Quantum Chemistry and Materials Algorithms

Dave Wecker
QuArC Chief Architect
Microsoft Research

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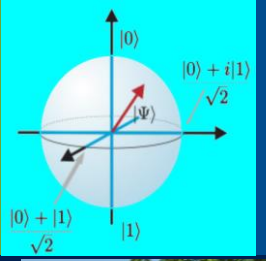
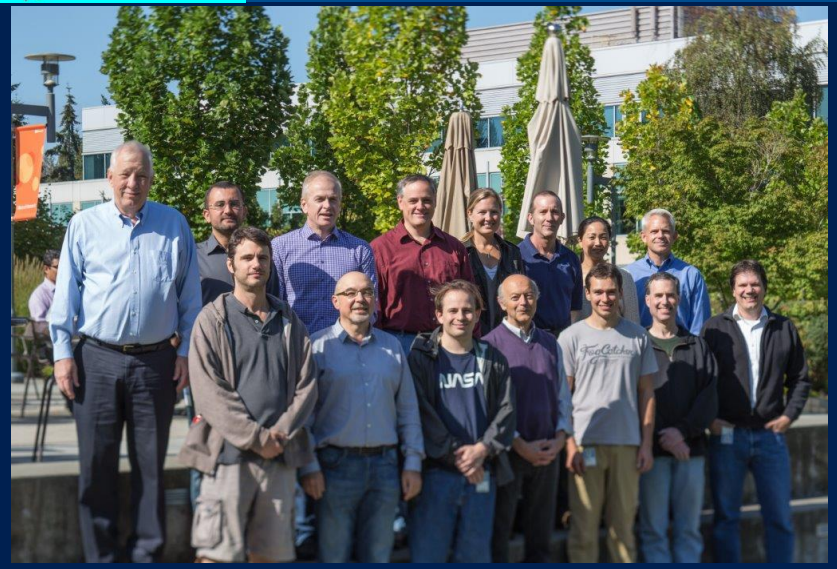
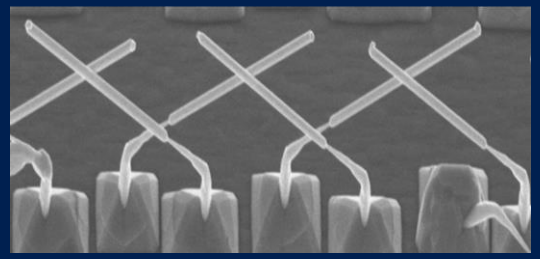
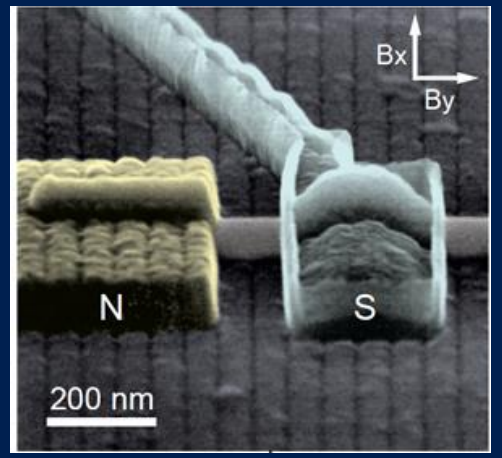
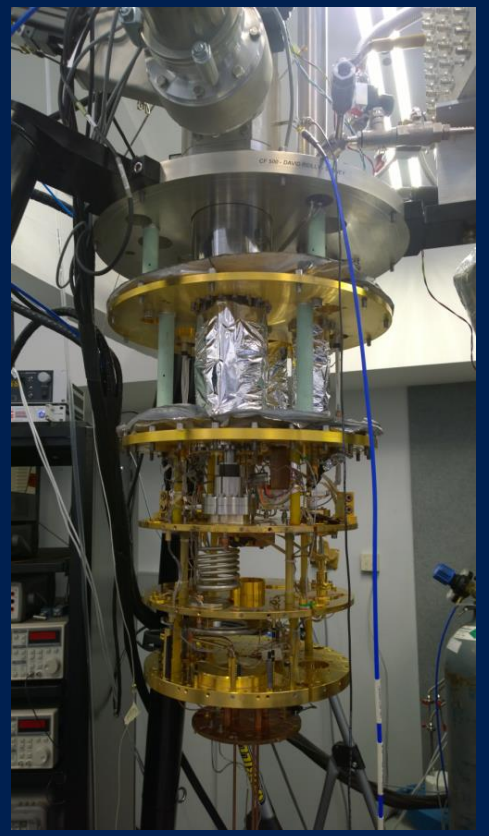


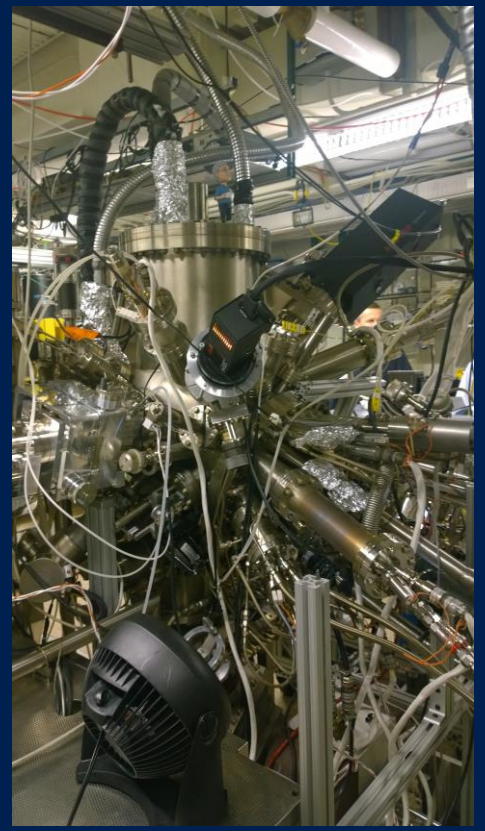
Microsoft QuArC and StationQ

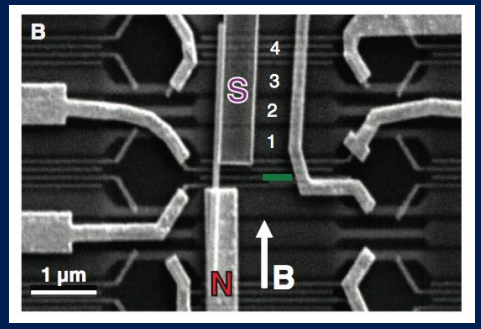












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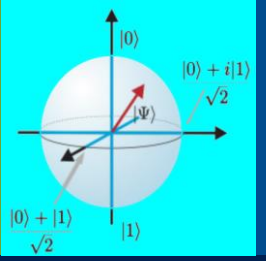
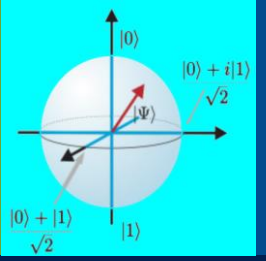


LIQ$Ui|\rangle$ Goals

- Simulation:
  - High enough level language to easily implement large quantum algorithms
  - Allow as large a simulation on classical computers as possible
  - Support abstraction and visualization to help the user
  - Implement as an extensible platform so users can tailor to their own requirements
- Compilation:
  - Multi-level analysis of circuits to allow many types of optimization
  - Circuit re-writing for specific needs (e.g., different gate sets, noise modeling)
  - Compilation into real target architectures



The LIQ$Ui|\rangle$ Simulation Platform

Langua

F# Script

Gates

Universa

Clie

LIQUi|>: A Software Design Architecture and Domain-Specific Language for Quantum Computing. Dave Wecker, Krysta M. Svore

Languages, compilers, and computer-aided design tools will be essential for scalable quantum computing, which promises an exponential leap in our ability to execute complex tasks. LIQUi|> is a modular software architecture designed to control quantum hardware. It enables easy programming, compilation, and simulation of quantum algorithms and circuits, and is independent of a specific quantum architecture. LIQUi|> contains an embedded, domain-specific language designed for programming quantum algorithms, with F# as the host language. It also allows the extraction of a circuit data structure that can be used for optimization, rendering, or translation. The circuit can also be exported to external hardware and software environments. Two different simulation environments are available to the user which allow a trade-off between number of qubits and class of operations. LIQUi|> has been implemented on a wide range of runtimes as back-ends with a single user front-end. We describe the significant components of the design architecture and how to express any given quantum algorithm.

