Achieving Practical Applications of Quantum Computers

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Quantum Supremacy

Article

Quantum supremacy using a programmable superconducting processor

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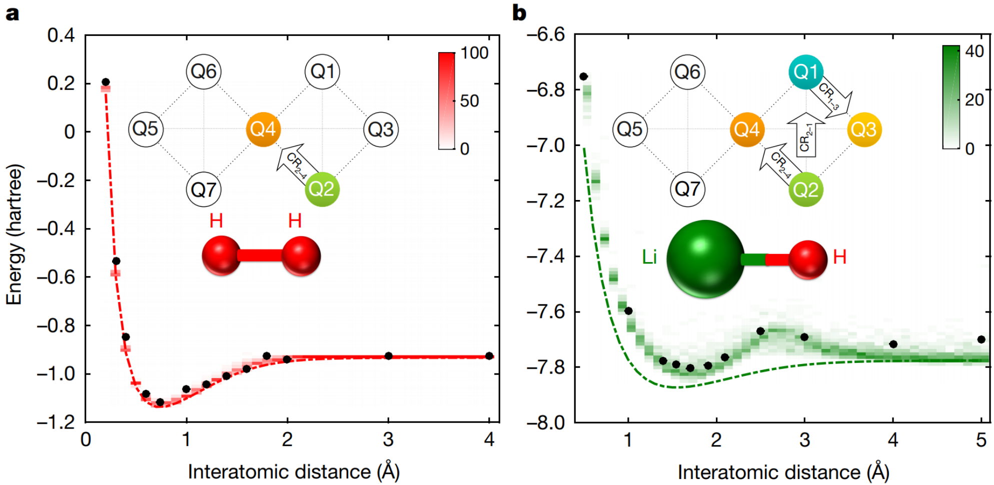
Frank Arute et al. “Quantum supremacy using a programmable superconducting processor”. In: *Nature* 574.7779 (2019), pp. 505–510.

Quantum Chemistry on Quantum Computers



Abhinav Kandala et al. "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets". In: *Nature* 549.7671 (2017), p. 242.

Outline

Hybrid Quantum/Classical Algorithms

Error Mitigation

Design of Novel Material and Chemical Systems for QIS Applications

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Hybrid Quantum/Classical Algorithms

Error Mitigation

Design of Novel Material and Chemical Systems for QIS Applications

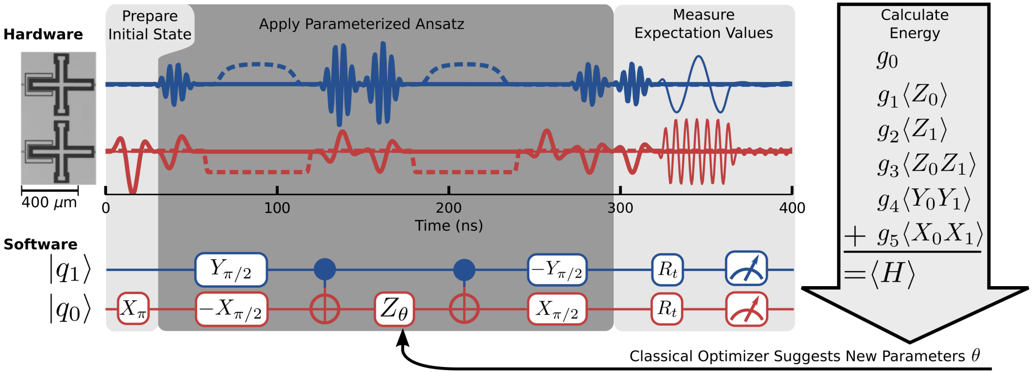
Variational Principle

- Solve for approximate, variational eigenvalue by optimizing the energy of a parameterized wavefunction ansatz $|\psi(\theta)\rangle$
- Variational principle ensures

$$E_0 \leq \frac{\langle \psi(\theta) | H | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle},$$

