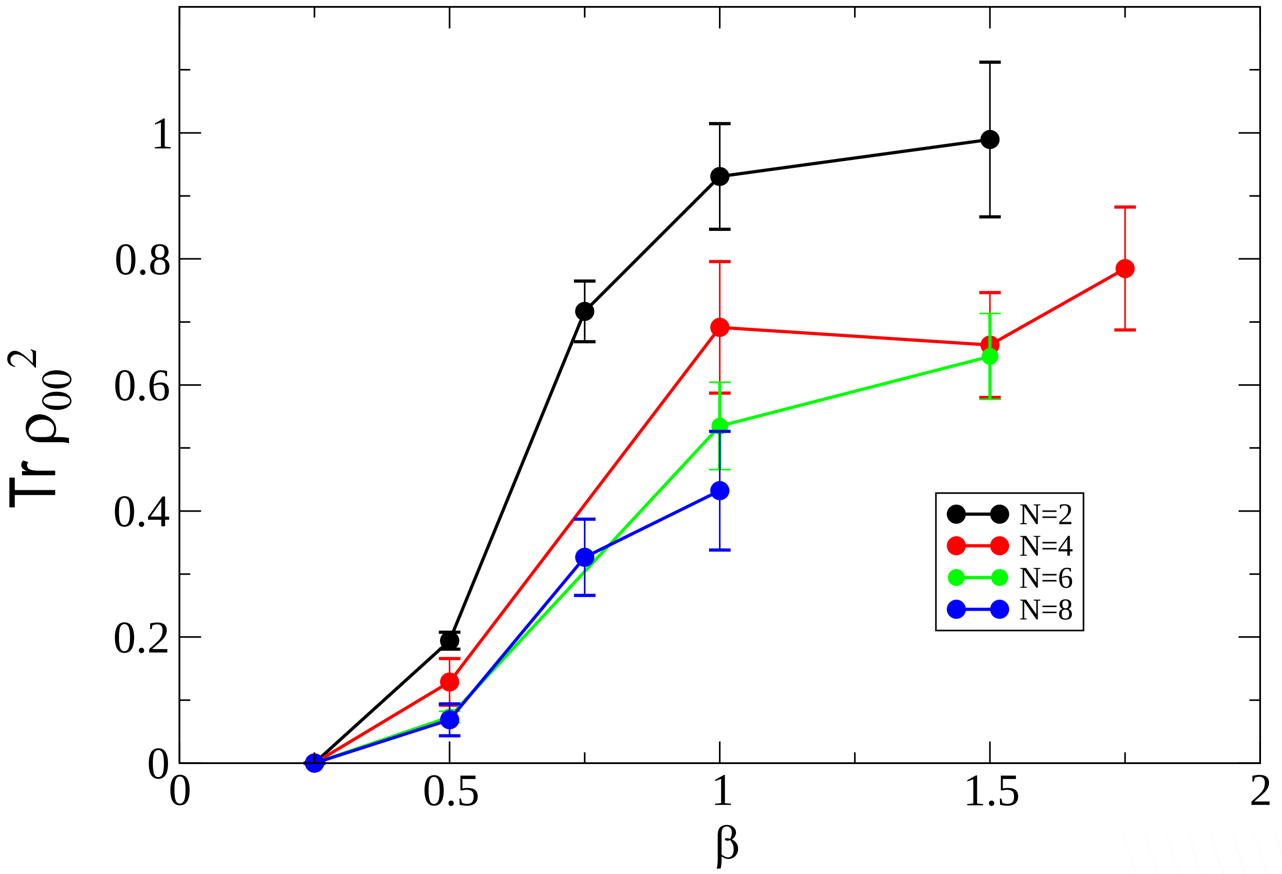


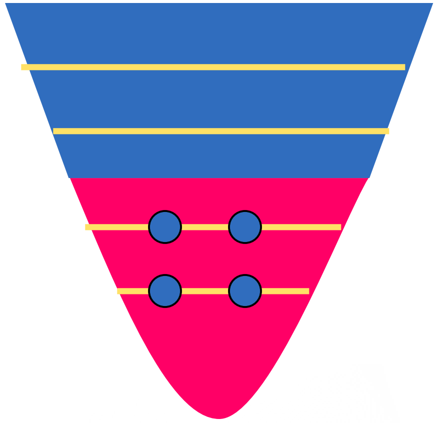
Standard observables:
one auxiliary field



