Noise Characterization and Utilization on IBM-Q Superconducting Quantum Computers

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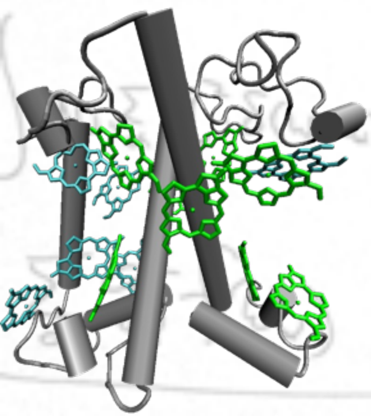
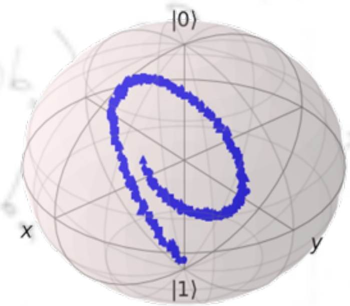
NCTS TG1.1: Quantum Computing and Interdisciplinary Applications





Workshop on Quantum Science and Technology

Physics Division, National Center for Theoretical Sciences

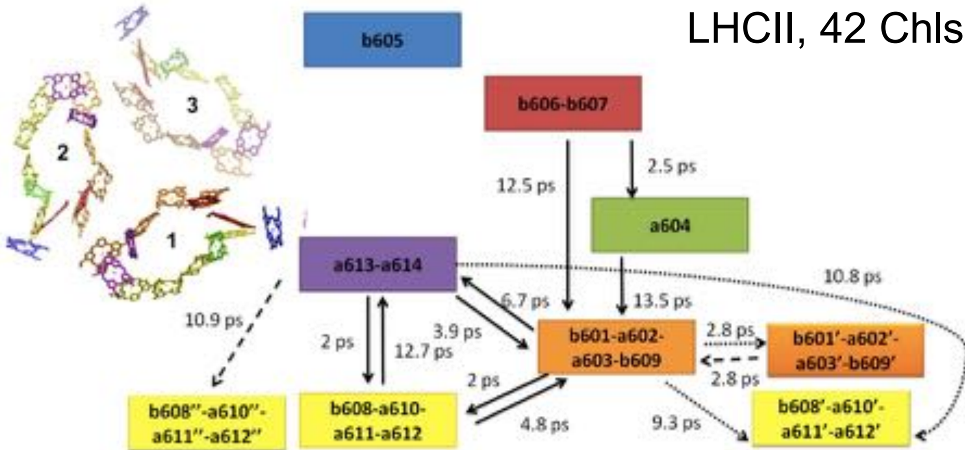
August 26, 2022

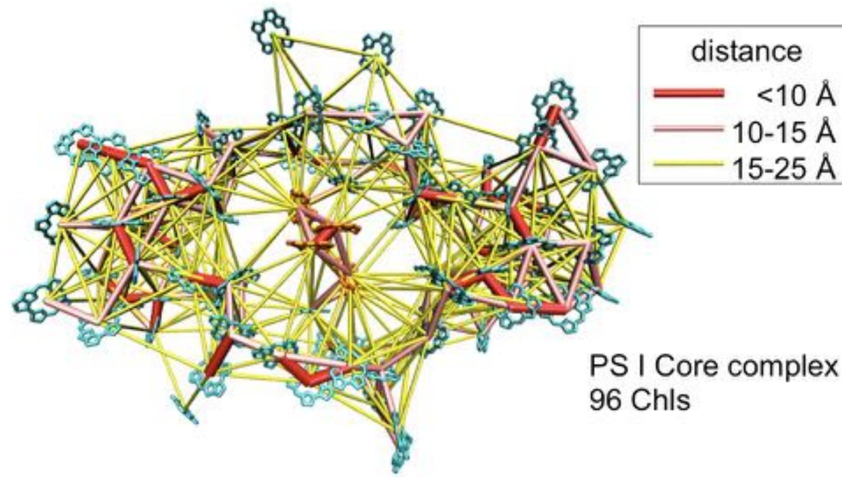
Molecular Modeling of Excitonic Dynamics

We combine molecular dynamics simulations/quantum chemistry with quantum dynamic calculations to study excitonic phenomena in molecular systems