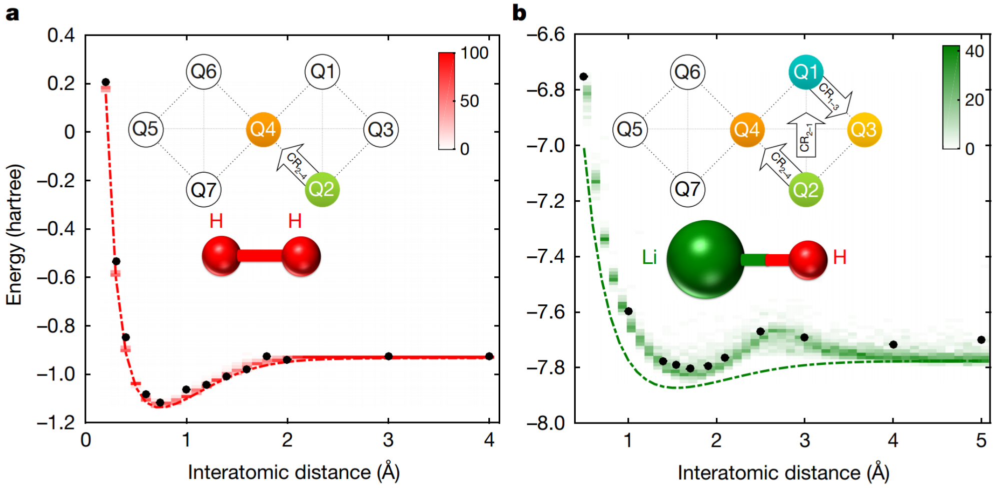
- Variational Monte Carlo does this on classical computers
- The hope is that a quantum realization can utilize non-trivial wavefunctions which would be much more difficult to prepare on a classical computer

Variational Quantum Eigensolver



PJJ O'Malley et al. "Scalable quantum simulation of molecular energies". In: *Physical Review X* 6.3 (2016), p. 031007.

Example VQE Calculation



Kandala et al., "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets".

Variational Quantum Eigensolver

- Hybrid quantum/classical algorithm
  - Quantum computer provides energy estimation, classical computer does optimization
- Currently limited to small molecules in small basis sets (sto-3g)
- Variational
  - Need good ansatz and efficient optimization
- Still limited by decoherence

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- Hybrid quantum/classical algorithm
  - Quantum computer provides energy estimation, classical computer does optimization
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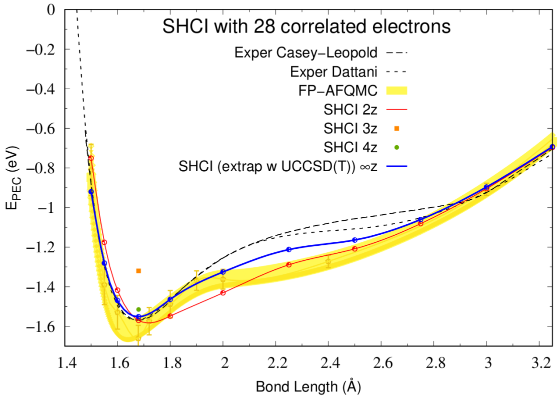
  - need good ansatz and efficient optimization
- Still limited by decoherence
- Classical quantum chemistry methods are very powerful

Selected Heat-Bath Configuration Interaction

- Full configuration interaction quality energies for Cr_2 28e, 4z basis (208 orbitals) – Hilbert space size of 10^{42}