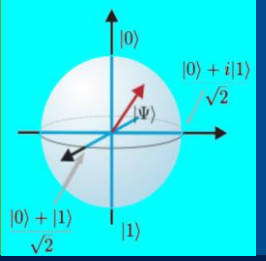
http://arxiv.org/abs/1402.4467

ise Export Render...

Back End ...

sical Quantum

Microsoft



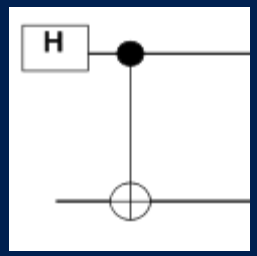
Teleport: User Code

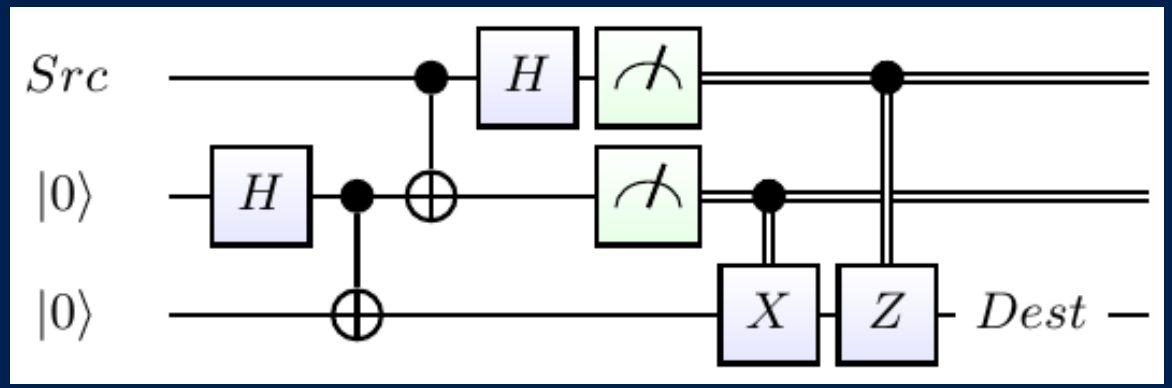
- Define a function to perform entanglement:

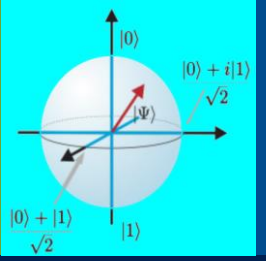
```
let EPR (qs:Qubits) = H qs; CNOT qs
```

- The rest of the algorithm:

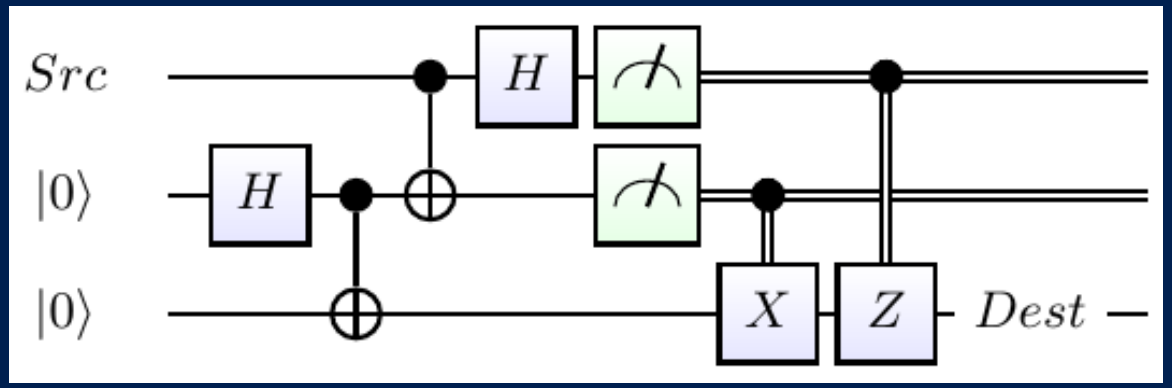
```
let teleport (qs:Qubits) =
    let qs'     = qs.Tail
    EPR qs'; CNOT qs; H qs
    M qs'; BC X qs'
    M qs ; BC Z !!(qs,0,2)
```



