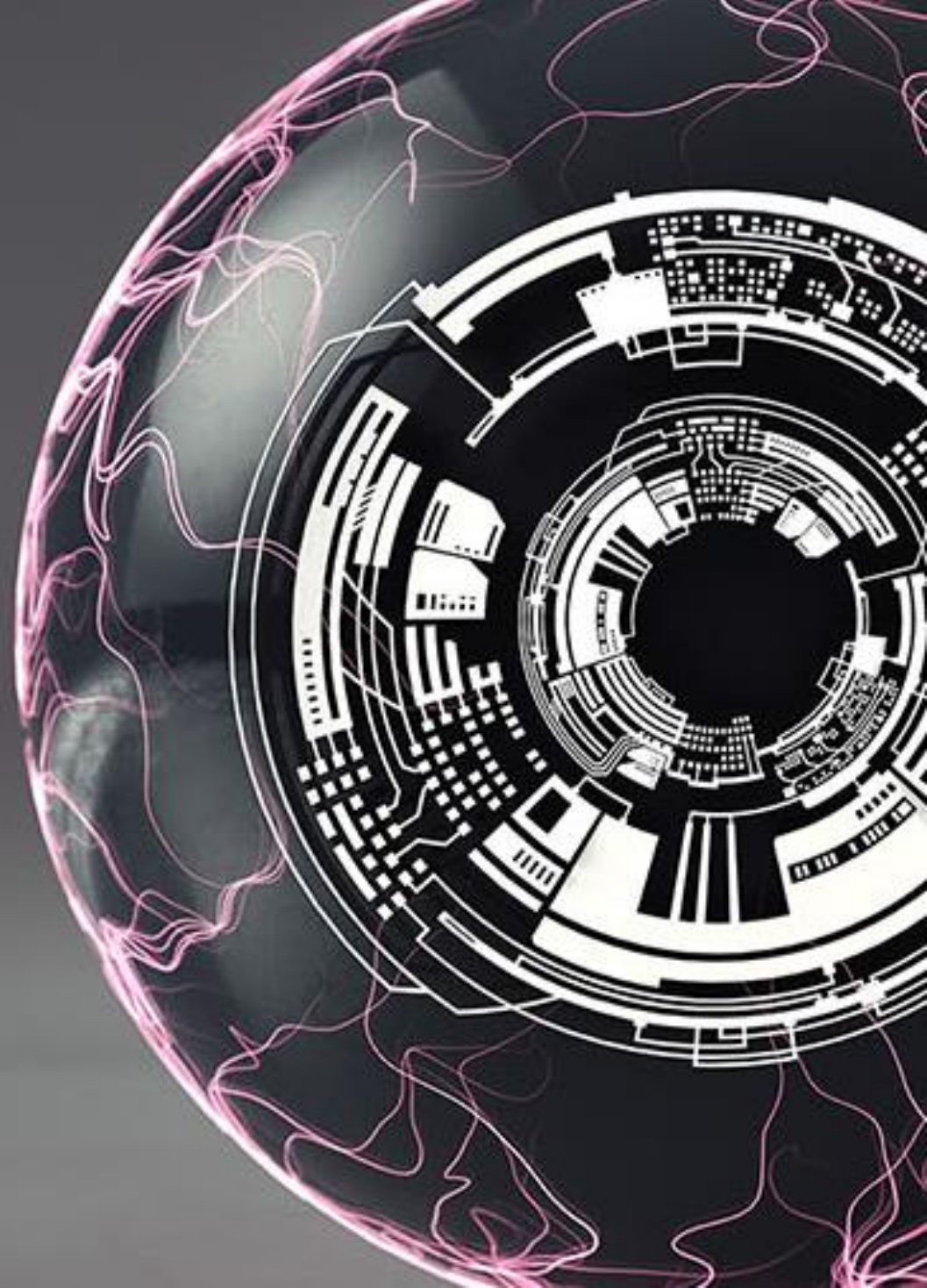


Microsoft Research
Faculty
Summit
2016



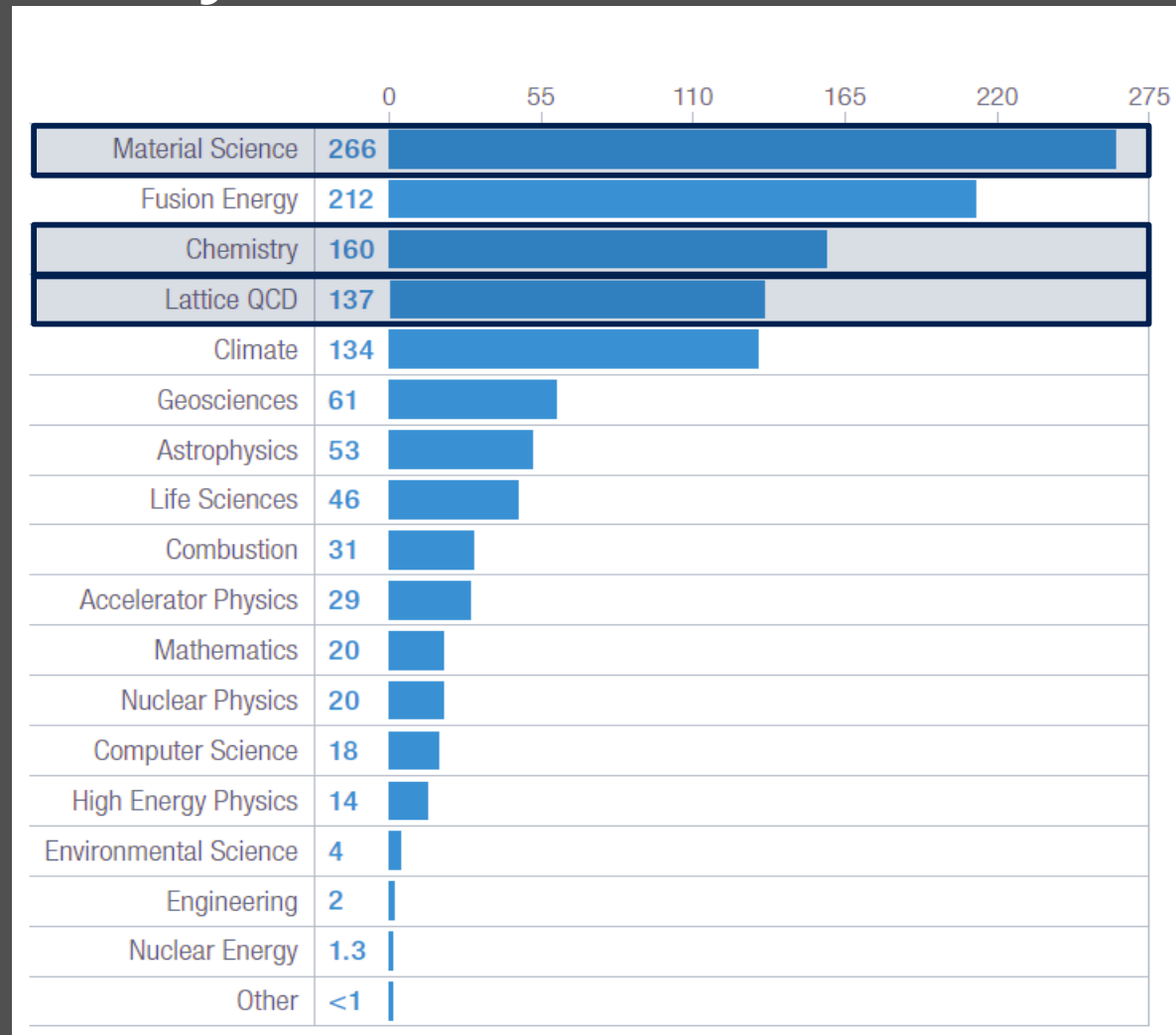
Quantum Algorithms: Today and Tomorrow

Dave Wecker
Microsoft Research, StationQ



Simulating physical systems

Hours (on Cray XE6)



The promise...

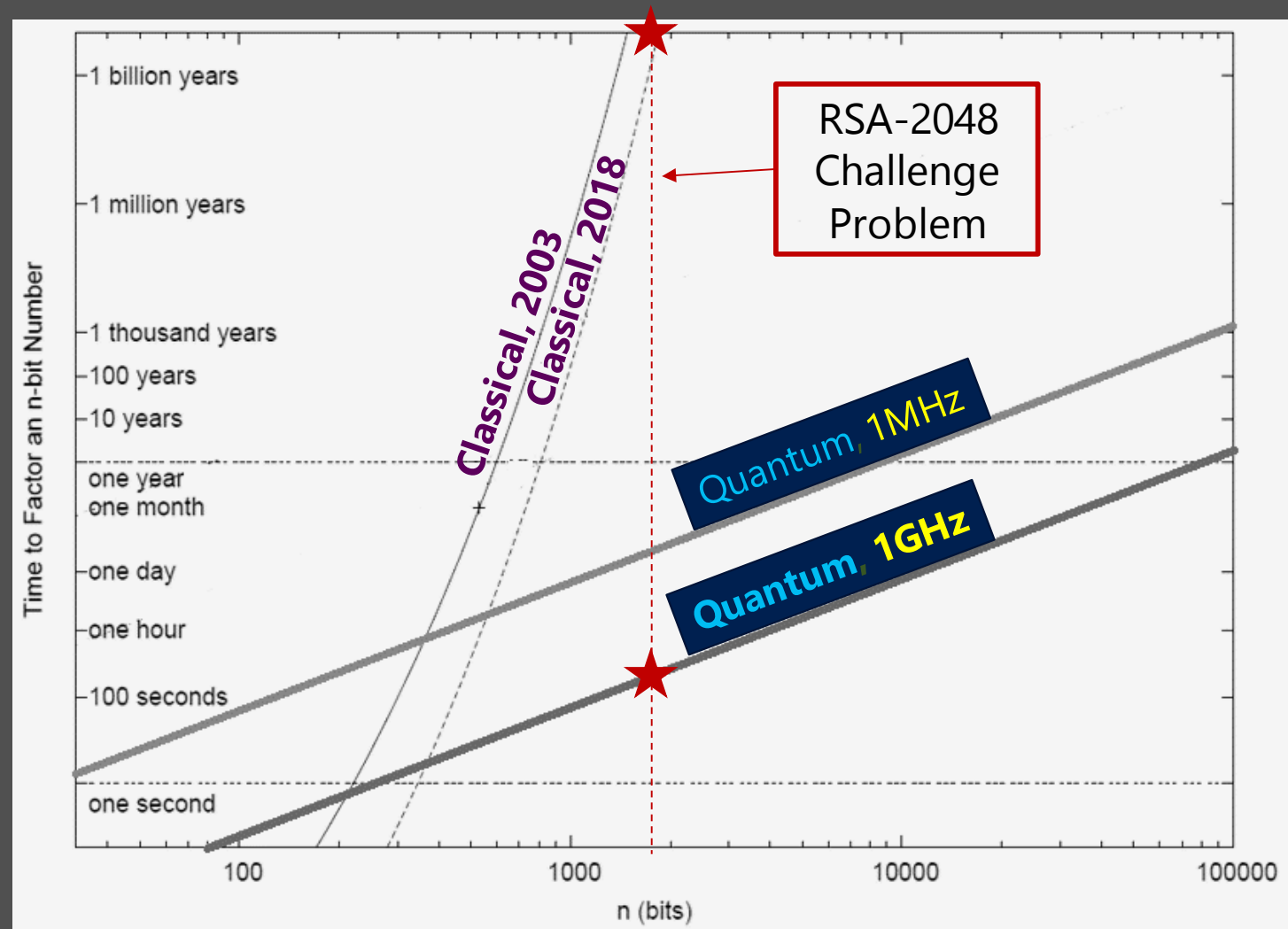
Simulating 250 interacting qubits
requires $\sim 10^{80}$ classical bits!