Dynamics of light harvesting

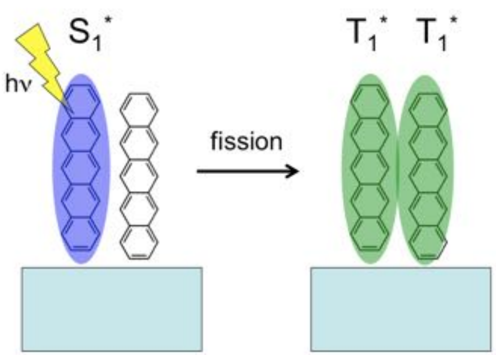
LHCII, 42 Chls



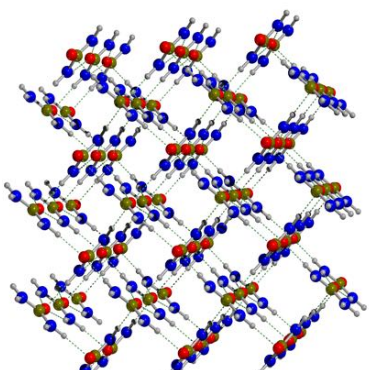


PS I Core complex
96 Chls

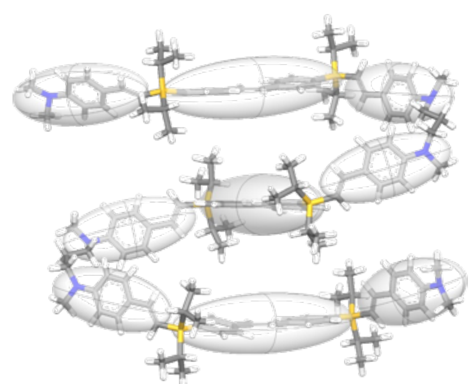
Exciton/charge dynamics in molecular materials



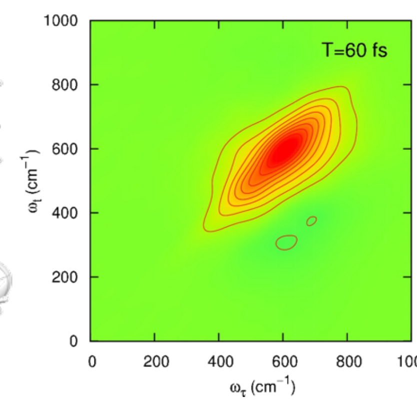
Singlet fission



Charge mobility



Donor/acceptor polymer

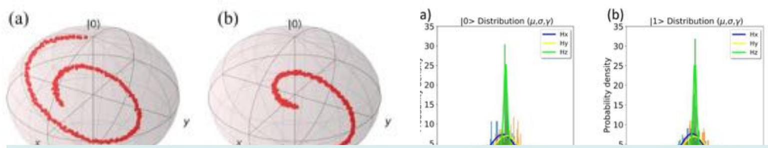


2D spectroscopy

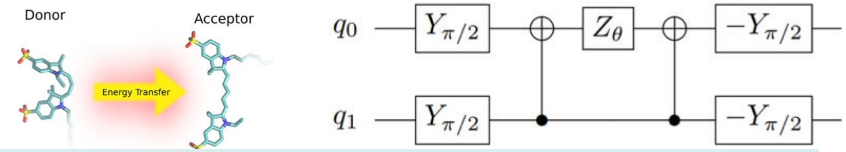
NISQ Quantum Computation for Quantum Chemistry

We also develop hybrid quantum/classical algorithms to enable simulations of molecular systems in the NISQ era.

Characterization of gate errors on IBM-Q



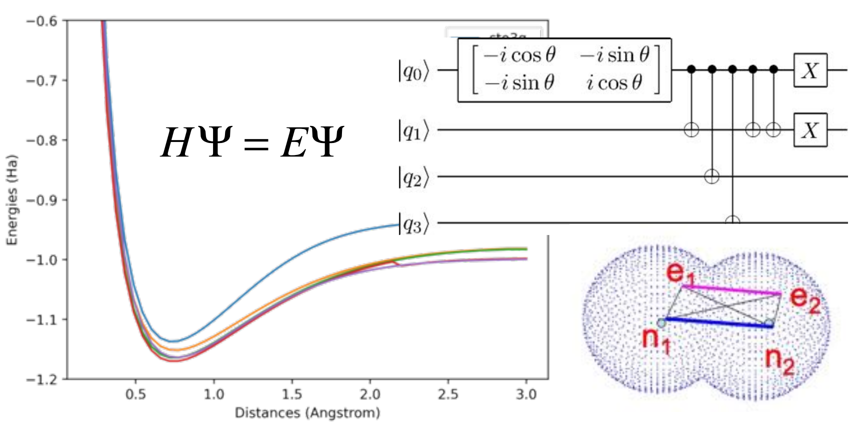
Energy transfer dynamics using quantum noises