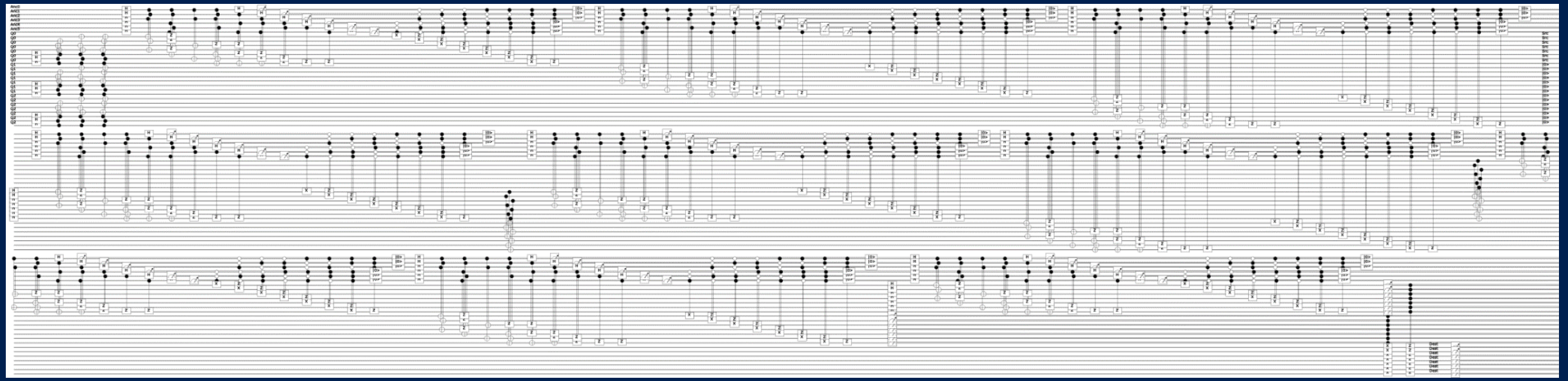




Full Teleport Circuit in a Steane7 Code



3 qubits go to 27



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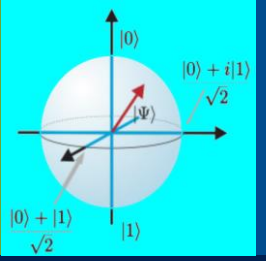
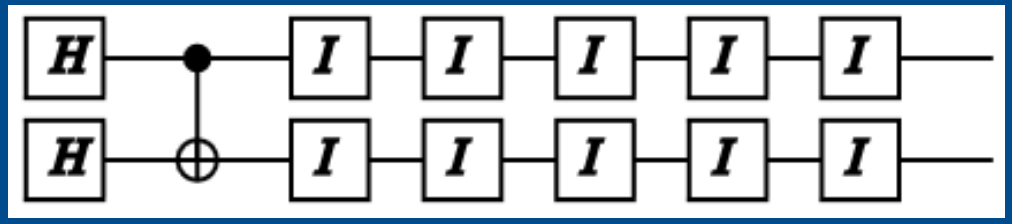
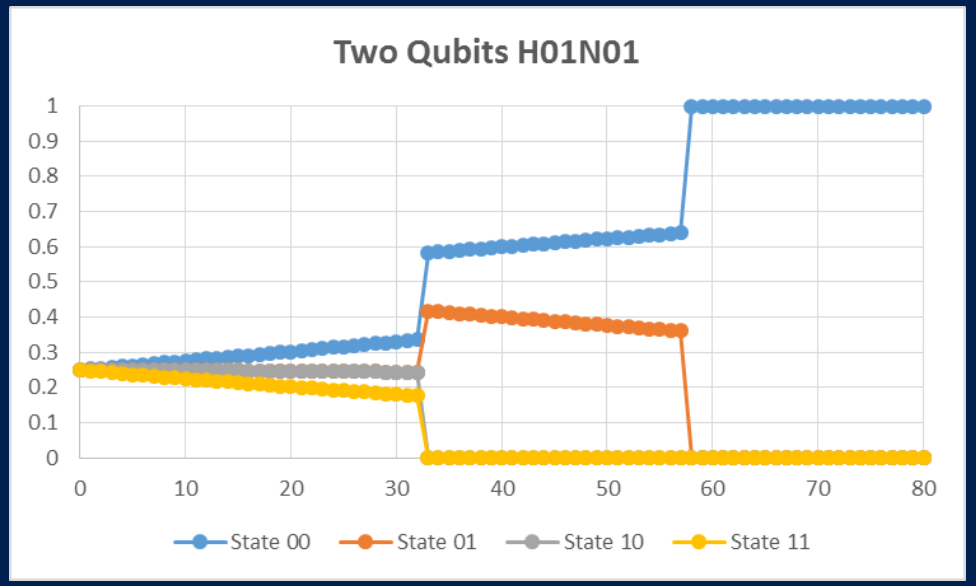
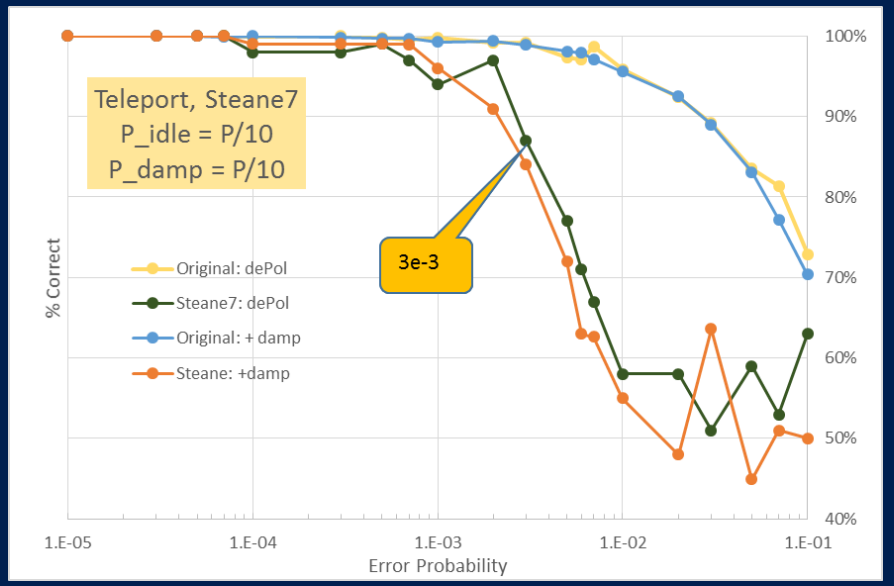


Advanced Noise Modeling




```
Noise(circ:Circuit,ket:Ket,models:NoiseModels)
type NoiseModel = {
    gate:                string       // Gate name (ending with "*" for wildcard match)
    maxQs:               int          // Max qubits that gate uses
    time:                float        // floating duration of gate (convention Idle = 1.0)
    func:                NoiseFunc    // Noise Model to execute
    gateEvents:          NoiseEvents  // Stats for normal gates
    ecEvents:            NoiseEvents  // Stats for EC gates
}
member n.DampProb                     // Get/Set damping probability on a qubit
```





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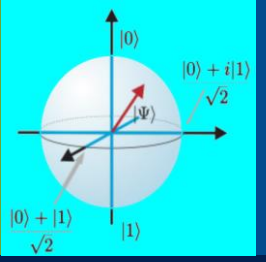
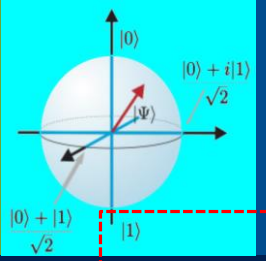


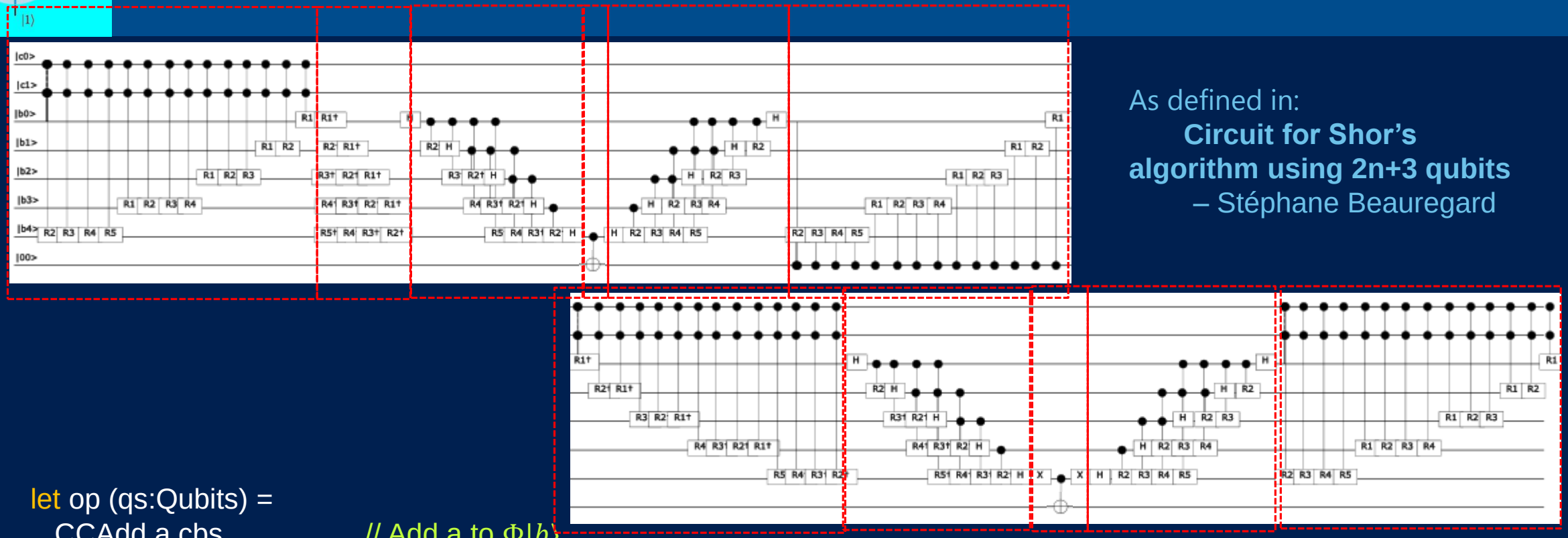
Shor's algorithm: Full Circuit: 4 bits ≅ 8200 gates