State of N interacting qubits: $\sim 2^N$ bits of info!



Breaking RSA

Time to Factor N-bit Number



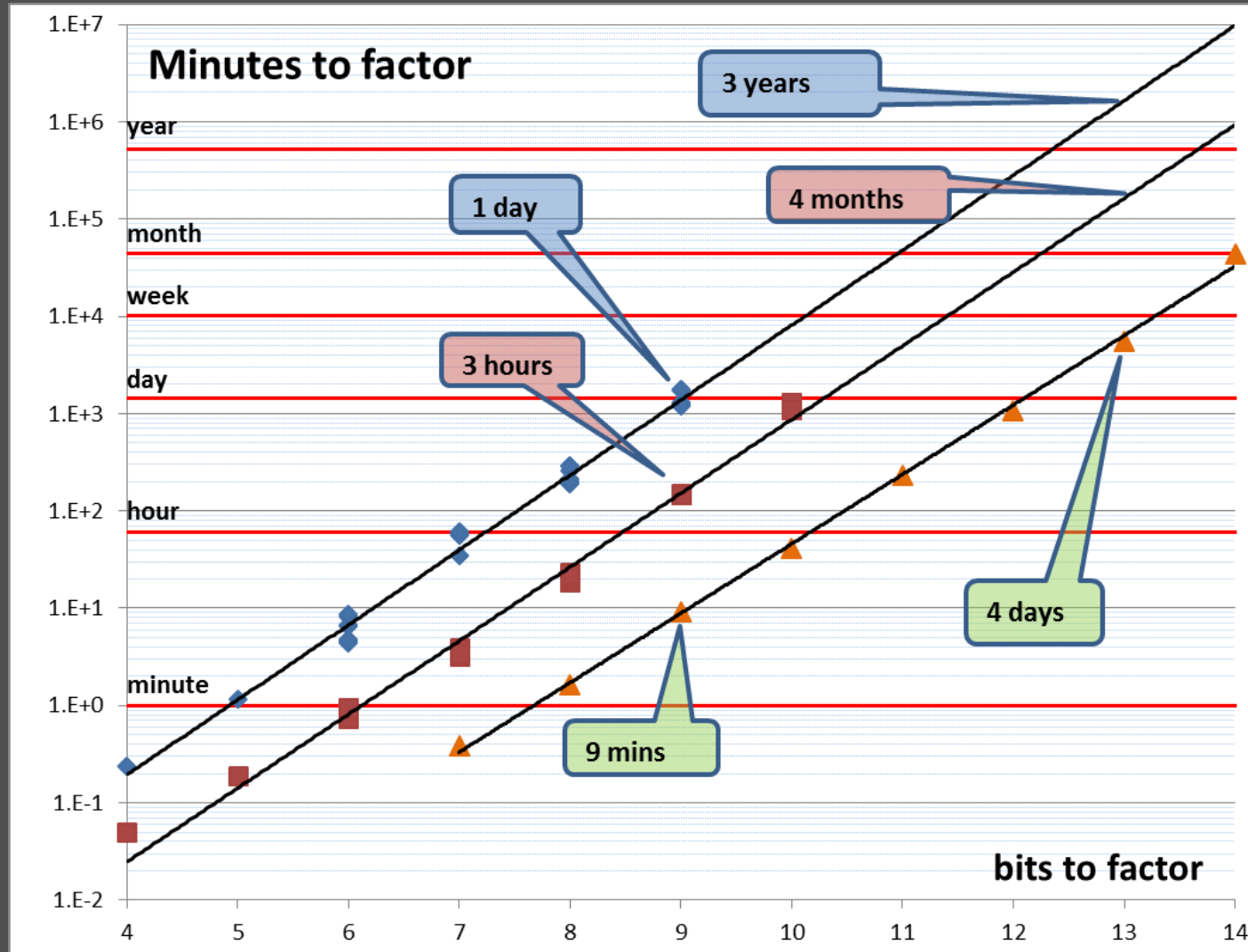
Number of bits N

LIQ*U*i| \rangle Efficient Classical Simulation of Quantum Algorithms

- Only materialize entangled parts of state vector (Skyline Vectors)
- Re-order tensor products of gates to keep gate matrix dense
- Permute state vector to block-diagonalize generated sparse matrix
- Permute gate matrix to keep from re-ordering state vector
- Grow gate matrix to keep from re-ordering state vector
- Keep a running permutation until measurement
- Use measurement to shrink memory usage of state vectors
- Coalesce gates into more efficient larger arrays
- For Hamiltonians only maintain physically achievable states
- Exponentiate system for Trotter and Phase Estimation calculations
- Re-unitarize exponentiated matrices to maintain accuracy



Shor's algorithm results



Quantum Chemistry

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

Can quantum chemistry be performed on a small quantum

computer: David
Hastings, Matthew

As quantum computers will appear feasible applications of frequently meeting simulating quantum structure of molecules computational perform quantum the quantum molecule twice exactly. We first increase in the required increase executed is more quantum computing problems, draft <http://arxiv.org/abs/1508.00410>

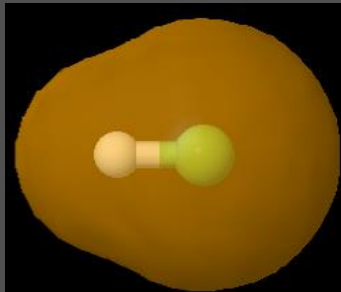
Ferredoxin (Fe_2S_2) used in many metabolic reactions including energy transport in photosynthesis

- *Intractable on a classical computer*
- *Assumed quantum scaling: ~24 billion years (N^{11} scaling)*
- *First paper: ~850 thousand years to solve (N^9 scaling)*
- *Second paper: ~30 years to solve (N^7 scaling)*
- *Third paper: ~5 days to solve ($N^{5.5}$ scaling)*
- *Fourth paper: ~1 hour to solve ($N^3, Z^{2.5}$ scaling)*

Molecules simulated in LIQUi|⟩



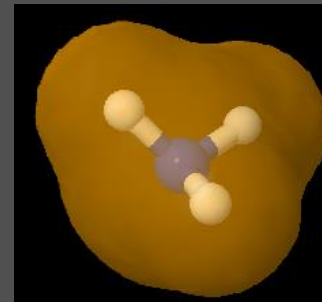
H_2



HF



H_2O



NH_3



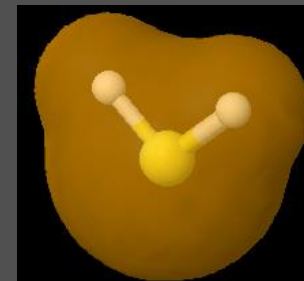
CH_4



HCl



F_2

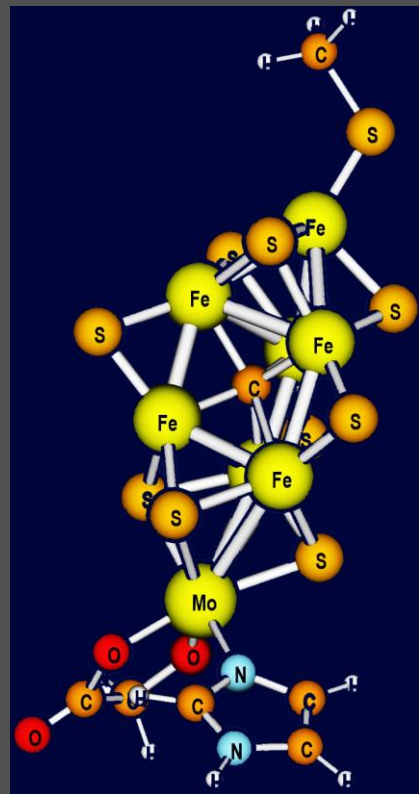
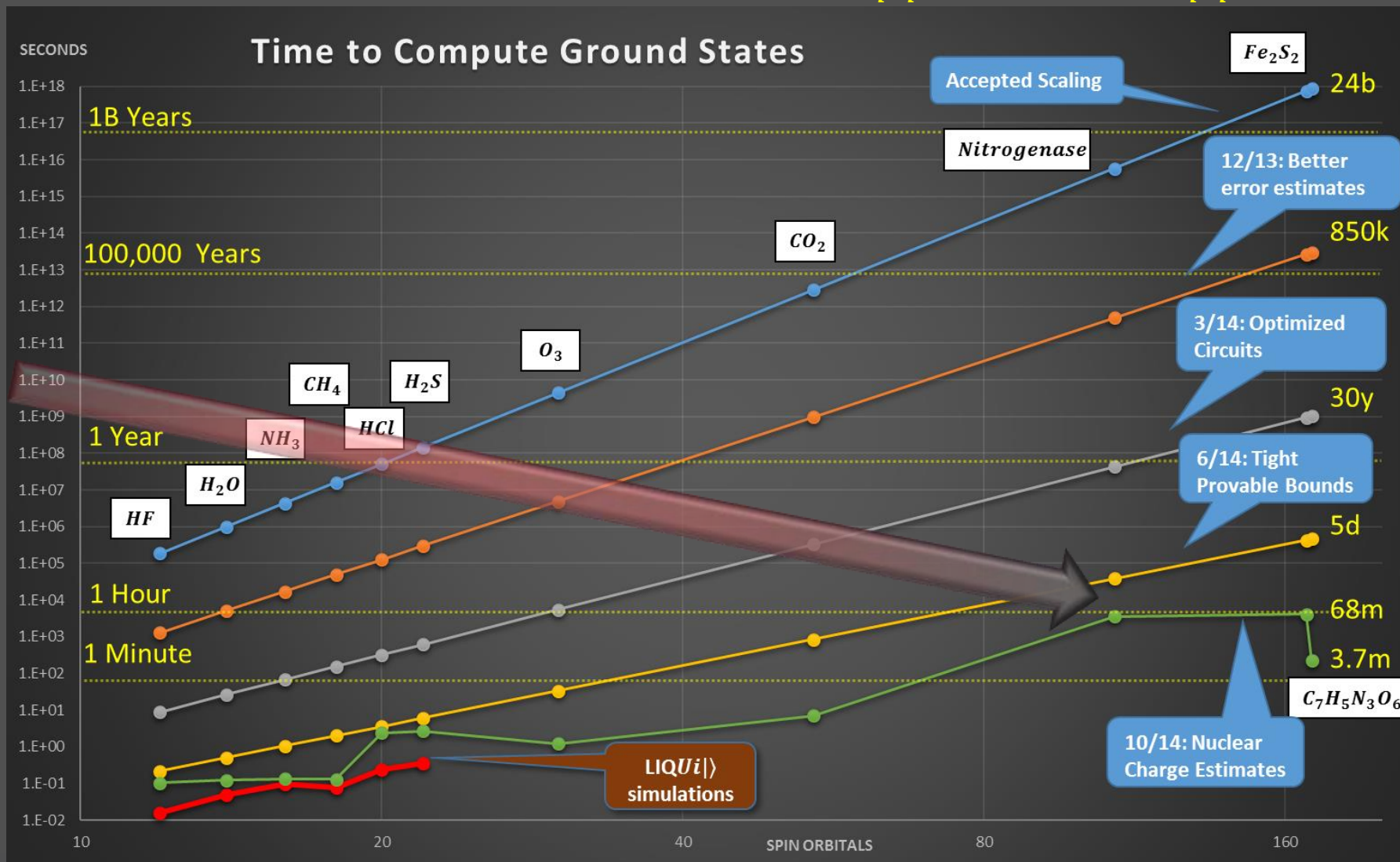