UU observables:
two auxiliary fields

Results: Pairing

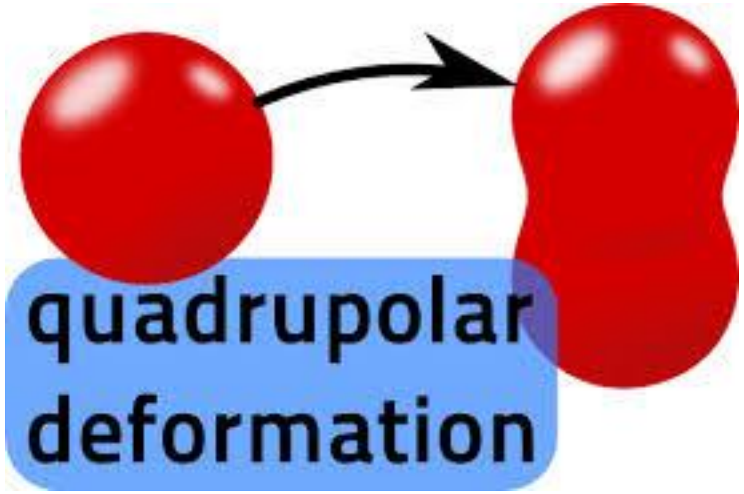




Spin ½ states
(24 levels)

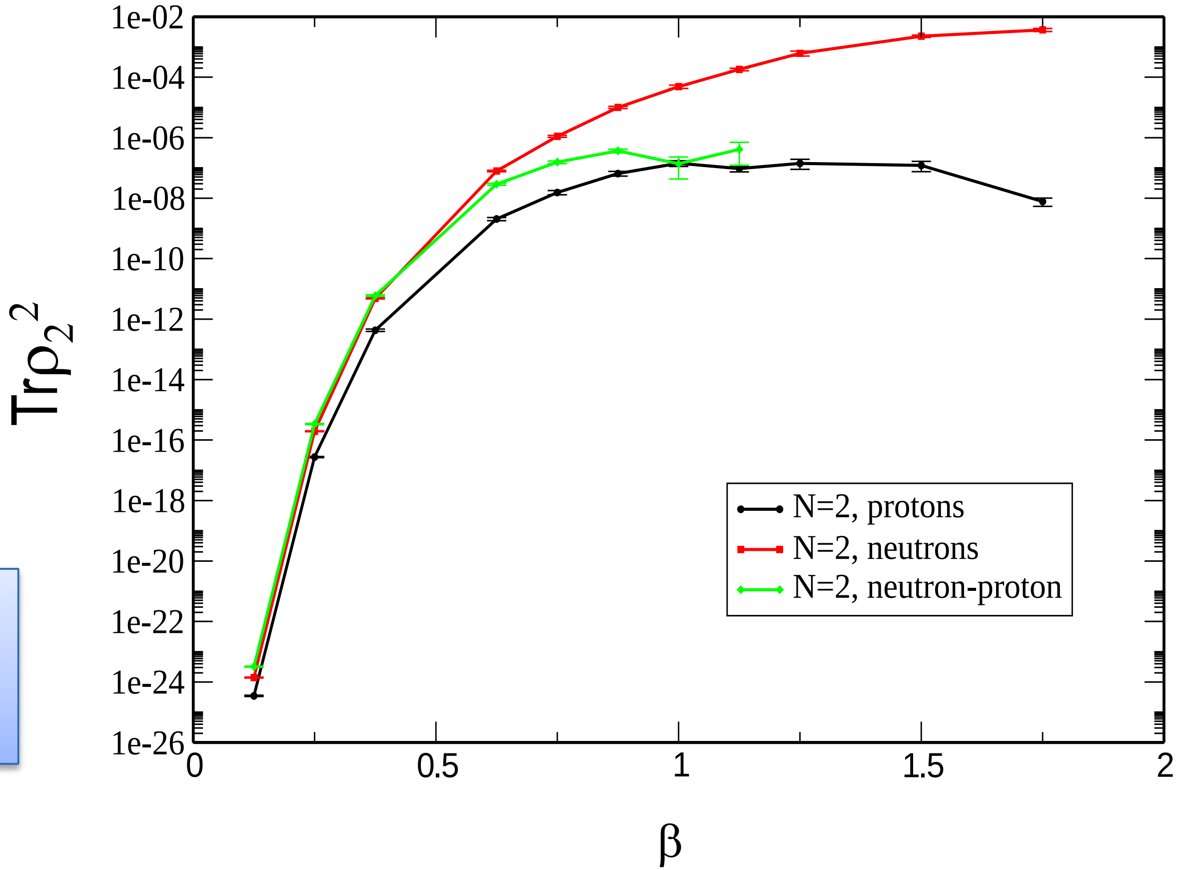
$$H = d\sum_{i=1}^{L} N_i a_i^+ a_i + G\sum_{i\le j} a_i^+ a_j^+ a_{\bar{j}} a_{\bar{i}} \qquad N_i = i$$

Collective effect in a nucleus…



Question: Do collective effects, which we have not yet anticipated, occur in multi-qubit systems?

68Ni enhanced quadrupole interaction, QMC calculation



Dean, in prep

Improvements

- Add SVD or UQ to give stable partial density calculation
- Do a deformed nucleus (like Zr80)
- Try this out on a slab of Si (from a DFT calculation) to simulate qubit entanglement
  - Add noise
- Use a time-dependent coupled-cluster approach to investigate coherence time in multi qubit systems (Pigg et al, PRC86, 014308 (2012) – *almost ready to show results, but not quite*