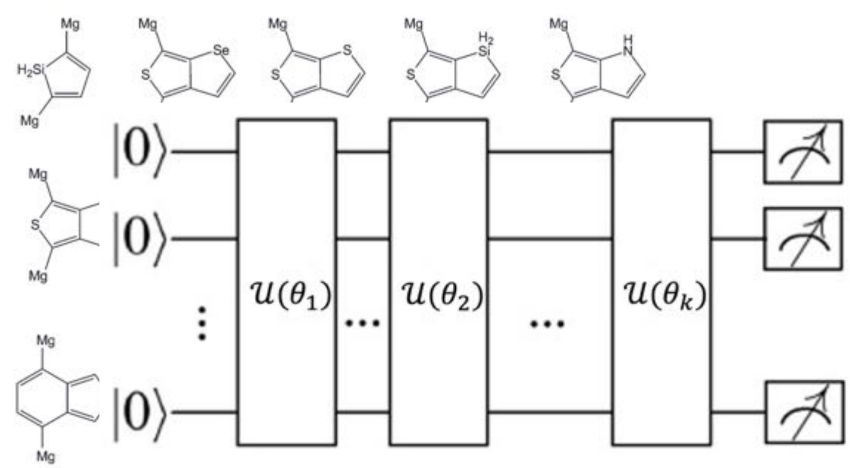


Postdoc/Ph.D. positions available now!