H_2S

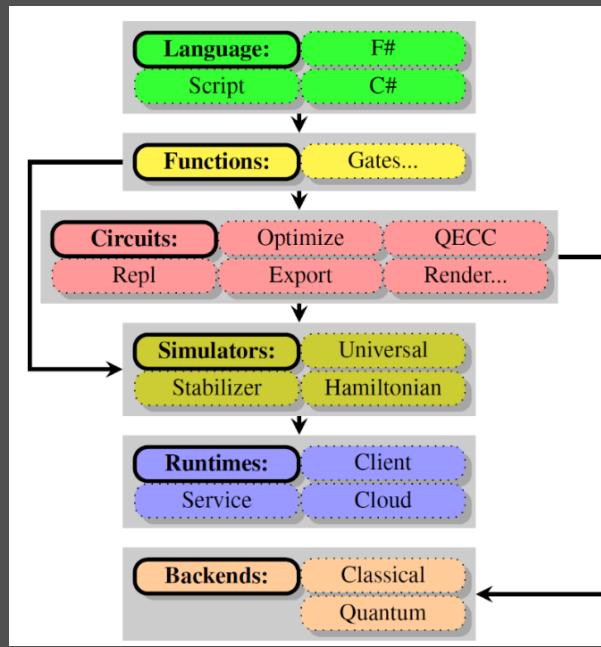
Geometries and molecular models from <http://www.colby.edu/chemistry/webmo/>

Simulation Evidence

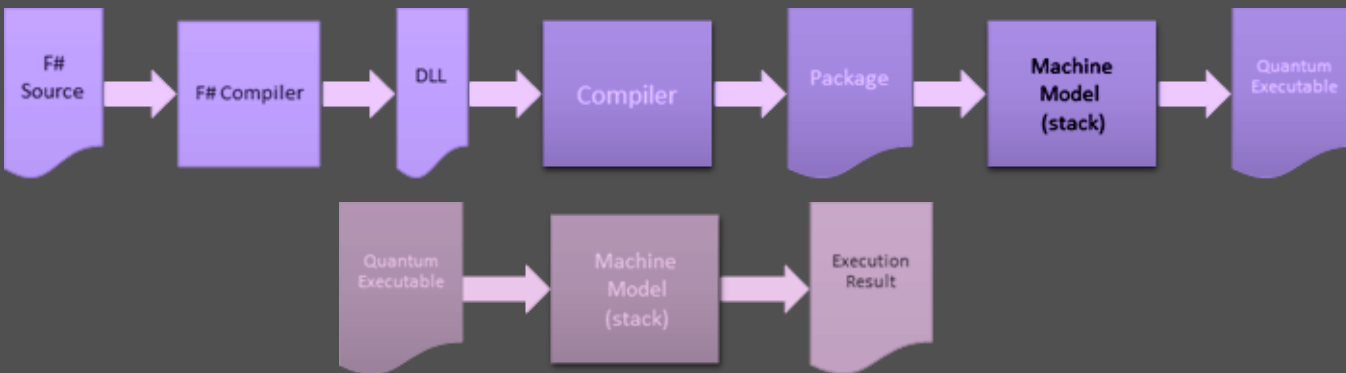
$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$