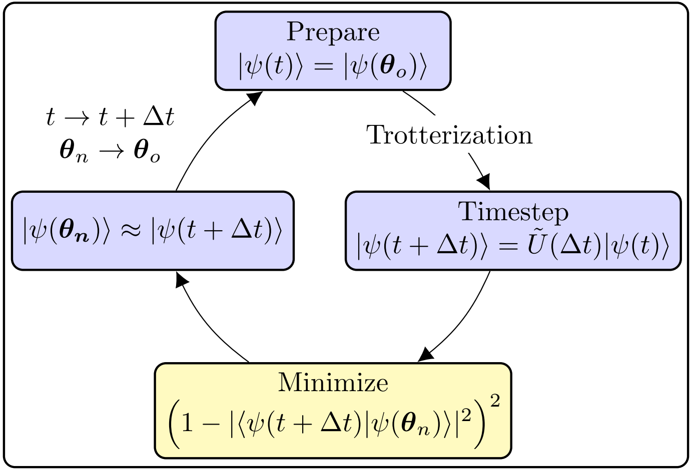


Junhao Li et al. “Accurate many-body electronic structure near the basis set limit: Application to the chromium dimer”. In: *Physical Review Research* 2.1 (2020), p. 012015.

Quantum Dynamics on Quantum Computers

- As opposed to eigenvalue estimation, fully quantum dynamics has been a much harder problem for classical computers
- State-of-the-art, fully quantum dynamics simulations are much more limited
- Quantum computers have the potential to solve these problems exponentially faster
- Algorithms specifically designed for noisy quantum devices (like VQE) will be necessary to use near-term quantum devices for chemical applications

Restarted Quantum Dynamics

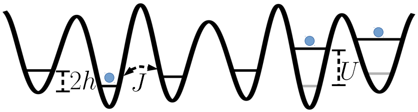


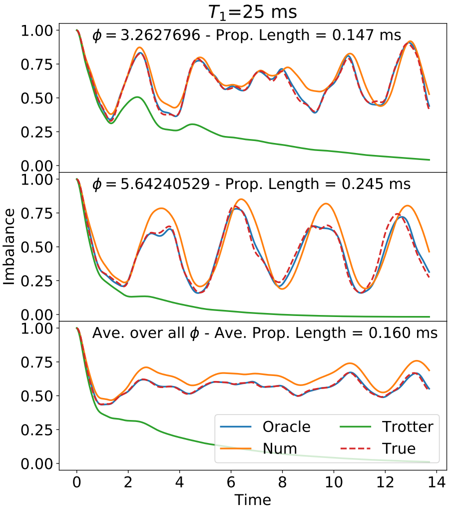
Matthew Otten, Cristian L Cortes, and Stephen K Gray. "Noise-Resilient Quantum Dynamics Using Symmetry-Preserving Ansatzes". In: *arXiv:1910.06284* (2019).

Restarted Quantum Dynamics

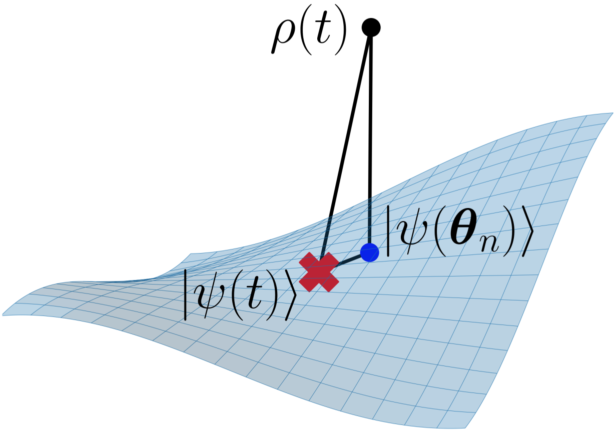
- Like VQE, RQD is a hybrid quantum/classical algorithm
  - Quantum computer provides time-stepping and fidelity estimation, classical computer does optimization
- Requires good ansatz and efficient optimization
- As long as long as a single time-step (via, e.g., a Trotterization procedure) can be taken with good fidelity, many time steps can be taken by restarting the dynamics from an optimized wavefunction
- Allows for much longer dynamical studies