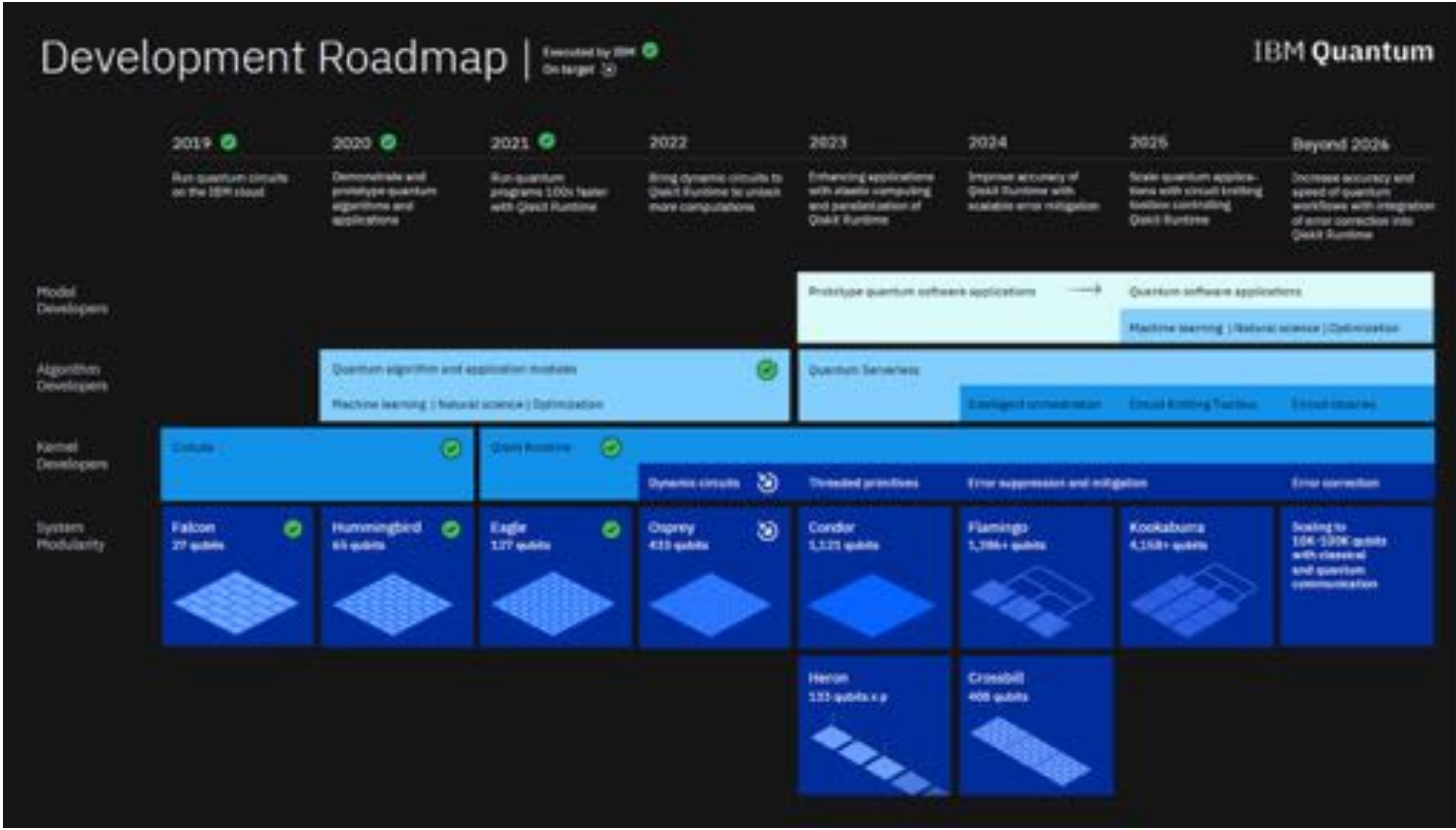
Ch

energies and structures





IBM Quantum Development Roadmap (2022/5)



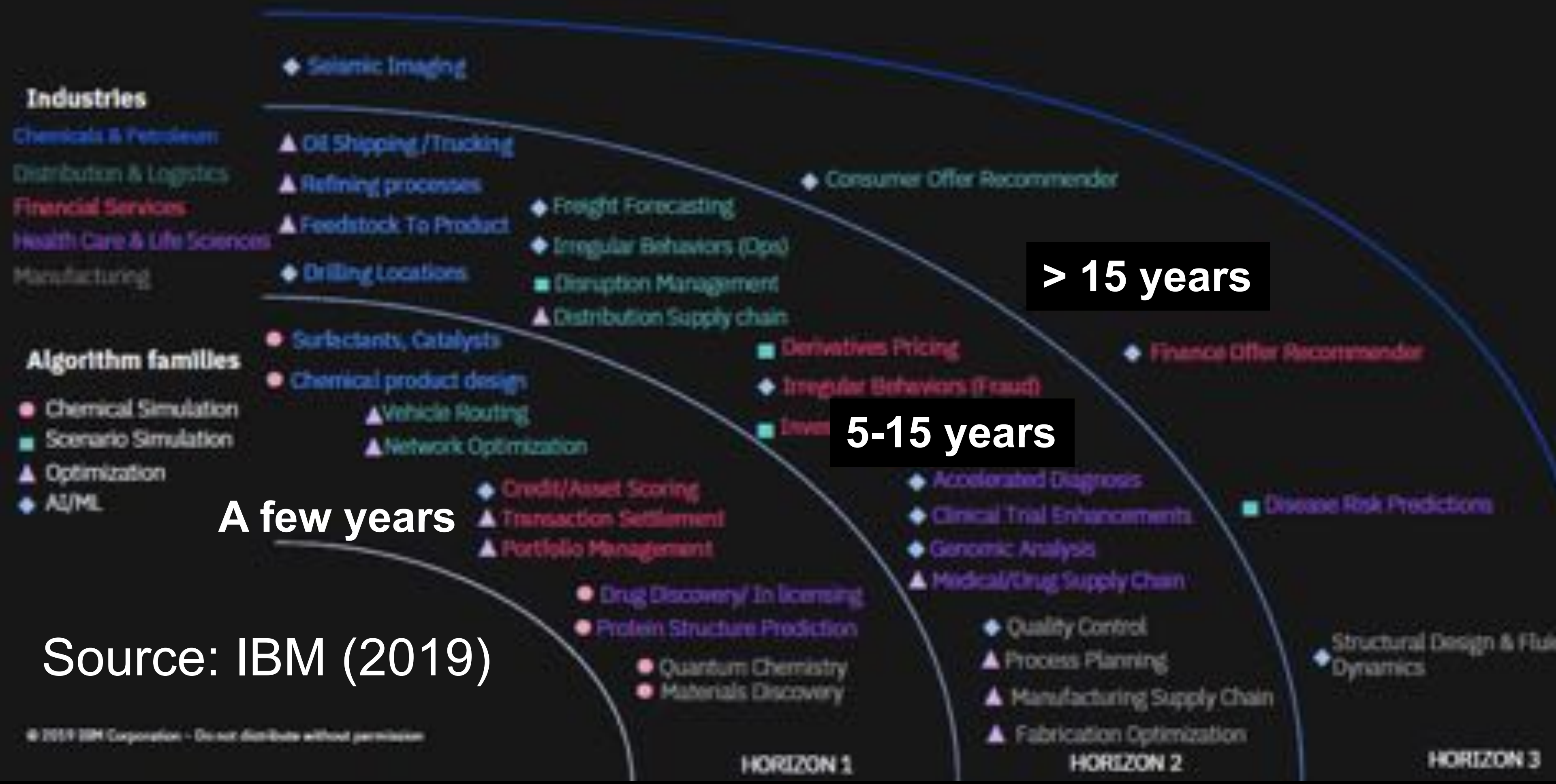
https://www.hpcwire.com/2021/02/04/think-big-ibm-shows-ambitious-roadmap-for-quantum-computing-ecosystem/

Exponential Growth in Quantum Performance

https://research.ibm.com/blog/quantum-volume-256

We will soon have quantum devices with > 100 qubits.
What do we do with it?