Largest we've done:
- 14 bits (factoring 8193)
- 14 Million Gates
- 30 days

Circuit for Shor's algorithm using 2n+3 qubits – Stéphane Beauregard



Shor's algorithm: Modular Adder

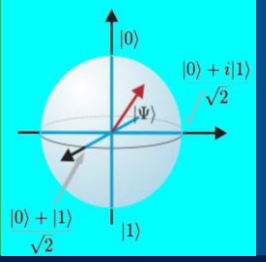


As defined in:

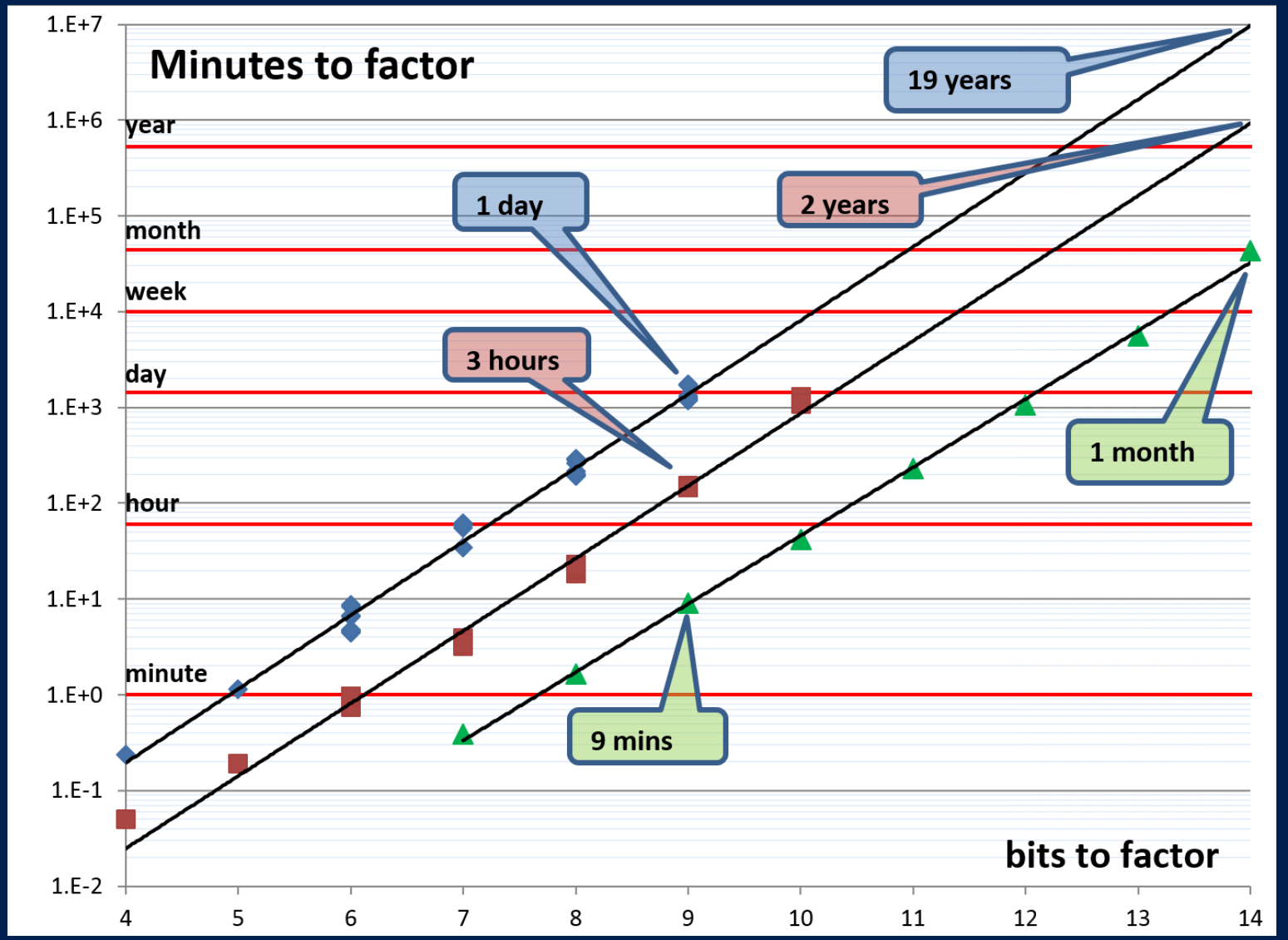
Circuit for Shor's algorithm using 2n+3 qubits

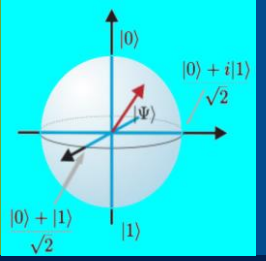
– Stéphane Beauregard

```
let op (qs:Qubits) =
    CCAdd a cbs          // Add a to Φ|b⟩
     AddA' N bs          // Sub N from Φ|a + b⟩
     QFT' bs             // Inverse QFT of Φ|a + b − N⟩
     CNOT [bMx;anc]      // Save top bit in Ancilla
     QFT bs              // QFT of a+b-N
     CAddA N (anc :: bs) // Add back N if negative
     CCAdd' a cbs        // Subtract a from Φ|a + b mod N⟩
     QFT' bs             // Inverse QFT
     X [bMx]             // Flip top bit
     CNOT [bMx;anc]      // Reset Ancilla to |0⟩
     X [bMx]             // Flip top bit back
     QFT bs              // QFT back
     CCAdd a cbs         // Finally get Φ|a + b mod N⟩
```



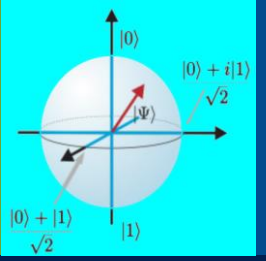
Shor's algorithm results





A Little Motivation

- Nitrogen Fixation:
  - Making fertilizer uses a process from 1909 and uses lots of energy (400^oC/200 atm)
  - Cost: 3-5% of the worlds natural gas production (1-2% of the world's annual energy)
  - Design of a new catalyst would take ~100-200 qubits (inexpensive fertilizer)
- Carbon Capture:
  - Cost: Capturing at point sources will result in 21-90% increase in energy cost
  - Design a new catalyst to extract CO_2 from the air would take ~200-400 qubits
- Design of new chemicals and materials:
  - Today 1/3 of all supercomputing time is spent on chemistry and materials modeling
  - Designs that can never be done classically are solvable with a few hundred qubits
  - Pharmaceuticals, High temperature Super Conductors (energy, transportation…)
    - Example: gain back current 6.5% transmission loss in power lines



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: D **Im**
Hastings, Ma

As quantum computers v appear feas applications frequently r simulating c of molecule computatio perform qua the quantur molecule tw exactly. We increase in t required inc executed is quantum co problems, di
http://arxi