LIQUi|>



SoLi|> and QCoDeS



<http://StationQ.github.io/Liquid>

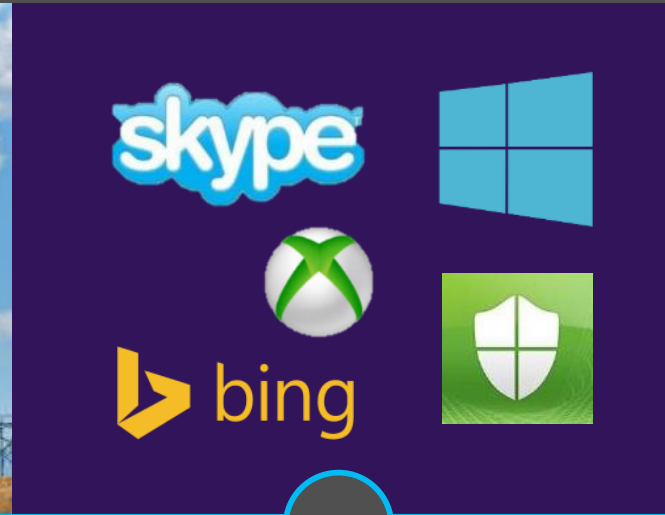
Initial applications

Nitrogen
fixation

Carbon
capture

Materials
science

Machine
learning



100-200
qubits

100-200
qubits

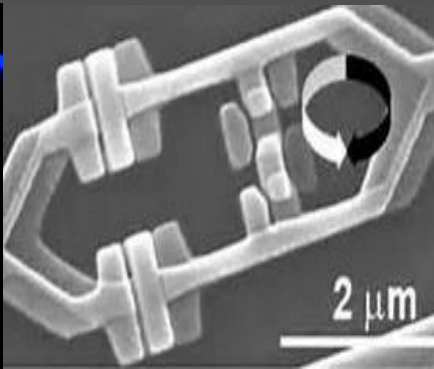
100s-1000s
qubits

100s-1000s
qubits

Quantum hardware technologies



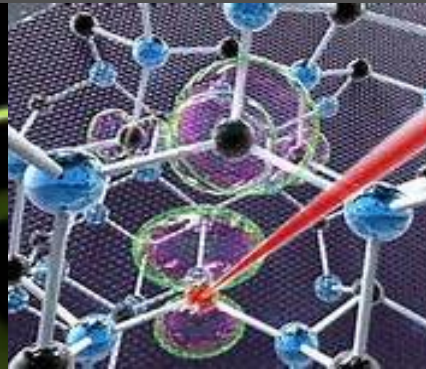
Ion traps



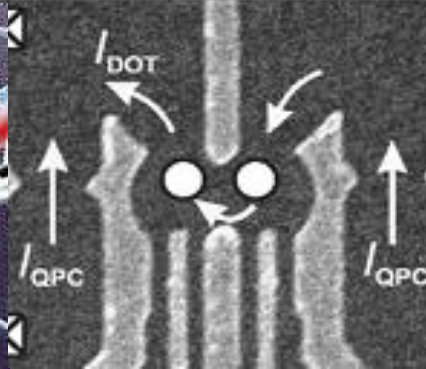
Superconductors



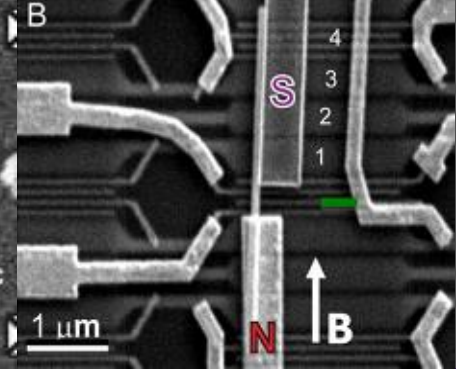
Linear optics



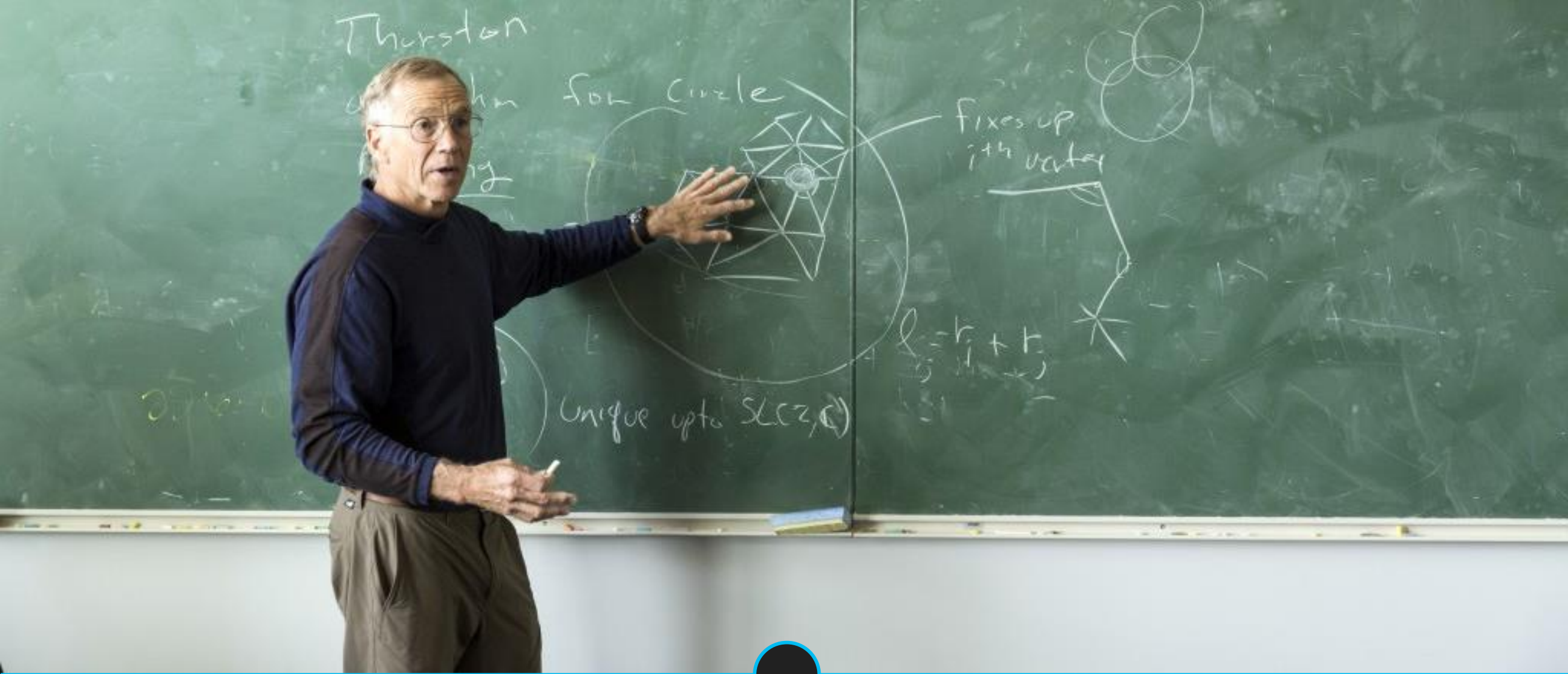
NV centers



Quantum dots



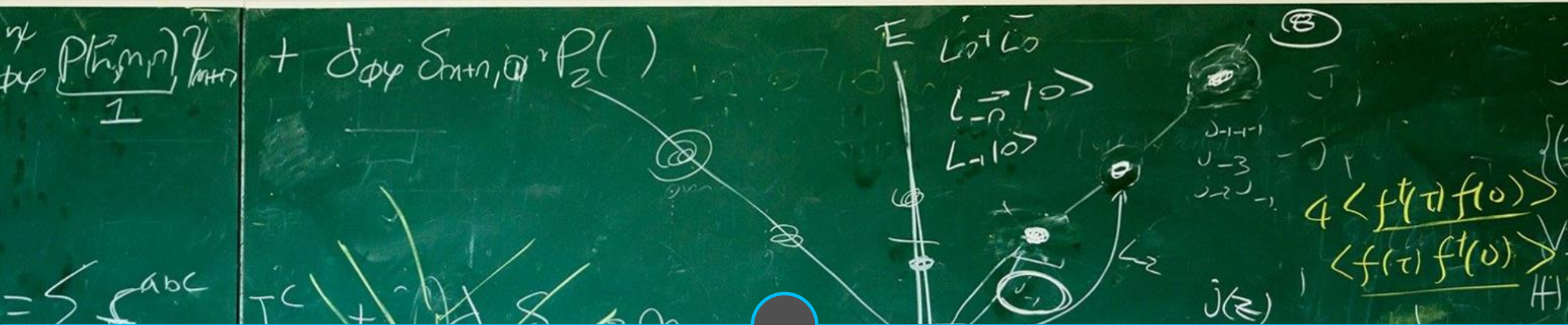
Topological



2000

STATION

Q



2006

“ MAJORANA PARTICLE
GLIMPSED IN LAB. ”

—
BBC NEWS

○
2012

Experimental Results

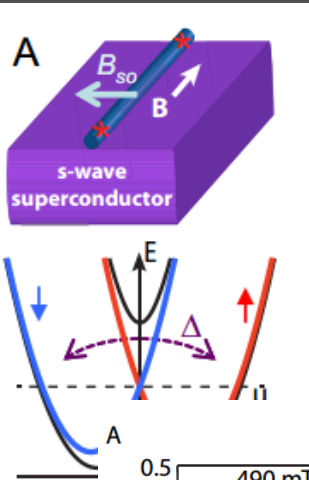
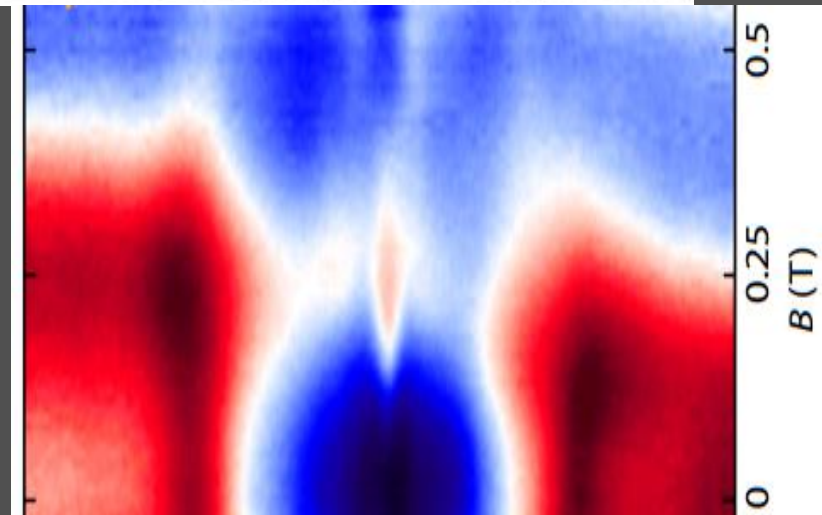
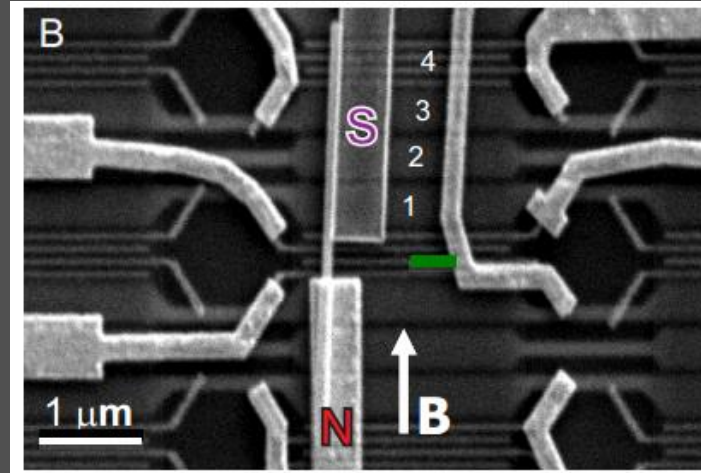
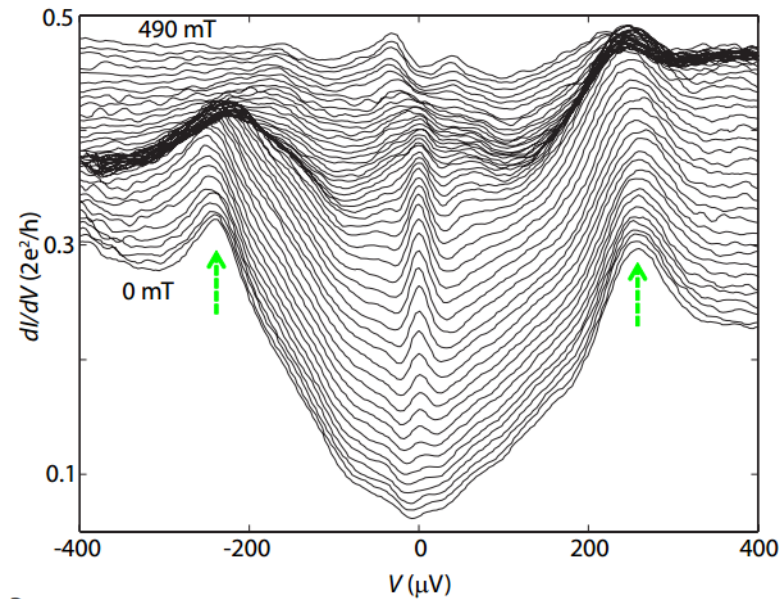


Figure 2



- Build experiment as described
- Measure zero-bias peak
- See that it goes away if we remove any of the necessary components

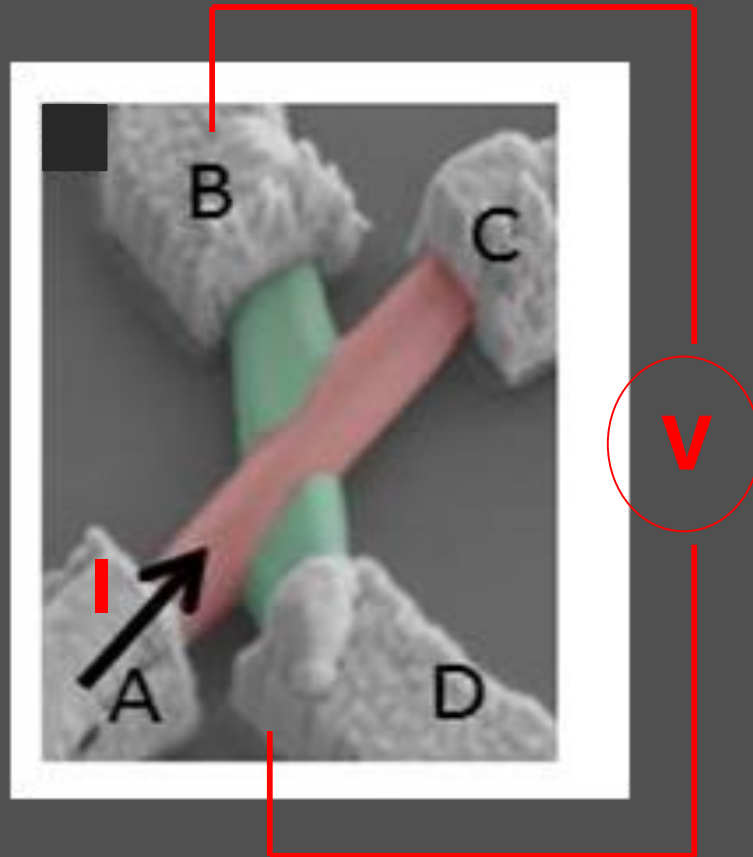
Mourik, ... Kouwenhoven 2012
<http://arxiv.org/abs/1204.2792>



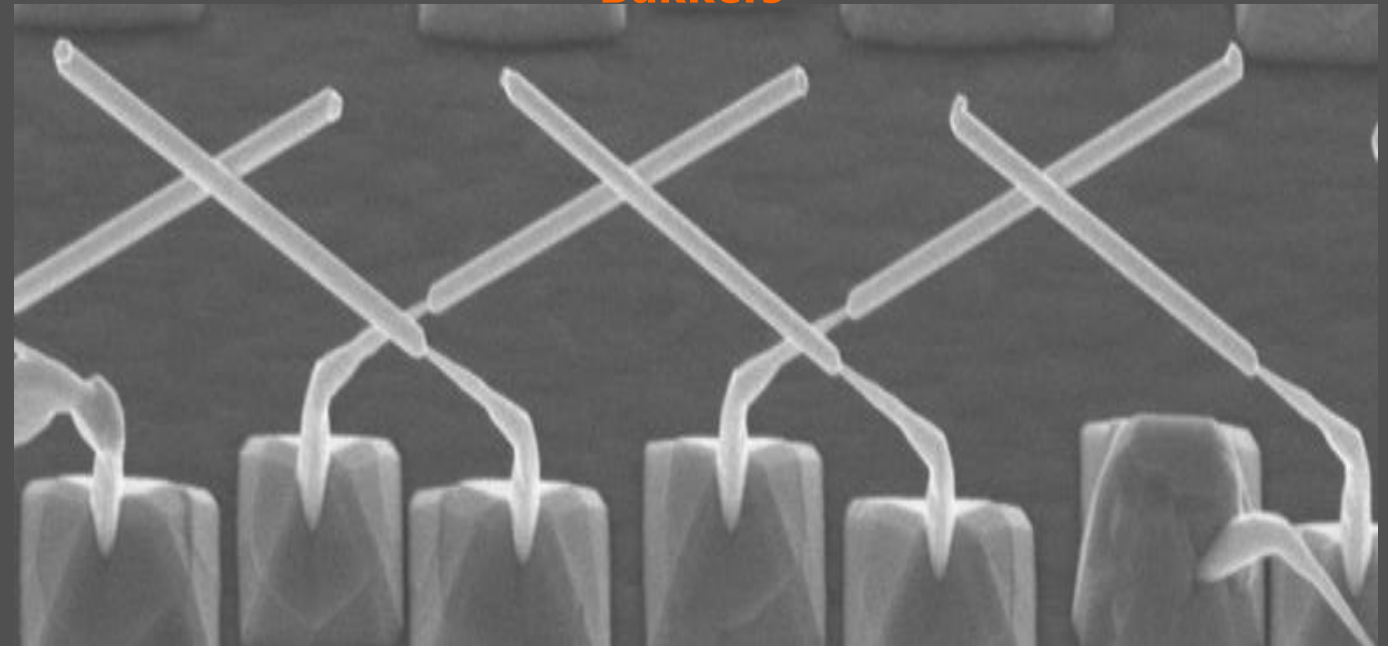
Charlie Marcus' lab in Copenhagen, Denmark
One of our primary experimental collaborators