IBM predicts quantum computing applications to evolve over ***3 horizons***



Source: IBM (2019)

IBM predicts quantum computing applications to evolve over ***3 horizons***

Quantum simulation and optimization tasks dominate near-term applications of quantum computers!!

Source: IBM (2019)

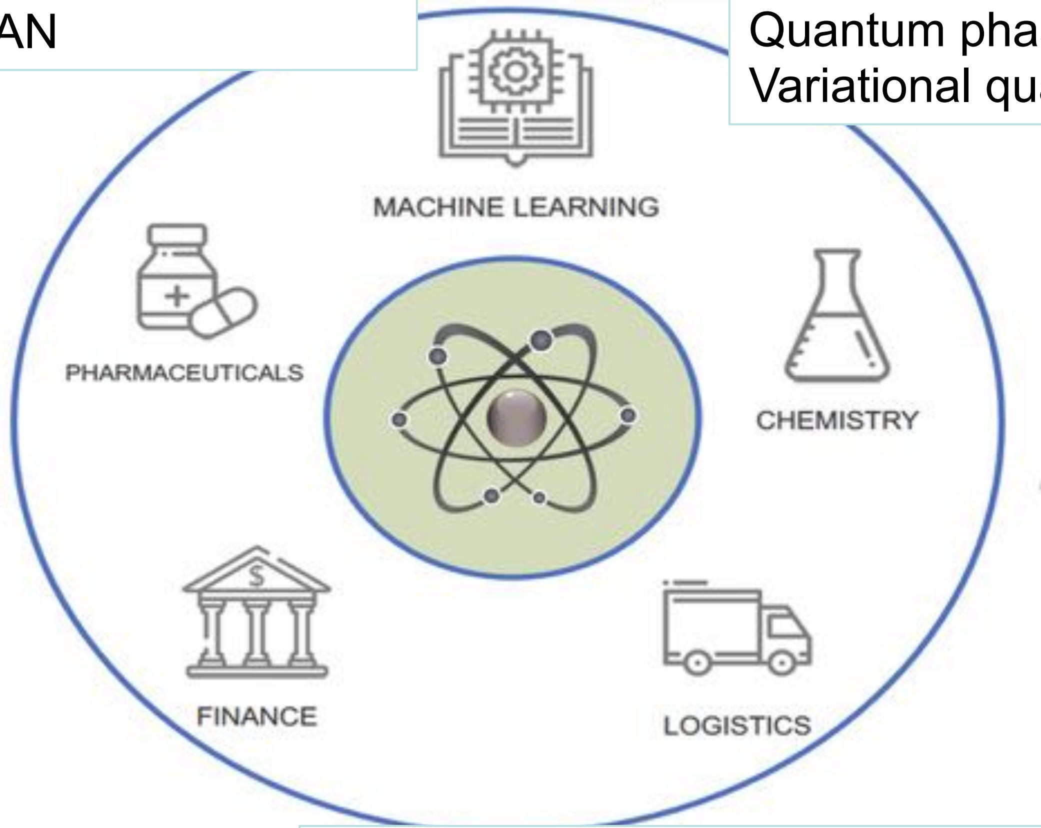
NISQ Devices

- Available near-term quantum computers (e.g. IBM-Q) are NISQ devices
- **NISQ** = Noisy Intermediate-Scale Quantum Computer
- Quantum algorithms designed for NISQ devices are available and currently a hot topic for research
- Suitable for specific tasks that can be performed with a small number of qubits and **limited circuit depth**