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)*

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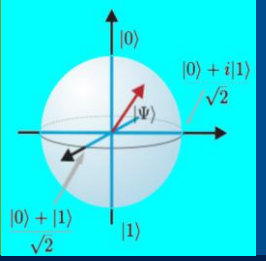
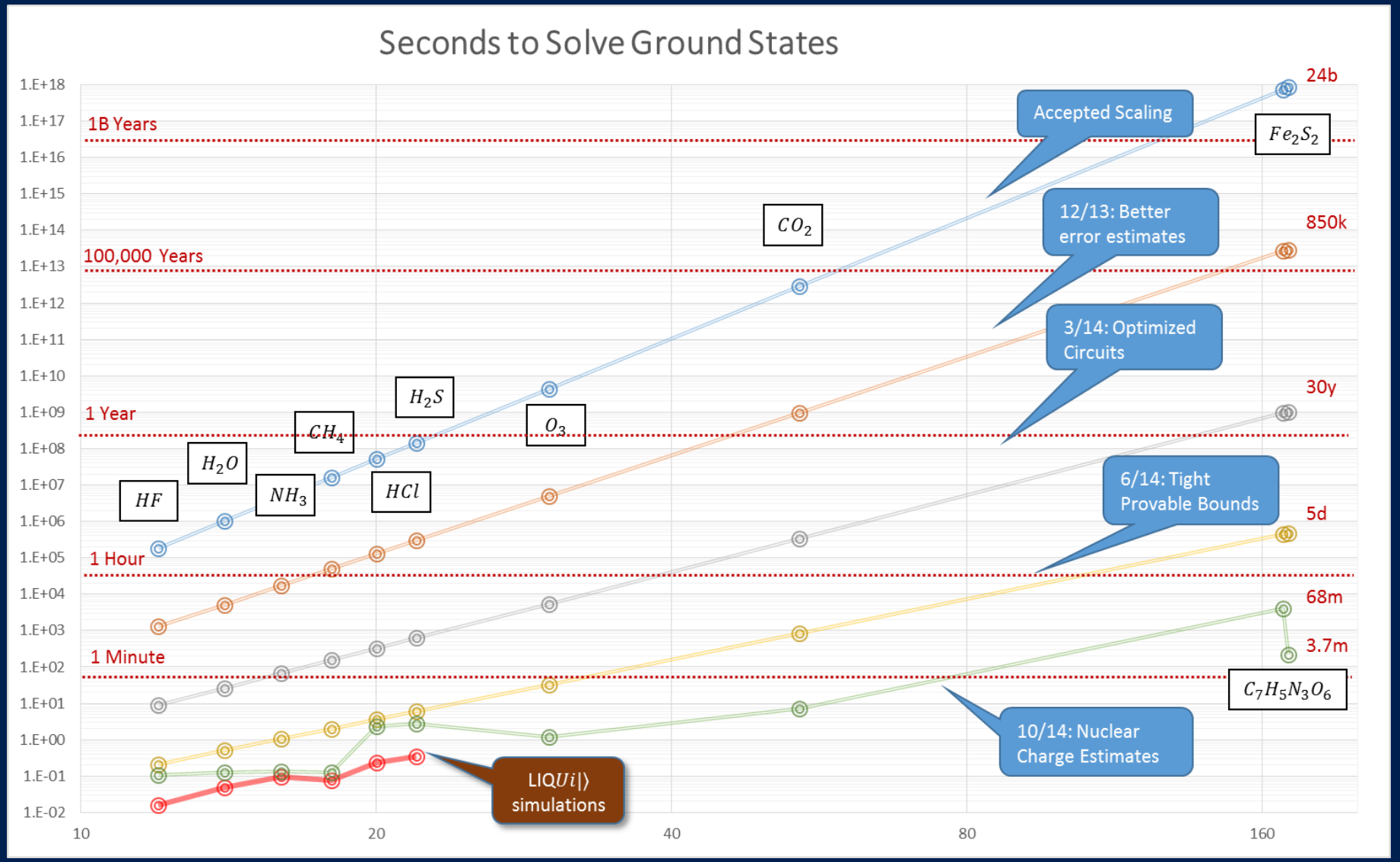


Simulation Evidence

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



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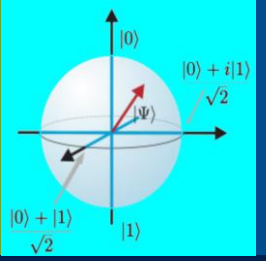
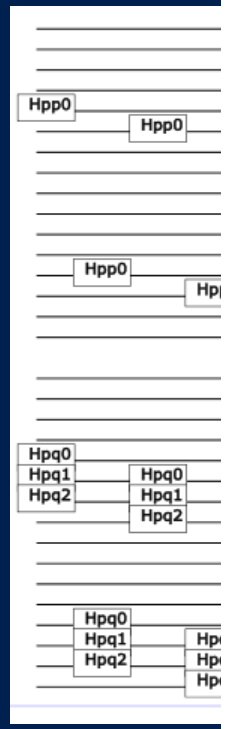


Simulation of Materials (on-going work)

$$H = -\sum_{\langle i,j\rangle}\sum_{\sigma} t_{ij}\left(c^{\dagger}_{i,\sigma}c_{j,\sigma} + c^{\dagger}_{j,\sigma}c_{i,\sigma}\right) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow} + \sum_{i}\epsilon_i\eta_i$$



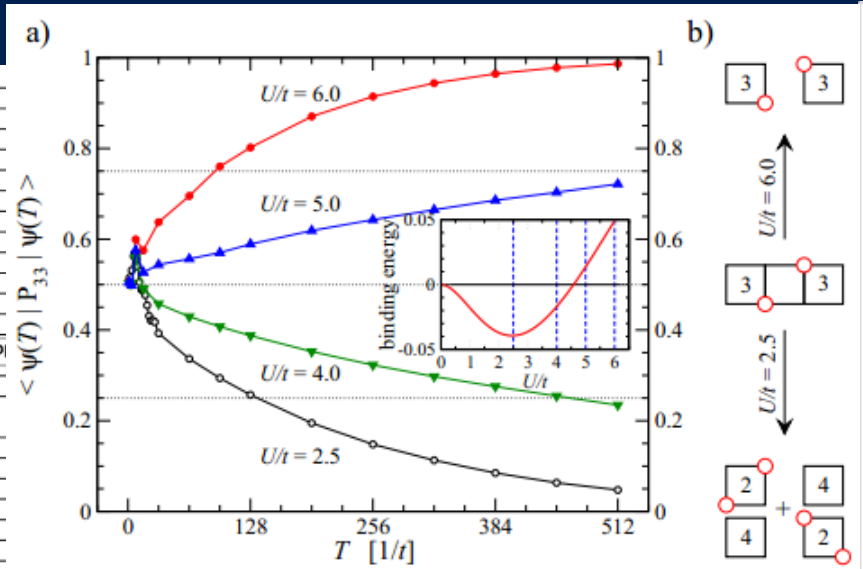
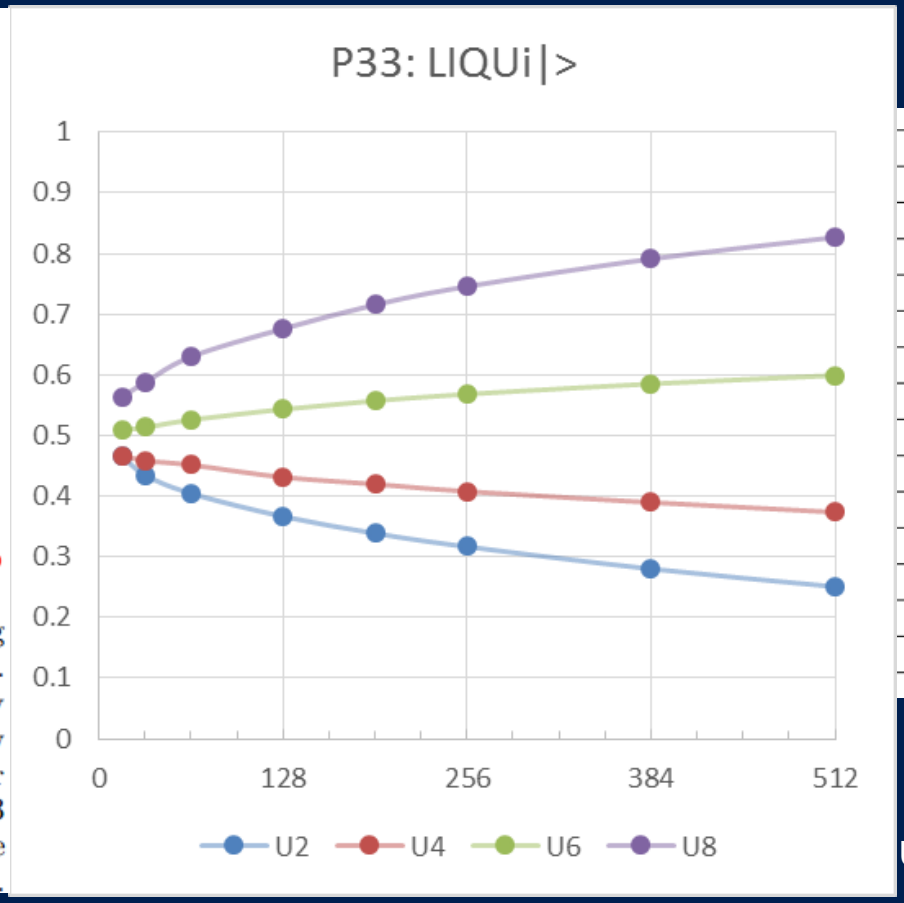
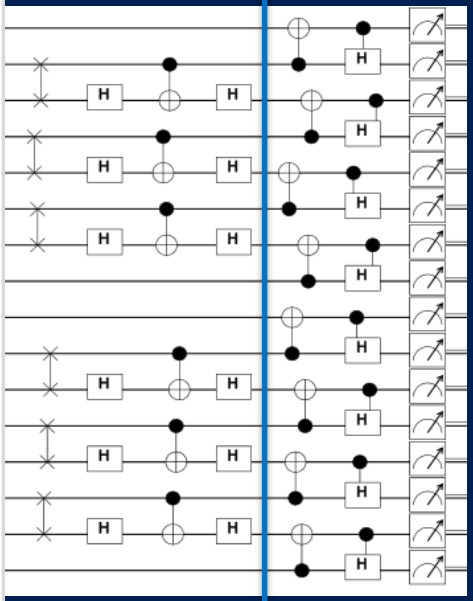