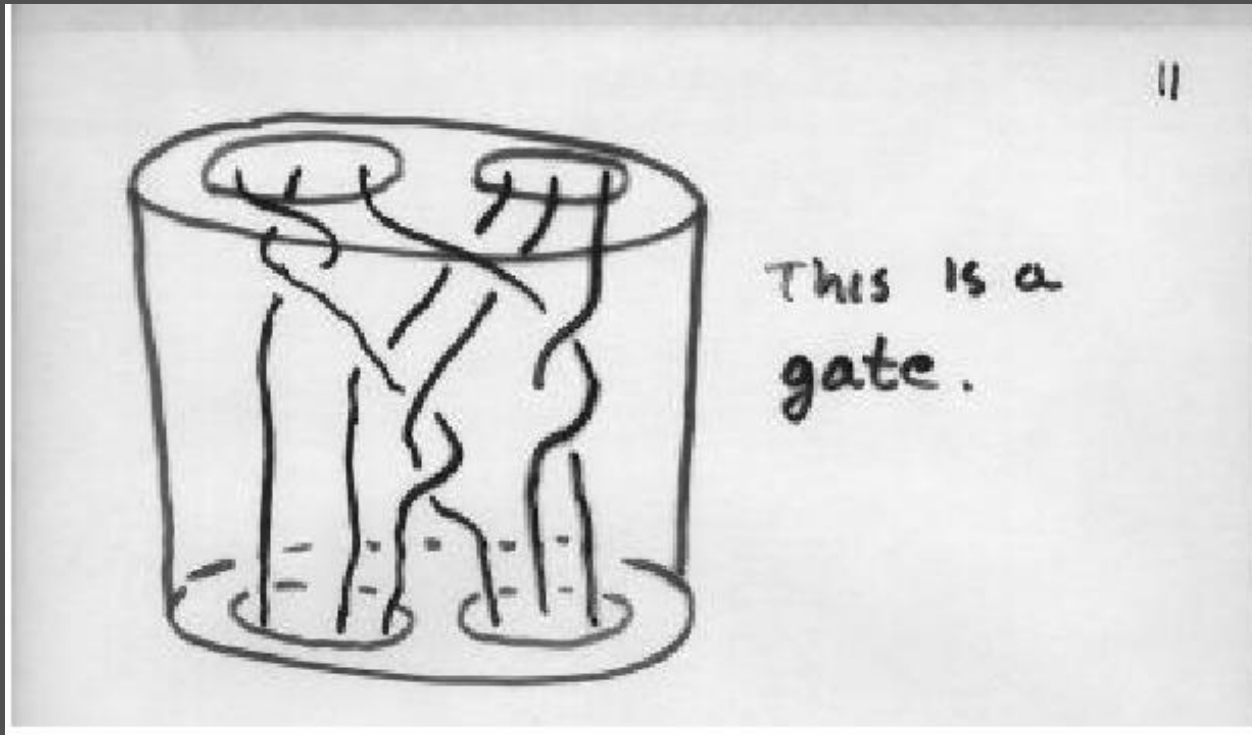
Junctions



Growth by Diana Car, Sébastien Plissard and Erik Bakkers



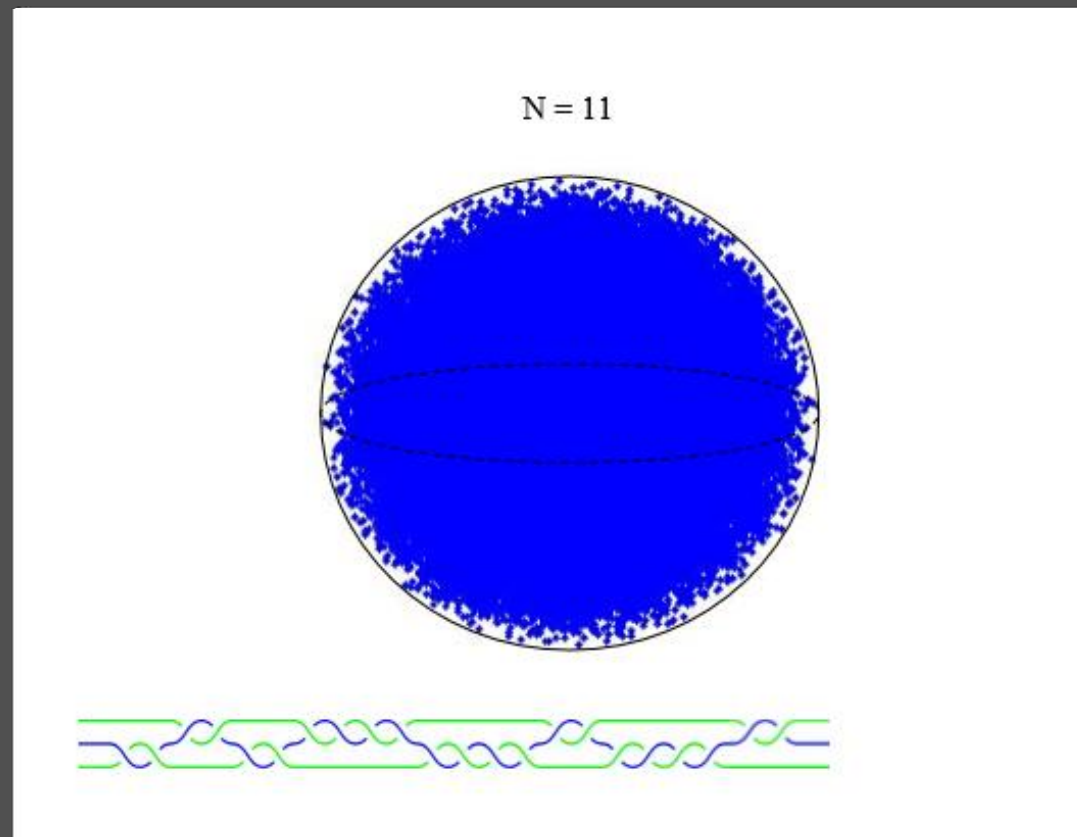
Inspiration



From “A topological modular functor which is universal for quantum computation”

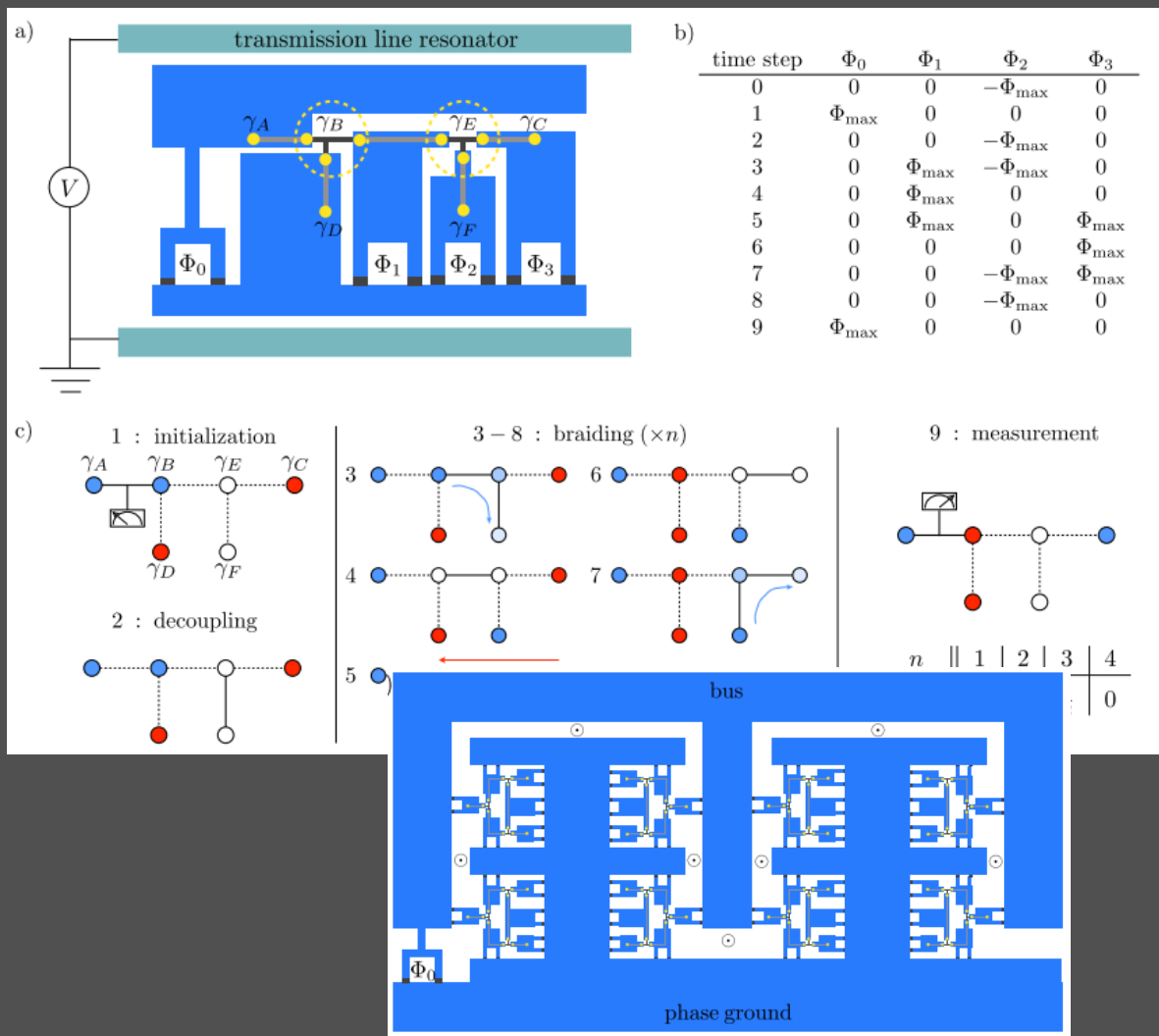
Talk given by
Michael Freedman at
“[Mathematics of Quantum Computation](#)”,
MSRI, Feb. 2000
(available online).