Quantum Advantage in the NISQ Era

Quantum Kernel estimation
Variational quantum classifiers
Quantum GAN

Quantum phase estimation
Variational quantum eigensolver



Challenges:
Noise mitigation
Space reduction
Hybrid computing
Barren plateau

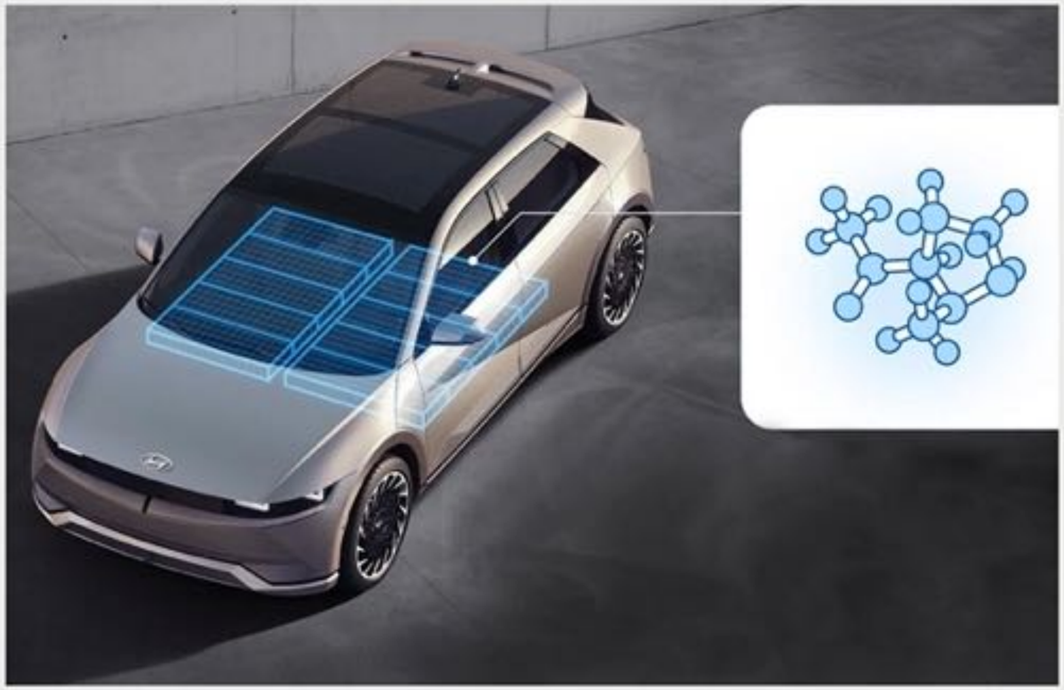
Quantum linear algebra
Quantum approximate optimization algorithm

https://quantumcomputingreport.com/quantum-advantage-with-nisq-devices/

Quantum Computing for Better Batteries

How Quantum Computers Can Make Batteries Better › Hyundai partners with IonQ to optimize lithium-air batteries

BY CHARLES Q. CHOI | 20 JAN 2022 | 3 MIN READ



HYUNDAI

https://www.ibm.com/case-studies/daimler/
https://ionq.com/posts/january-21-2022-improving-battery-chemistry-quantum-computing
Ho et al., Joule 2, 810 (2018); Kim et al., Phys. Rev. Research 4, 023019 (2022)
https://doi.org/10.48550/arXiv.2204.11890