Restarted Quantum Dynamics Results

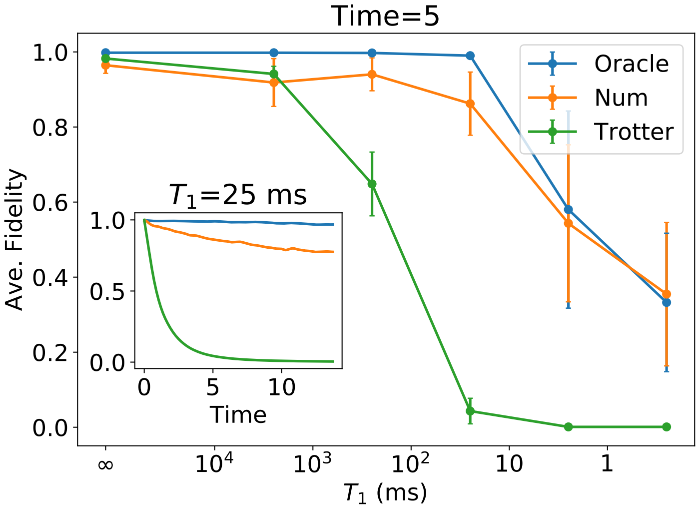




Noise-Resilience of RQD



Restarted Quantum Dynamics



Applications of RQD

- Interacting spins/fermions on lattices (e.g., Hubbard models)
- Quantum field theory dynamics (e.g., Schwinger models)
- Chemical systems
  - Electronic wave packet dynamics
  - Photosynthetic complexes, such as Fenna-Matthews-Olson (FMO), and other excitonic systems
  - Fully quantum nuclear wave packet dynamics on a Born-Oppenheimer potential surface (e.g., reactive chemistry of $H + H_2$)

Outline

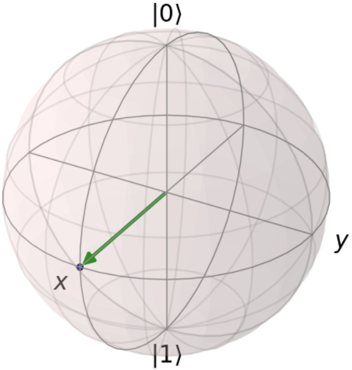
Hybrid Quantum/Classical Algorithms

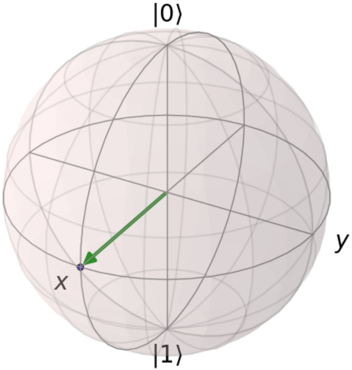
Error Mitigation

Design of Novel Material and Chemical Systems for QIS Applications

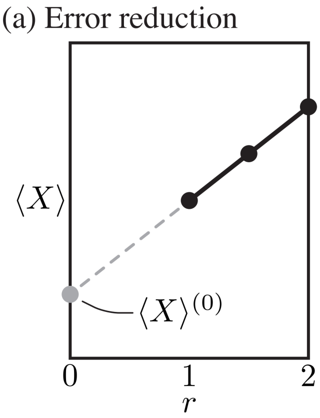
Decoherence

- Inevitable in near-term quantum hardware
- Represents the undesirable coupling to the outside world
- Can be fixed via error correction, but at an extremely high overhead in number of qubits