Braiding



From: Nick Bonesteel talk at KITP UCSB

Proposed Architecture

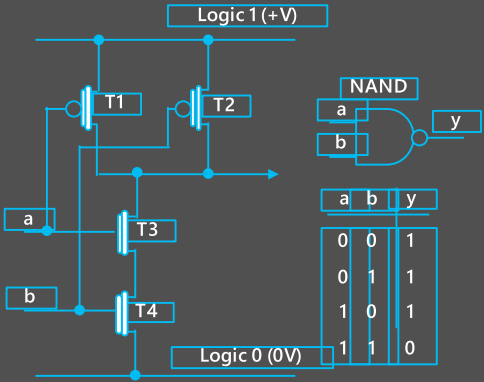

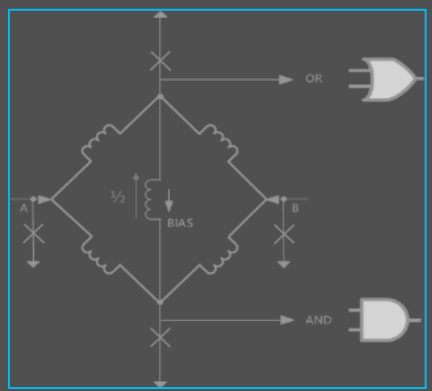
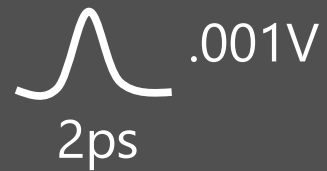


- Proposed experiment to braid Majoranas
- The same control structure is used for initialization, braiding and measurement
- Instead of moving Majoranas, they are coupled and de-coupled to de-localize them and then get them to appear at the desired location
- Must be done adiabatically
- May be scaled to much larger system

After Hyart et al 2013

<http://arxiv.org/abs/1303.4379>

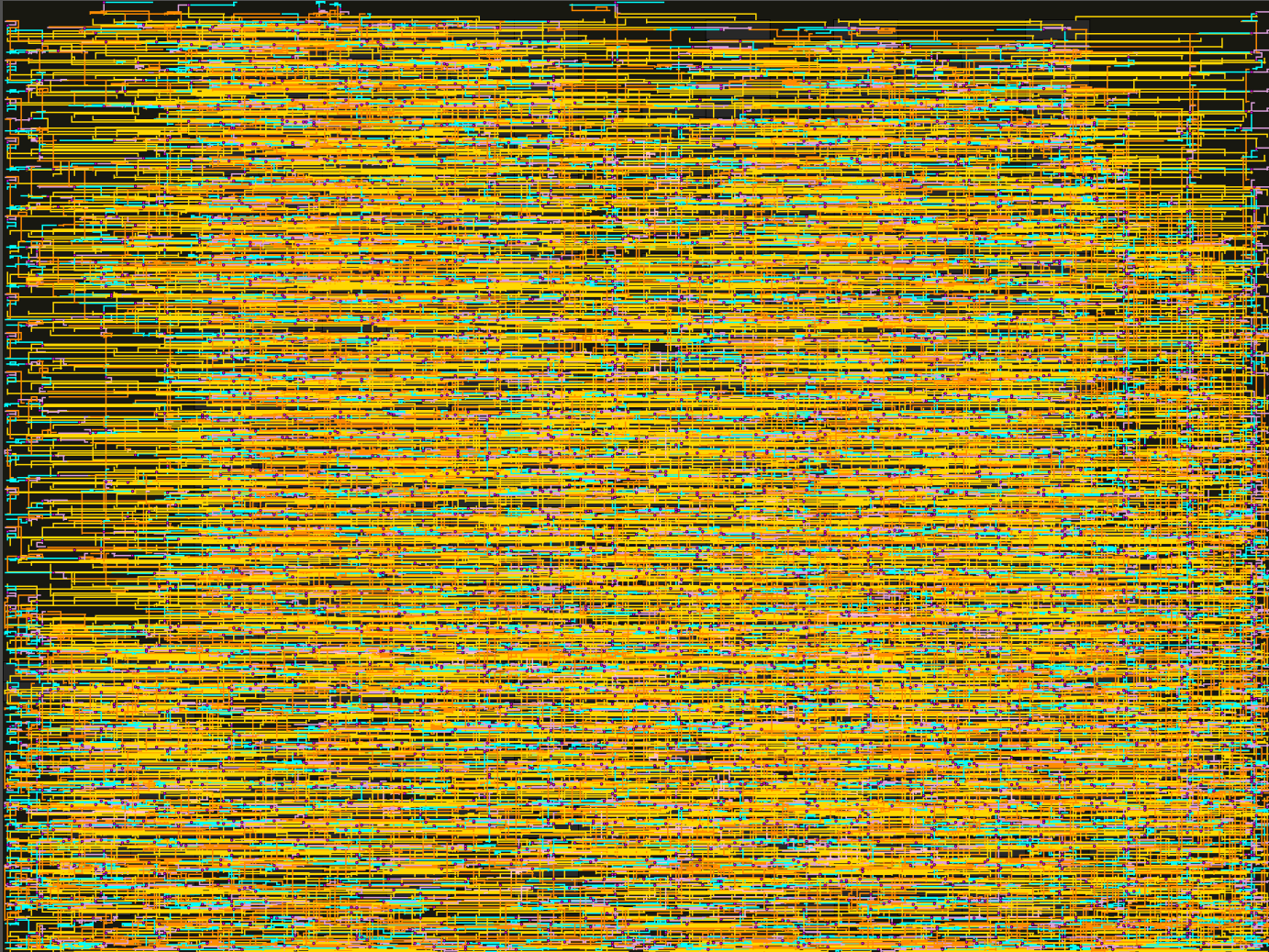
Reciprocal Quantum Logic (RQL)

CMOS	Data	Energy															
 <p>Logic 1 (+V) Logic 0 (0V)</p> <p>NAND</p> <table border="1"><thead><tr><th>a</th><th>b</th><th>y</th></tr></thead><tbody><tr><td>0</td><td>0</td><td>1</td></tr><tr><td>0</td><td>1</td><td>1</td></tr><tr><td>1</td><td>0</td><td>1</td></tr><tr><td>1</td><td>1</td><td>0</td></tr></tbody></table>	a	b	y	0	0	1	0	1	1	1	0	1	1	1	0	 <p>1.3V 300ps</p>	10^{-15}J
a	b	y															
0	0	1															
0	1	1															
1	0	1															
1	1	0															
RQL	Data	Energy															
 <p>OR</p> <p>AND</p>	 <p>.001V 2ps</p>	10^{-19}J															

Reached limits of technology scaling
Significant energy in wires
Frequency limited to 3-4GHz
Not efficient at low temperatures

Memory technology unproven
CAD tools, methodology needed
Relatively small scale demonstrations

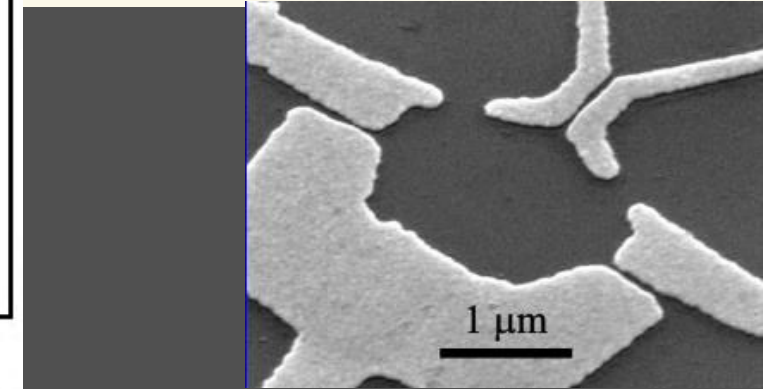
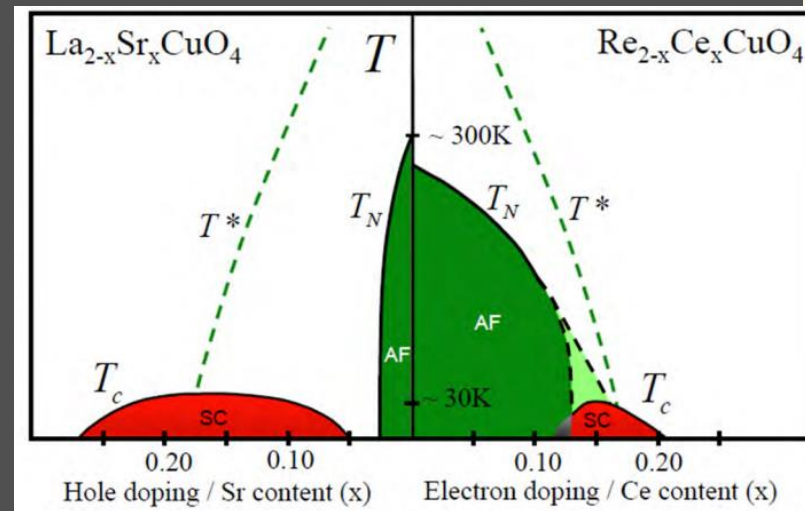
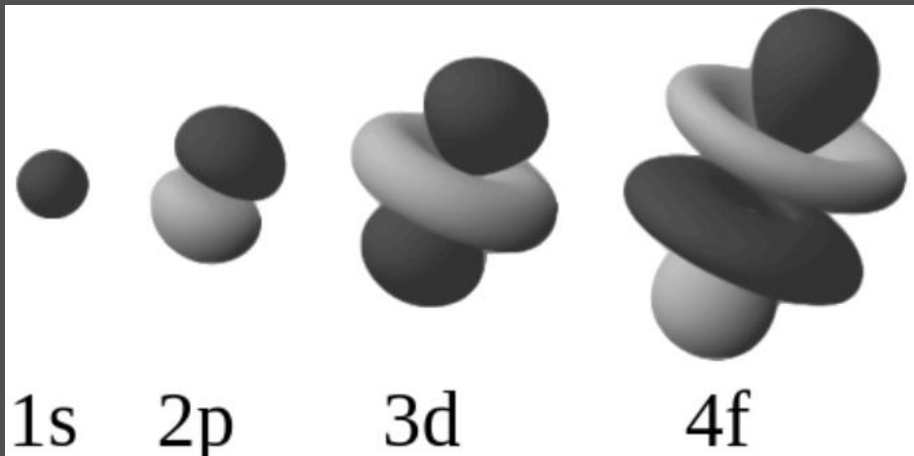
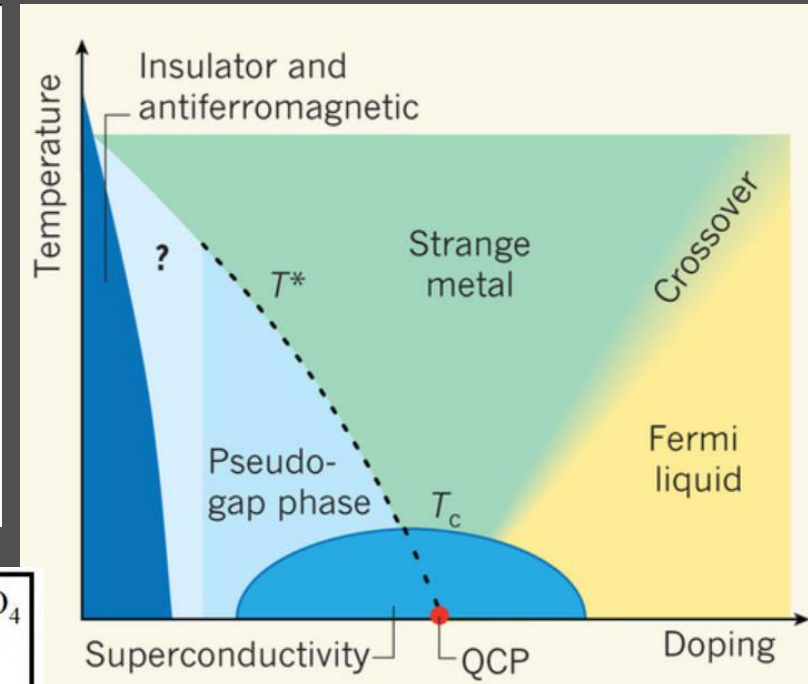
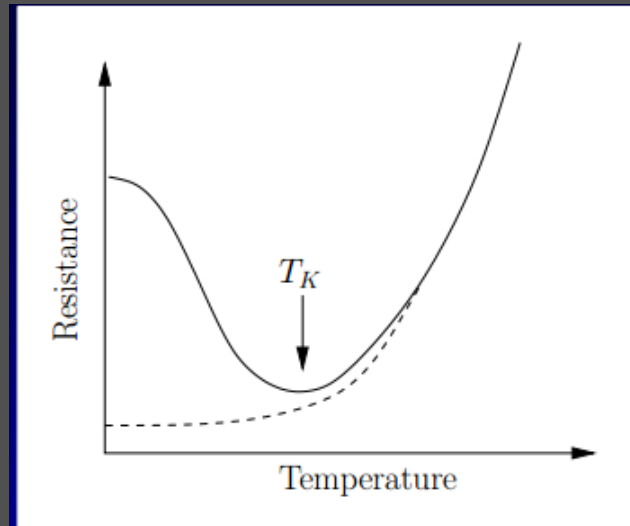
Reciprocal Quantum Logic (RQL)