Google’s Quantum Milestone

RESEARCH

QUANTUM COMPUTING

Hartree-Fock on a superconducting qubit quantum computer

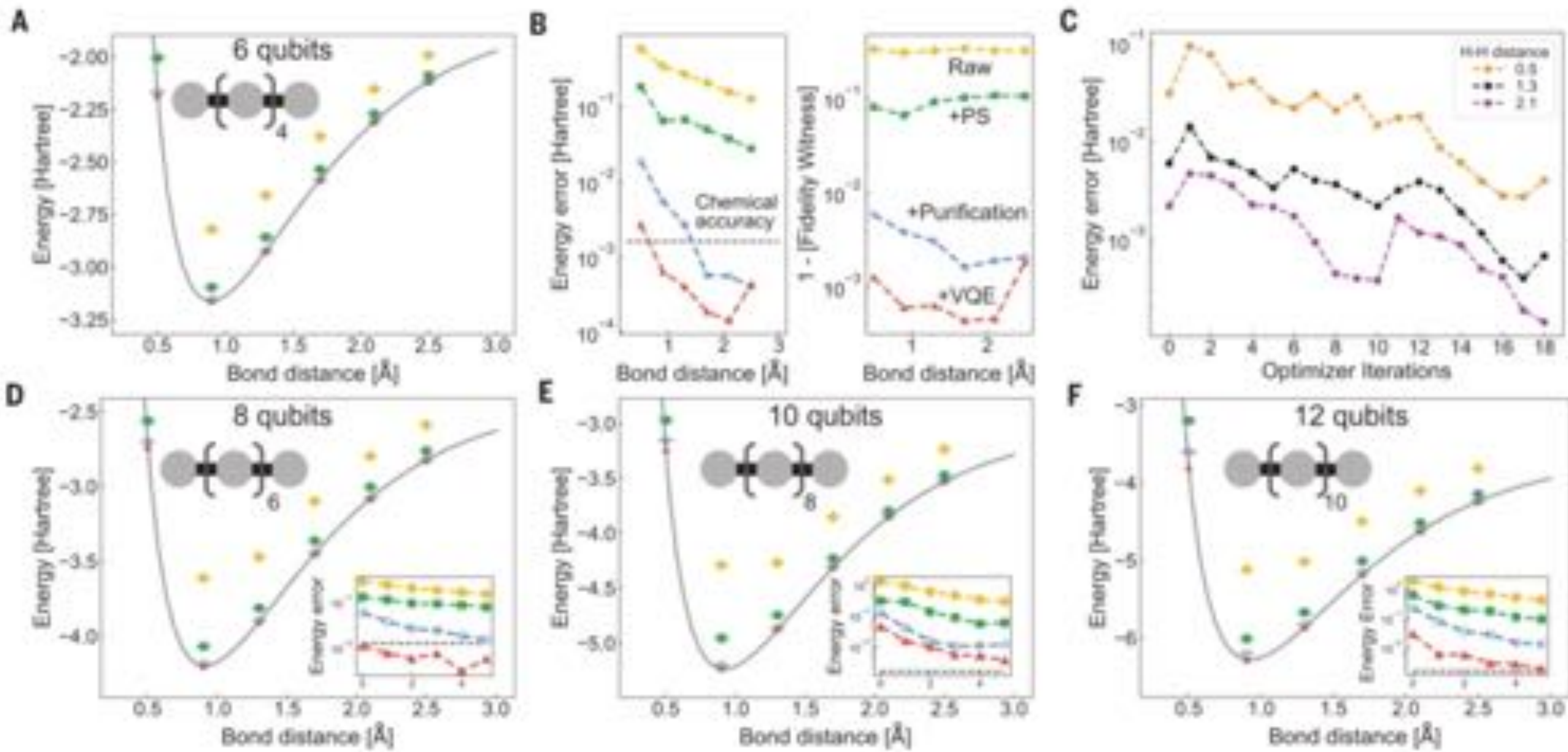
Science **369**, 1084 (2020).

Google AI Quantum and Collaborators*†

The simulation of fermionic systems is among the most anticipated applications of quantum computing. We performed several quantum simulations of chemistry with up to one dozen qubits, including modeling the isomerization mechanism of diazene. We also demonstrated error-mitigation strategies based on *N*-representability that dramatically improve the effective fidelity of our experiments. Our parameterized ansatz circuits realized the Givens rotation approach to noninteracting fermion evolution, which we variationally optimized to prepare the Hartree-Fock wave function. This ubiquitous algorithmic primitive is classically tractable to simulate yet still generates highly entangled states over the computational basis, which allowed us to assess the performance of our hardware and establish a foundation for scaling up correlated quantum chemistry simulations.

Google's Quantum Milestone

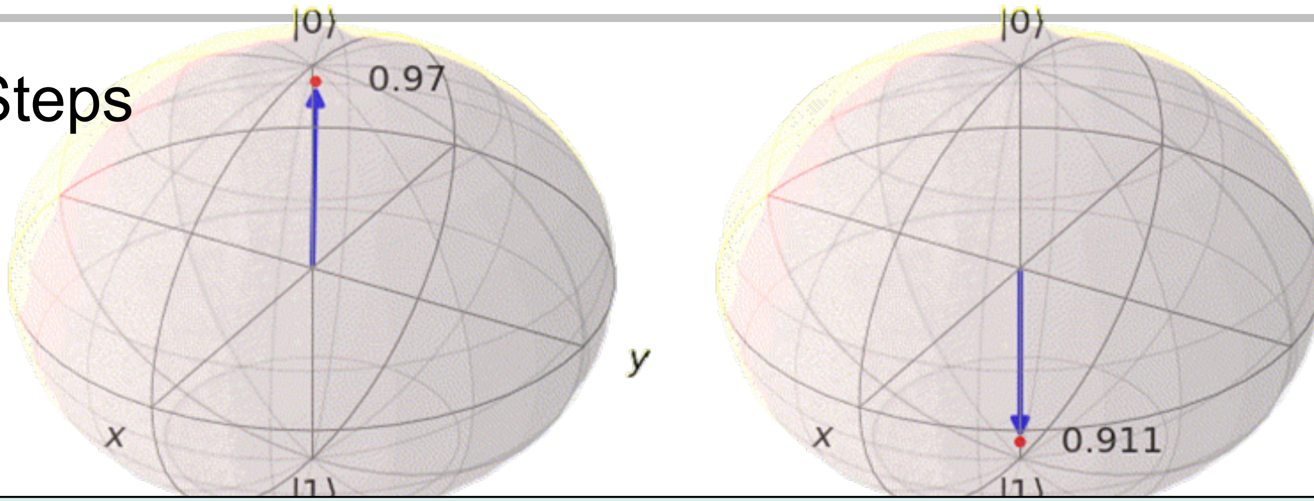
Hartree-Fock calculations of hydrogen chains