FIG. 3: Signature for d-wave RVB pairing when decoupling two plaquettes with 6 atoms for varying onsite repulsion U/t. b) For $U/t \lesssim 4.5$ pairs are formed with a small binding energy shown in the inset. In the final state after sufficiently slow decoupling the hole pair is located on one plaquette, while for large repulsion $U/t \gtrsim 4.5$ the unpaired holes separate into 3 atoms on each plaquette (right panel). a) Projection of the final state onto the subspace with 3 atoms on each plaquette.



Basis Change



urement

See: d-wave resonating valence bond states of fermionic atoms in optical lattices

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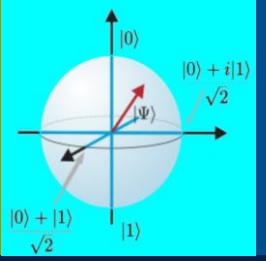
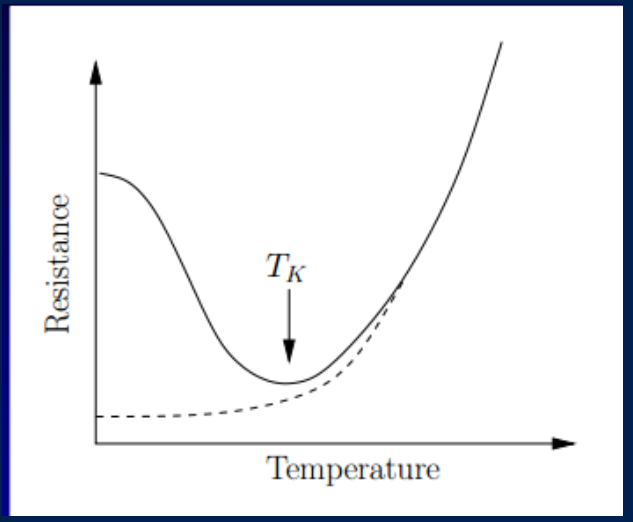
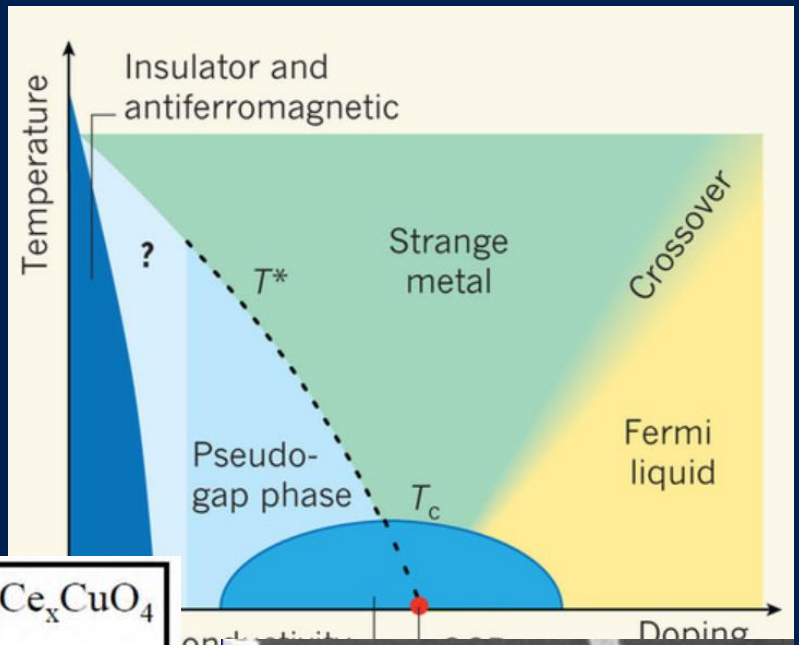
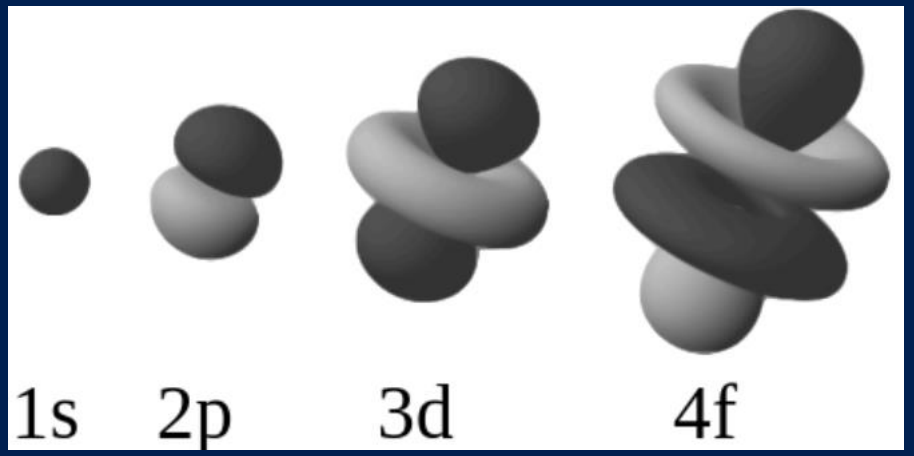