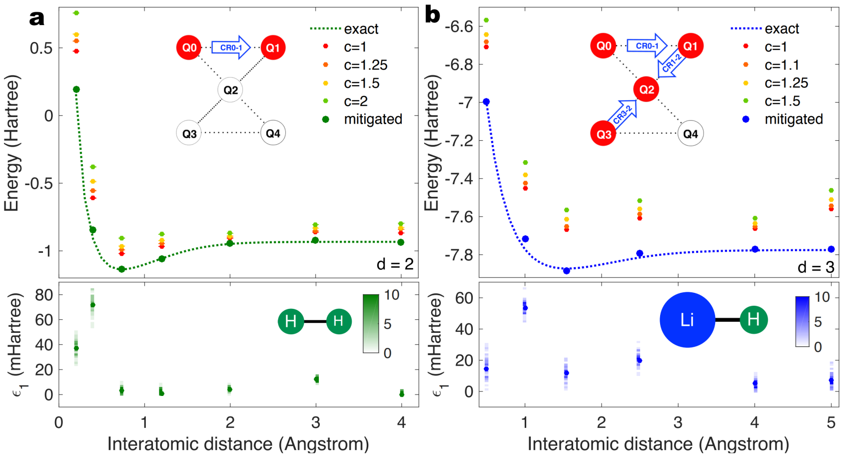


Noise Extrapolation



Ying Li and Simon C Benjamin. "Efficient variational quantum simulator incorporating active error minimization". In: *Physical Review X* 7.2 (2017), p. 021050.

Noise Extrapolation for Quantum Chemistry



Abhinav Kandala et al. "Error mitigation extends the computational reach of a noisy quantum processor". In: *Nature* 567.7749 (2019), p. 491.

Generalization to Many Noise Sources

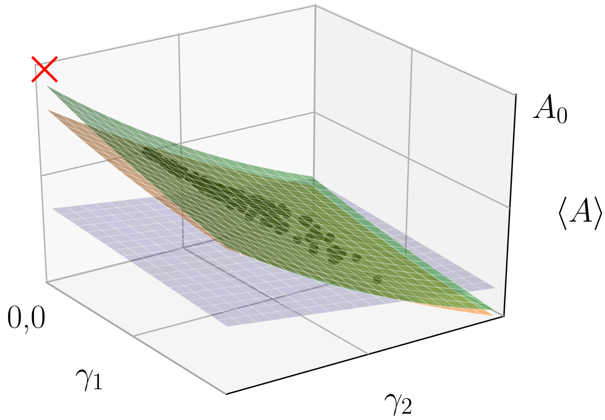
- Instead of a single noise source with rate γ, we consider many noise sources with rates γ_j
  - Think of this as T_1 and T_2 times for each qubit

$$\langle A \rangle = A_0 + \sum_j \gamma_j A_j + \sum_j \sum_k \gamma_j \gamma_k A_{jk} + \cdots ,$$

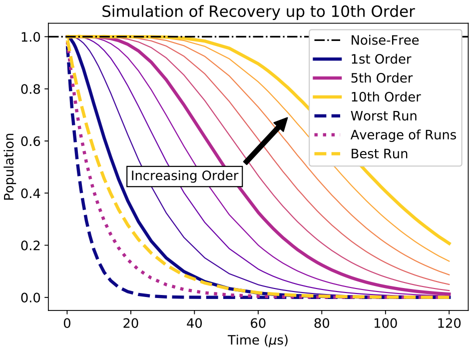
- where A_0 is the noise-free observable value and A_j is the effect of noise rate j on the observable.
- We do not have knowledge of A_0 and A_j, A_{jk}, etc, but we can vary γ_j and, with truncation, fit these values

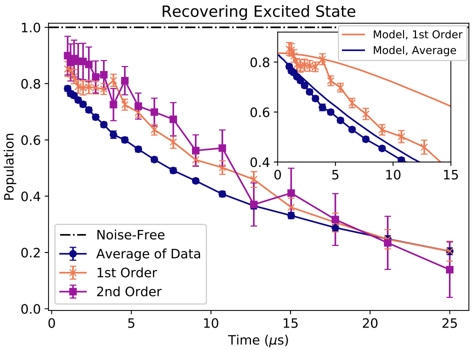
Matthew Otten and Stephen K Gray. "Recovering noise-free quantum observables". In: *Physical Review A* 99.1 (2019), p. 012338.