The Data Path
Compiler (DPC)

Quantum Algorithms for Quantum Impurity Problems

- Mott Insulators
- Transition Metal Compounds
 - Cuprates (e.g., High T_c SC)
- Lanthanides and Actinides
- Kondo Physics (Low temperature Resistance) from Magnetic Impurities
 - Quantum Dots

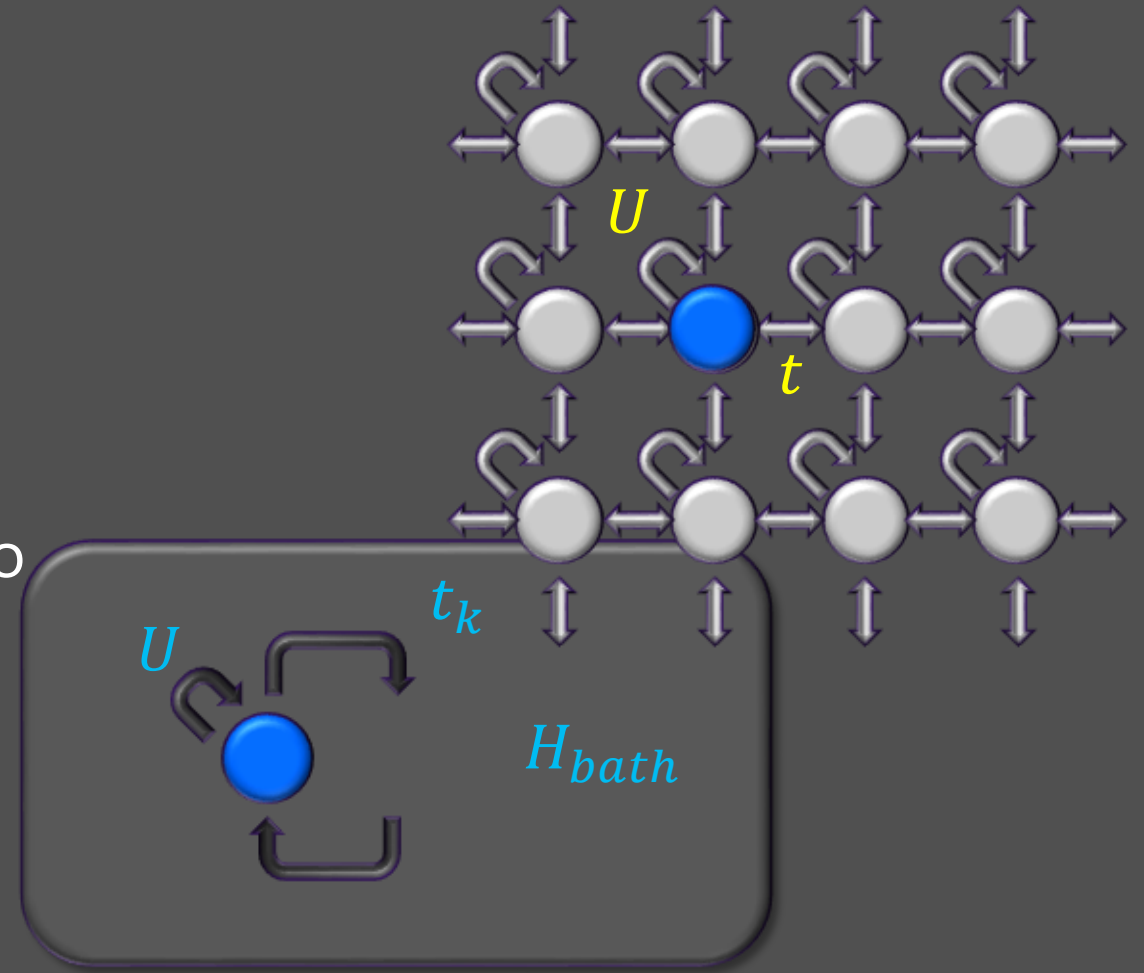


Materials Modeling

$$H_{hub} = U \sum_i n_{i\uparrow} n_{i\downarrow} - t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma}$$

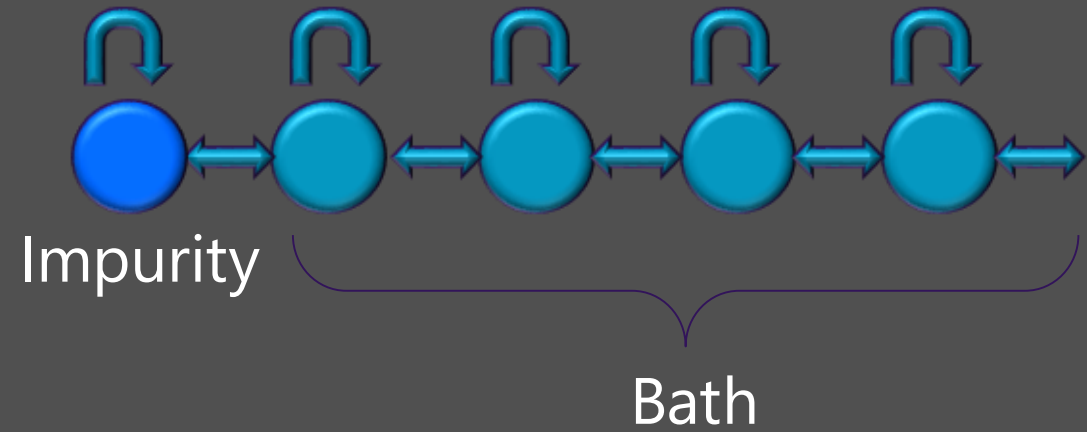
$$H_{imp} = U n_{\uparrow} n_{\downarrow} - \sum_{k, \sigma} (t_k c_{\sigma}^\dagger a_{k, \sigma}^{bath} + h.c.) + H_{bath}$$

- Solids have regular structure that can be modeled as lattices
- The Hubbard model only implements H_{pp} and H_{pqqp} terms
- This doesn't cover many of the materials we're interested in
- One can choose a single site in the lattice to model
- The effect of the rest of the lattice can be modeled in terms of its effect on this site



Anderson Impurity Model

- Choose a single place in the lattice to model (the impurity). This may contain a collection of local sites
- The impurity is typically a full two-body model
- The effect of the rest of the lattice can be modeled in terms of its effect on the impurity (the bath) via a Dynamic Green's function $G(\omega)$
- The bath may have many sites and interconnections

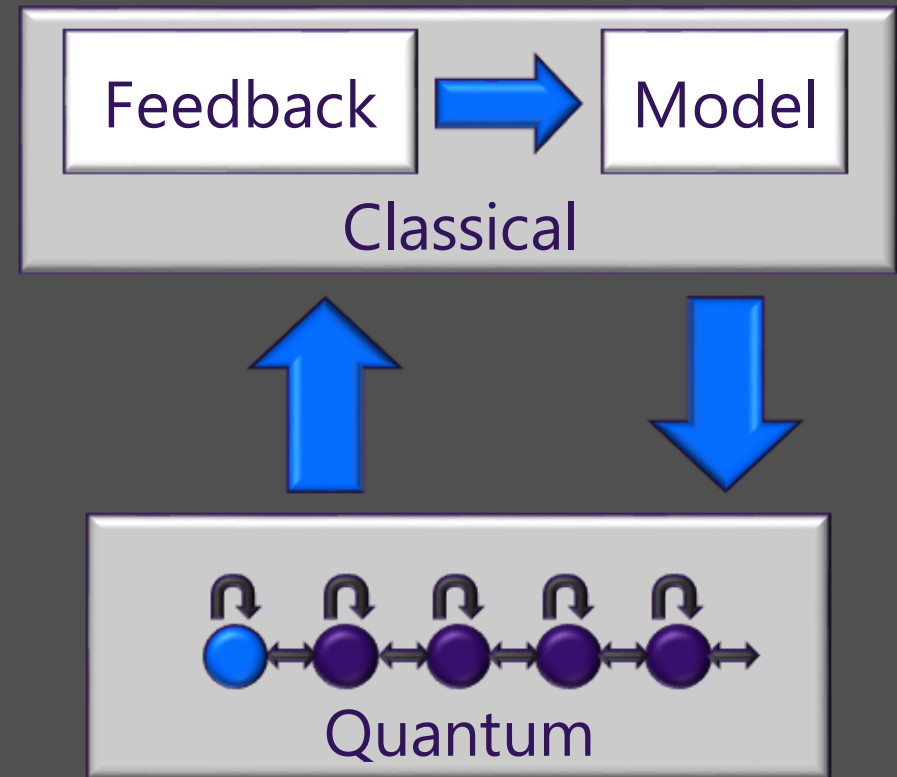


$$H = \sum_{ij} t_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} w_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \sum_{ip} V_{ip} (a_i^\dagger a_p + a_p^\dagger a_i) + \sum_{pq} \epsilon_p a_p^\dagger a_q$$

Dynamical Mean Field Theory (DMFT)

$$G_{\text{solver}}(\omega) \rightarrow \Sigma(\omega) \rightarrow G(k, \omega) \rightarrow G_n(\omega) \rightarrow \Delta_n(\omega)$$