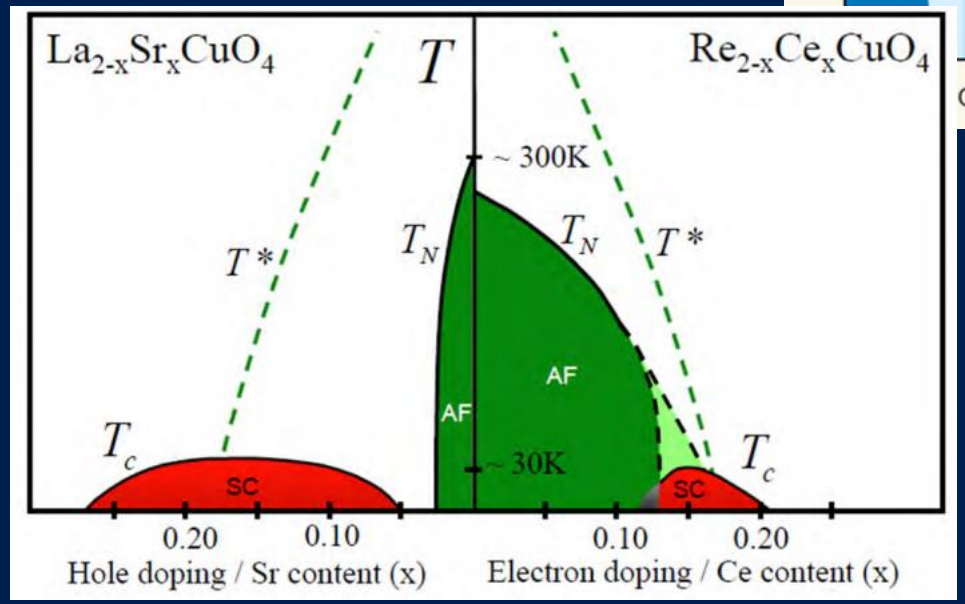
Quantum Algorithms for Quantum Impurity Problems

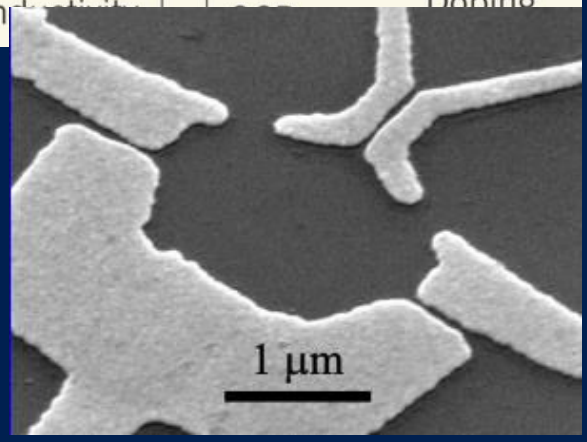
- Mott Insulators
- Transition Metal Compounds
  - Cuprates (e.g., High Tc SC)
- Lanthanides and Actinides
- Kondo Physics (Low temperature Resistance) from Magnetic Impurities
  - Quantum Dots











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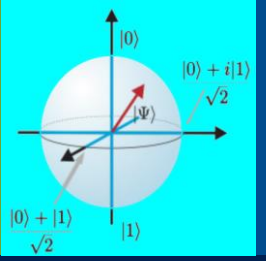
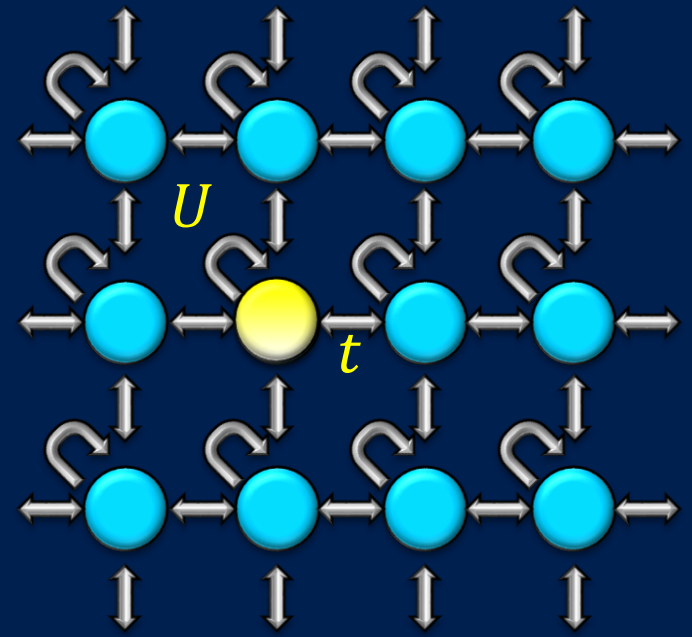


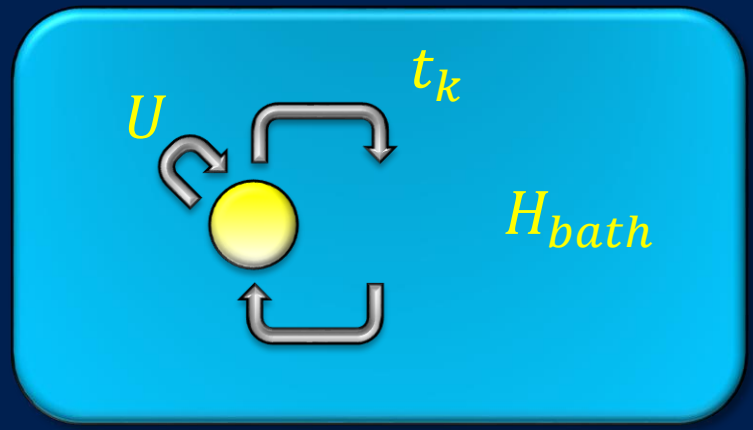
Materials Modeling

$$H_{hub} = U\Sigma_i n_{i\uparrow} n_{i\downarrow} - t\Sigma_{<i,j>,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}$$

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

- 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





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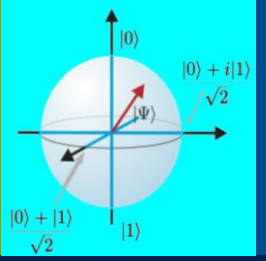
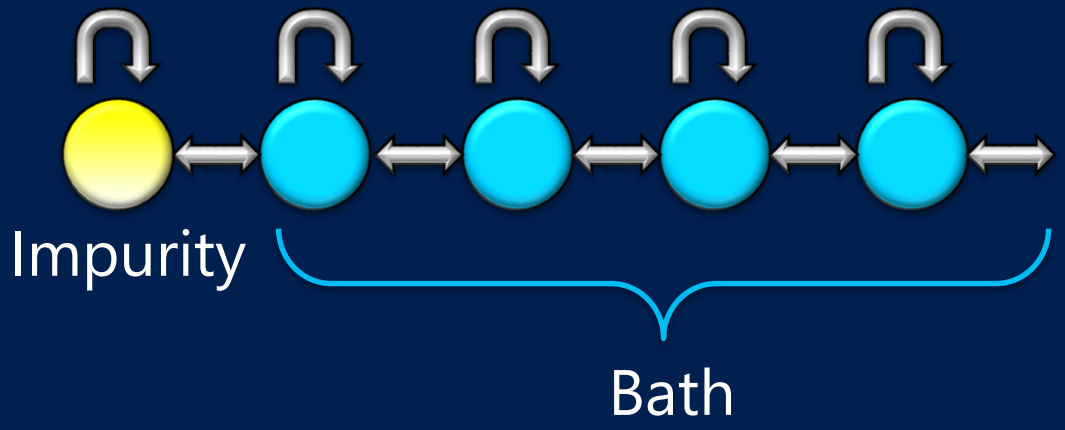
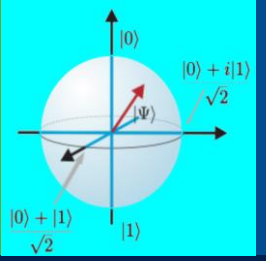