Example ‘Hypersurface’

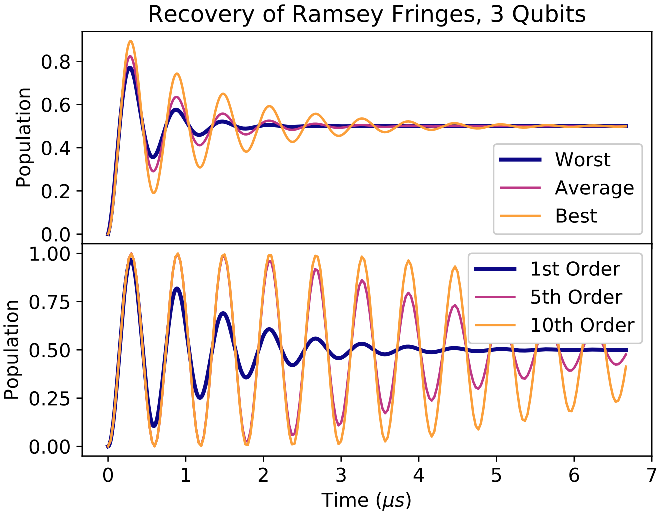


Hypersurface Error Recovery





NV Center Magnetometer



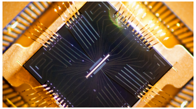
Hypersurface Recovery

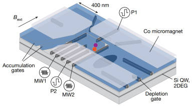
- Different Regimes:
  - Quantum Sensor: very high order, small number of noise terms
  - Quantum Computer: low order, very large number of noise terms
- Allows for another type of 'parallelism'; run one algorithm on many slightly different quantum computers
  - Combine results in post processing
- A good understanding of the noise sources is important
- Well characterized noise rates, $\{\gamma\}$, are necessary
- The resulting extrapolation can be ill-behaved

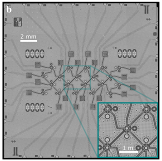
Outline

Many Different Quantum Architectures

- Trapped ion, silicon quantum dot, superconducting qubit, photons, etc, have all demonstrated limited use in quantum computing applications
- Novel qubits are still being developed and could have interesting technological advantages
  - Chemical and materials systems are at the forefront of novel qubit technologies







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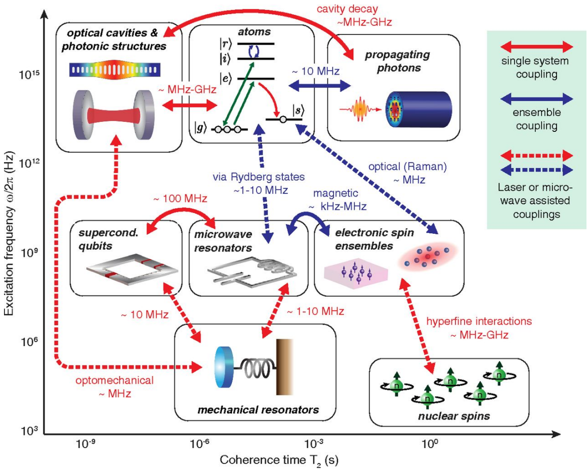
TF Watson et al. "A programmable two-qubit quantum processor in silicon". In: *Nature* (2018).
JS Otterbach et al. "Unsupervised Machine Learning on a Hybrid Quantum Computer". In: *arXiv preprint arXiv:1712.05771* (2017).

Hybrid Quantum Systems

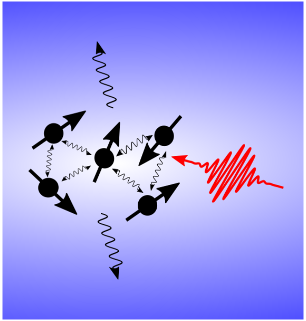


Gershon Kurizki et al. "Quantum technologies with hybrid systems". In: *Proceedings of the National Academy of Sciences* 112.13 (2015), pp. 3866–3873.