- We can posit an initial model for a material
- Measure quantum simulations at many sites and frequencies deriving a dynamical Green's function
- Use feedback to update model
- Repeat until converged
- The resulting model is defined classically and may be used to efficiently investigate many questions about the material



<http://arxiv.org/abs/1012.3609>

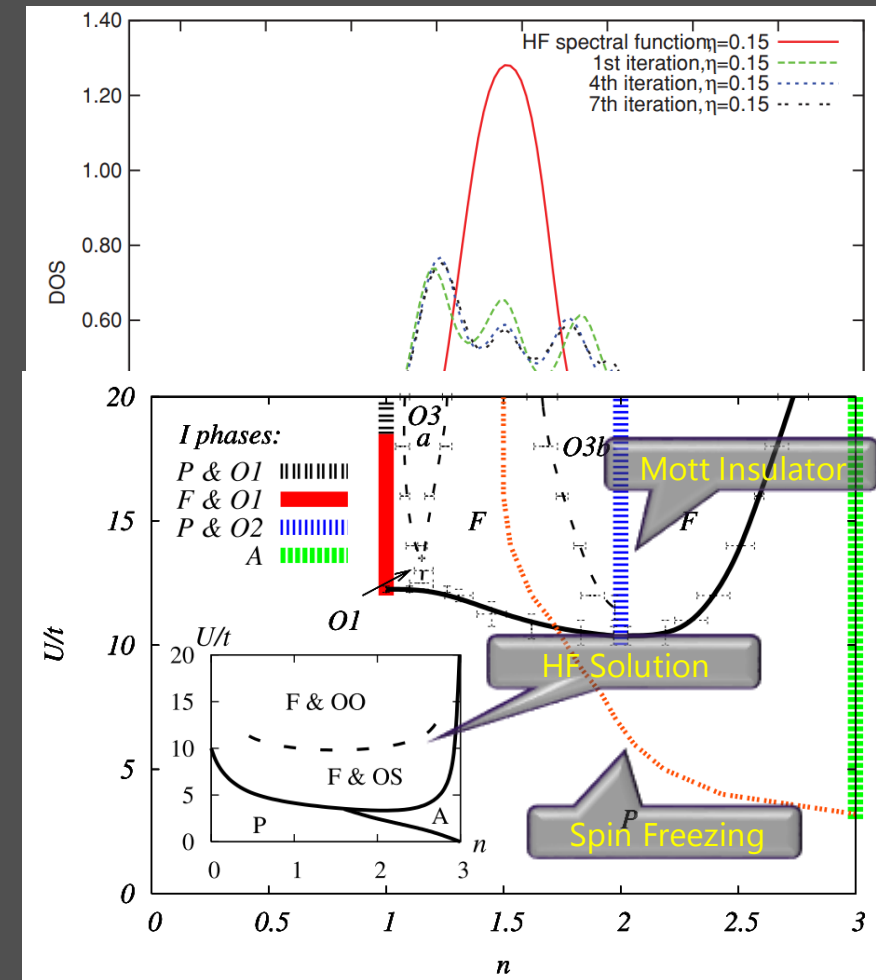
$$G_{\text{solver}}(\omega) = \langle c_i^\dagger(\omega) c_j(-\omega) \rangle$$

Dynamical Mean Field Theory (DMFT)

$$G_{imp}(\omega)^{-1} = (\omega + \mu + i0_{\pm})S - h_{imp} - \Sigma(\omega) - \Delta(\omega)$$

- Cubic Hydrogen (H_2 crystal structure)
- Simulate at 2.5 Å with a bath of 9 orbitals
- Density of States plot for different frequencies. Red curve is the Hartree-Fock solution (used as initial guess). DMFT Converges after 7 iterations
- 5-7 total orbitals for a single site is state-of-the-art.
- Example from Troyer et al [the diagram](#) shows a 3 shell degenerate solution (need 5 for D and 7 for F)
- A Quantum Computer could do a 4x larger impurity or 4x more orbitals than state-of-the-art with 200 qubits

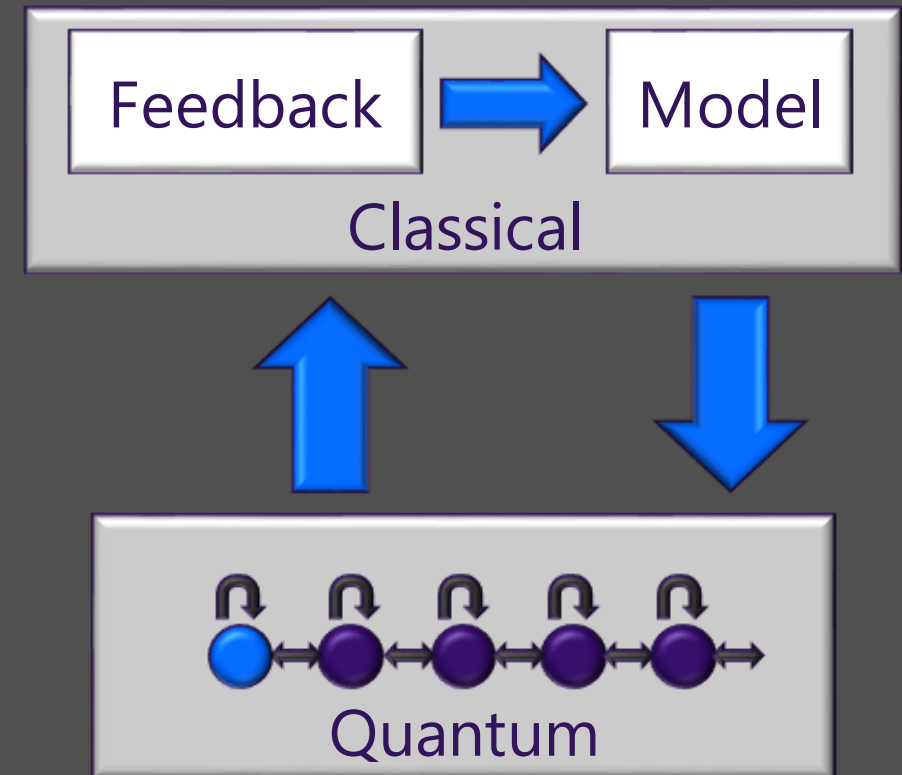
<http://arxiv.org/abs/1012.4474>



Variational Eigensolver

$$E_{gs} = \sum_k \left(H_{FF} + \sum_i \sum_j \theta_{ij} H_j + M(H_k) \right)$$

- **Good:** Only need to stay coherent for prep, evolution and measurement
- **Bad:** Parameters discovered by sampling (quadratically worse than PE)
- Useful for small machines with physical qubits that have relatively short coherence times.
- Only needs few thousand gate executions before losing coherence



<http://arxiv.org/abs/1012.3609>

Two Hubbard Plaquettes (16 qubits)

Gates	Samps/Pt	Samps	Evals	Energy	Overlap	Error	Hours
1000	91680	4.64E+07	506	-8.40204553	0.97616926	0.07625777	6.4
Measures	89395	4.52E+07	506	-8.44653127	0.98536880	0.03177203	6.3
5	86170	4.36E+07	506	-8.43120304	0.98722563	0.04710026	6.1
Speed	91652	4.64E+07	506	-8.45373504	0.98680546	0.02456826	6.4
1.00E-07	77749	3.93E+07	506	-8.32567973	0.97155555	0.15262357	5.5
eGS	92597	4.69E+07	506	-8.43120606	0.98206797	0.04709724	6.5
-8.4783	92404	4.68E+07	506	-8.42695124	0.98382985	0.05135206	6.5
	53207	2.69E+07	506	-8.38545966	0.96754805	0.09284364	3.7
	86289	4.37E+07	506	-8.44177206	0.99095627	0.03653124	6.1
	89696	4.54E+07	506	-8.43294365	0.98231876	0.04535965	6.3
Average	85084	4.31E+07	506	-8.41775273	0.98138456	0.06055057	6.0

SoLi|⟩ - Son of LIQUi|⟩



SoLi|⟩

300 Kelvin - Room


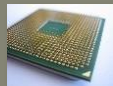
77K-Nitrogen

4K-Helium

.02K-He₃/He₄


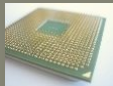
CMOS

CPU Memory





Superconducting

CPU Memory



Quantum

Control Qubits



Understanding of Classical + Quantum

```
let R (k:int) (q:Qubit) =  
  Op.Unitary <-  
    let phi      = (2.0*Math.PI)/(pown 2.0 k)  
    let phiR     = Math.Cos phi  
    let phiI     = Math.Sin phi  
    CSMat(2, [(0,0,1.,0.);(1,1,phiR,phiI)])  
  
let CR (k:int) (c:Qubit) (t:Qubit) = Control1 R c k t  
  
let QFT (qs:Qubits) =  
  let n      = qs.Length  
  for aIdx in n-1..-1..0 do  
    let a    = qs.[aIdx]  
    H a  
    for k in 2..aIdx+1 do  
      let c = qs.[aIdx-(k-1)]  
      CR k c a
```

- Unitary Operations are defined by their matrices
- Meta-operations (**control, adjoint**) understand how to re-write the AST (including the classical generators)
- Joint Measurement is a fundamental operation (depends on Machine Model for implementation)
- Target code will be unrolled at the discretion of the target Machine Model
- **Adjoint QFT** will reverse the code order, run the loops backwards and adjoint all the unitary operations

Compilation

- The compiler front end maps the quantum algorithm to “quantum intermediate language” (QIL)
- The back end rewrites the QIL for execution on actual hardware
- Different quantum computers will require different rewrites of the original QIL
- We have designed and built a layered architecture to support flexible rewriting

```
Push symbol n =
  Property: qs.Length
Push symbol inputSequence =
  Call function Operators.op_RangeStep
  Args:
    Call function Operators.op_Subtraction
    Args:
      Var: n
      Int: 1
    Int: -1
    Int: 0
For each aIdx
  In: inputSequence
  Do:
    Push symbol a =
      Property: qs.Item[aIdx]
    Invoke operation H with args:
      Var: a
    For k
      From: 2
      To:
        Call function Operators.op_Addition
        Args:
          Var: aIdx
          Int: 1
      By: 1
      Do:
        Push symbol c =
          Property: qs.Item[(expr)]
        Invoke operation CR with args:
          ...
```

QCoDeS

Where we are now:

- Igor (based on Alex Johnson code circa 2002)
- QTLab (Delft Python package circa 2008)
- LabVIEW + Mathematica
- MATLAB (various ad-hoc efforts)
- Some other lightweight Python code



QCoDeS Measurement Syntax

```
data = Loop(c0[-20:20:0.1], 0.1).run()

data2 = Loop(c1[-15:15:1], 0.1).each(
    Task(c0.set, -10),
    qubit1.t1,
    fridge.mc_temp,
    Loop(c0[-15:15:1], 0.01).each(meter.amplitude),
    Task(c0.set, -10),
    wait(0.1),
    Loop(c2[-10:10:0.2], 0.01),
    Task(c2.set, 5)
).run()
```

More information...

<http://StationQ.com>

<http://StationQ.github.io/Liquid>