Anderson Impurity Model

- 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



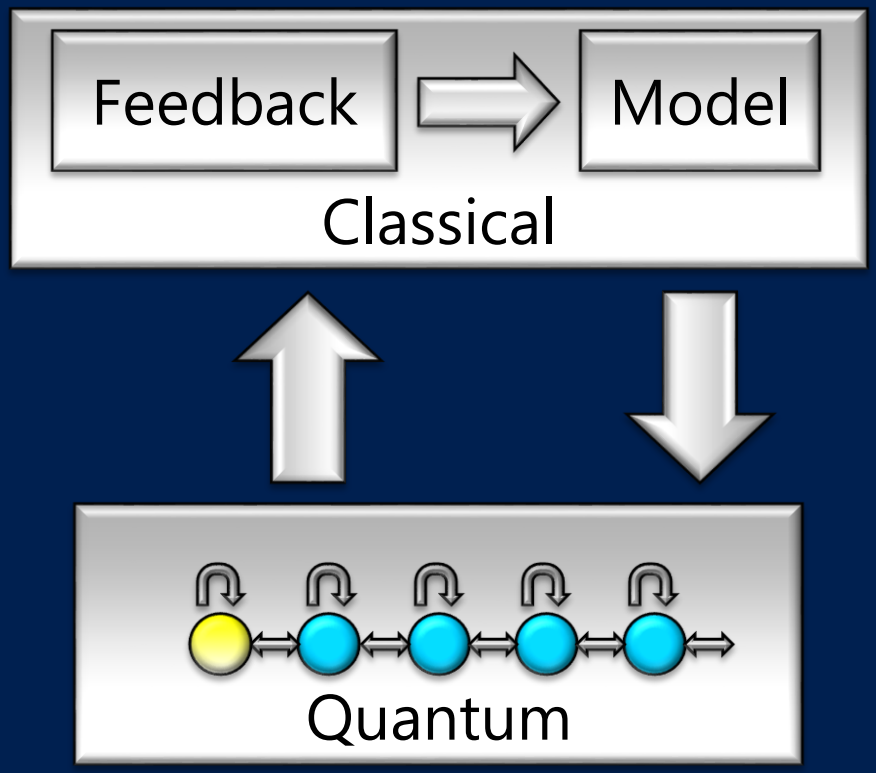
$$H = \sum_{ij} t_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} w_{ijkl} a_i^\dagger a_j^\dagger a_k a_l + \sum_{ip} V_{ip} (a_i^\dagger a_p + a_p^\dagger a_i) + \sum_{pq} \epsilon_p a_p^\dagger a_q$$



Dynamical Mean Field Theory (DMFT)

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

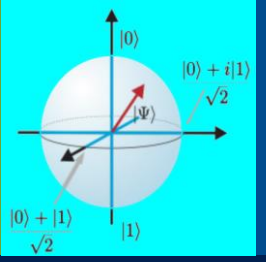
- We can posit an initial model for a material
- Measure quantum simulations at many sites and frequencies deriving a dynamical Green's function
- Use feedback to update model
- Repeat until converged
- The resulting model is defined classically and may be used to efficiently investigate many questions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



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

http://arxiv.org/abs/1012.3609

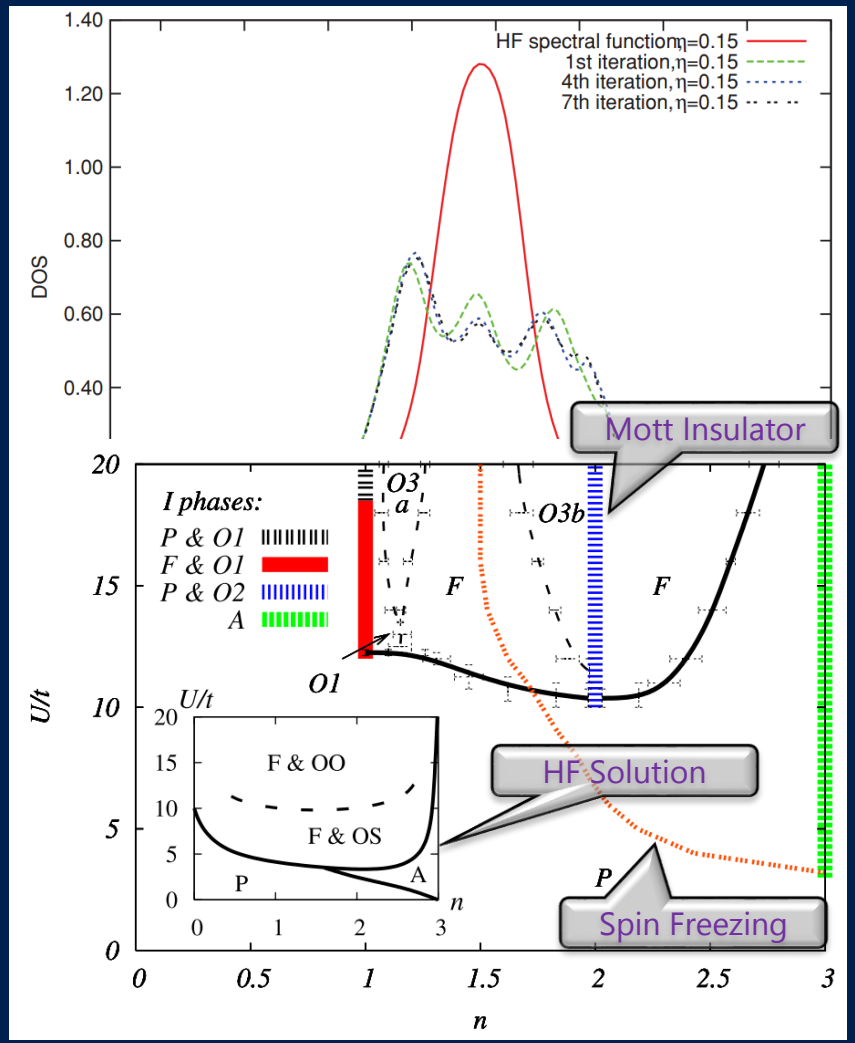
Microsoft



Dynamical Mean Field Theory (DMFT)

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

- 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 Gull 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

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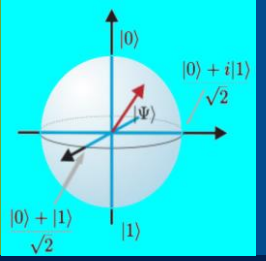


SoLi|⟩ - Son of LIQui|⟩

SoLi|⟩

300 Kelvin - Room

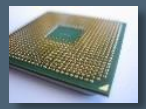
77K-Nitrogen

4K-Helium

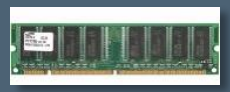
.02K-He_3/He_4

CMOS

CPU

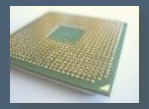


Memory

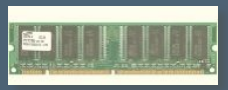


Superconducting

CPU



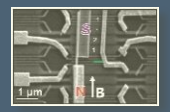
Memory



Quantum

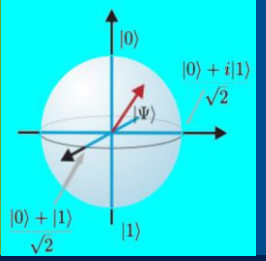
Control

Qubits



STATION Q

Microsoft

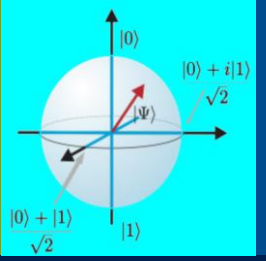


Compilation for Hardware Execution

Algorithm

- Mixed Classical and Quantum
- F# Syntax, Domain Specific Language

```
let QFT (qs:Qubits) = …
```



Thank You

Dave Wecker
QuArC Chief Architect
Microsoft Corporation

Referenced papers may be found at:
http://arxiv.org (Search: wecker_d)