Open Quantum Systems

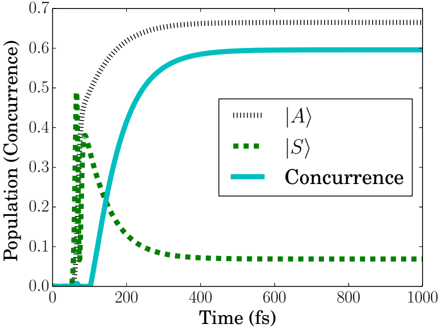
- All qubit technologies share one key feature: the control and processing of quantum information in time and the inevitable decoherence
- This can be modeled with the Lindblad master equation

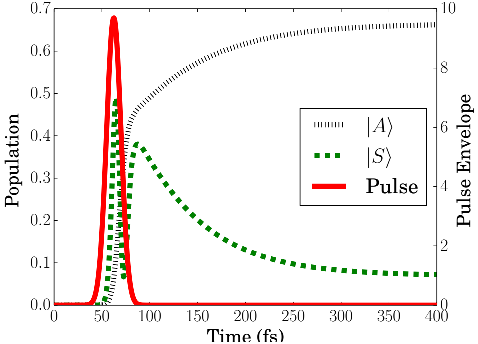
$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H + H(t), \rho] + L(C)[\rho],$$



- where H is the natural system Hamiltonian, $H(t)$ represents the physical application of gates, and $L[C](\rho)$ represents decoherence from coupling with the environment

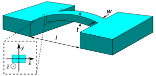
Quantum Dot Entanglement

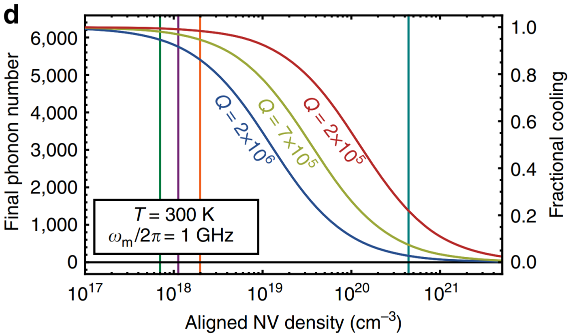




Matthew Otten et al. "Origins and optimization of entanglement in plasmonically coupled quantum dots". In: *Physical Review A* 94.2 (Aug. 2016), p. 022312.

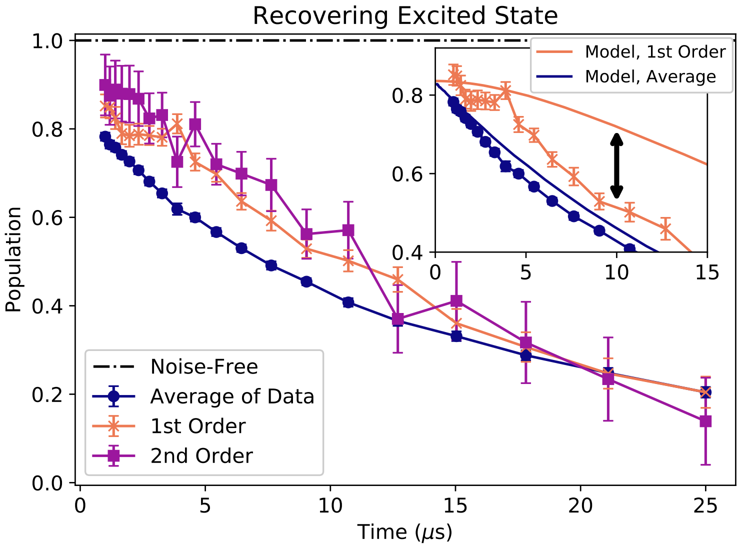
NV Center Cooling of a Mechanical Resonator





E R MacQuarrie et al. "Cooling a mechanical resonator with nitrogen-vacancy centres using a room temperature excited state spin–strain interaction". In: *Nature Communications* 8 (Feb. 2017), p. 14358.

Missing Error Sources?



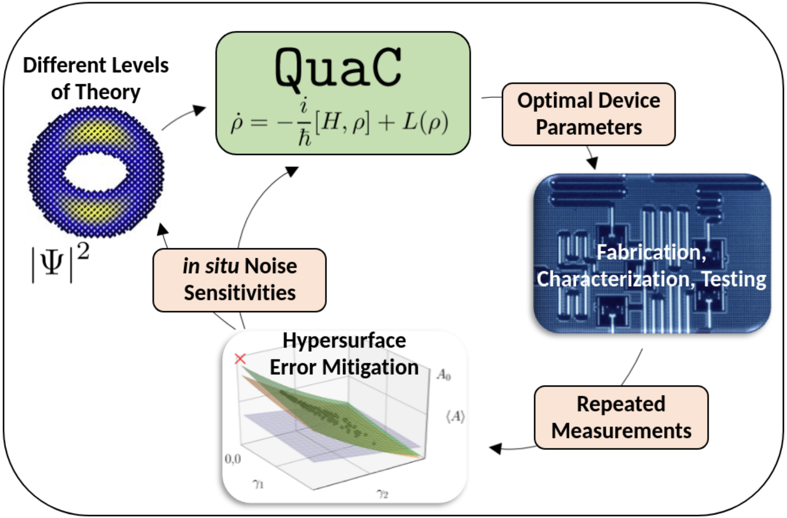
Simulating Realistic Quantum Information Devices

- Density matrix is $2^n \times 2^n$
  - Much more memory intensive than wavefunction
  - Need high-performance computing (QuaC)
- Careful understanding of the important physics for the given architecture is necessary
  - What are the Hamiltonian parameters? What pulse represents what gate? What noise terms are dominant?
  - Other levels of theory (e.g., electronic structure) or experimental data often necessary
- But, we can gain substantial understanding and better performance with high-fidelity simulations

QuaC Features

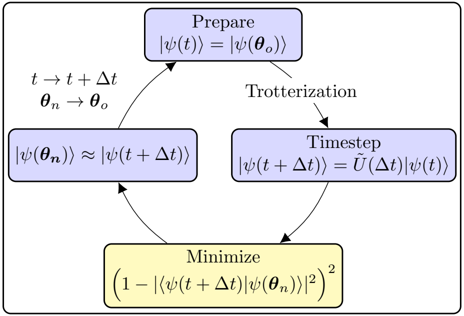
- Simulate arbitrary (and possibly time-dependent) Hamiltonians and Lindbladians
  - n level systems, not just qubits
  - microwave pulses, etc
- Distributed memory parallelism
- 'Easy to use' interface
- Read circuits generated from cirq, qiskit, Forest (Rigetti), ProjectQ

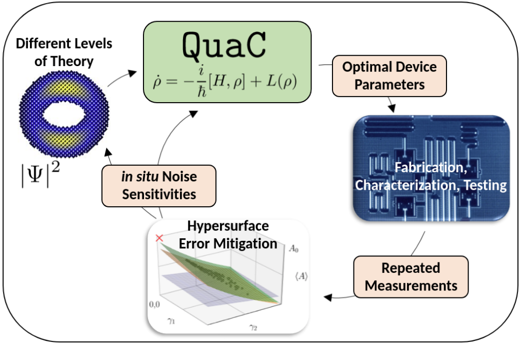
Iterative Design



Conclusion

- Practical applications of quantum computers, especially within chemistry, are within reach
- New algorithms, less expensive error mitigation, and better hardware are necessary to achieve these applications





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