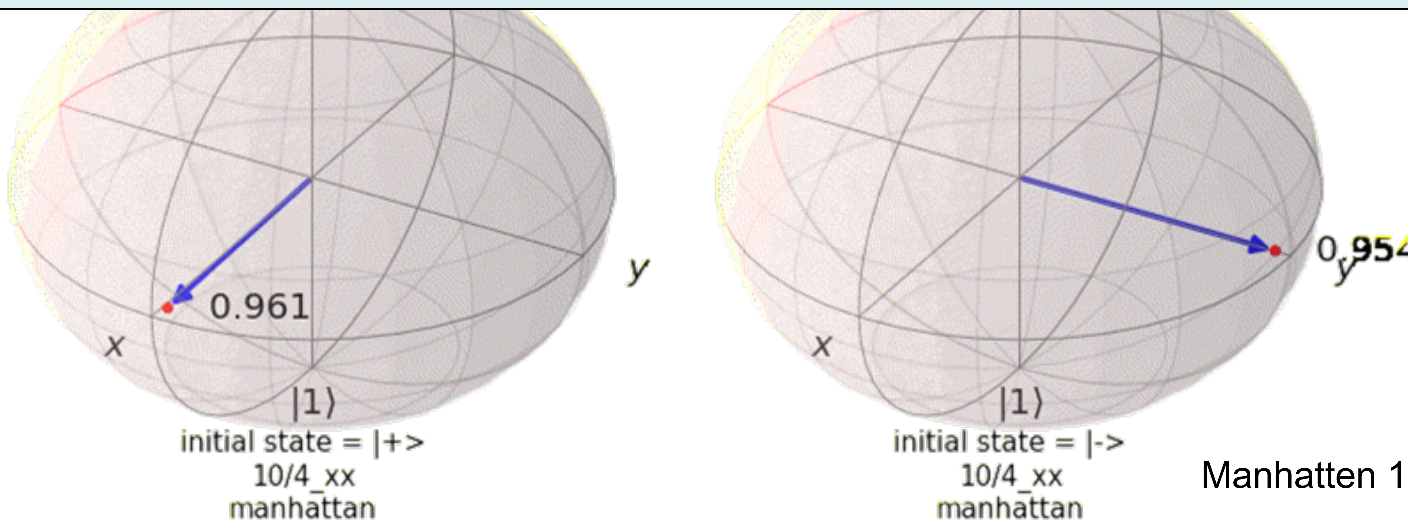
All these calculations still suffer from errors in the quantum devices and it is extremely difficult to scale up.

Errors on a IBM-Q System

300 XX Steps



Nontrivial non-Markovian noises that can not be described by simple error rate models!



Manhatten 10/4/2020

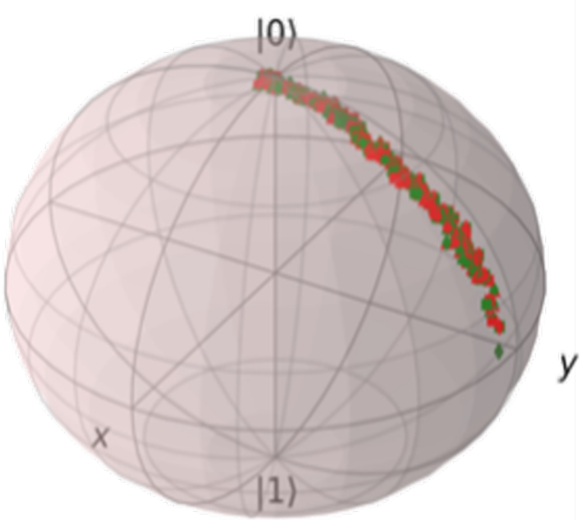
Error Characterization via QST

- Apply repetitive contracted-identity gates + quantum state tomography → $\rho(t)$
- Propagate Liouville dynamics that matchs observed time evolutions → $h_x(t), h_y(t), h_z(t)$

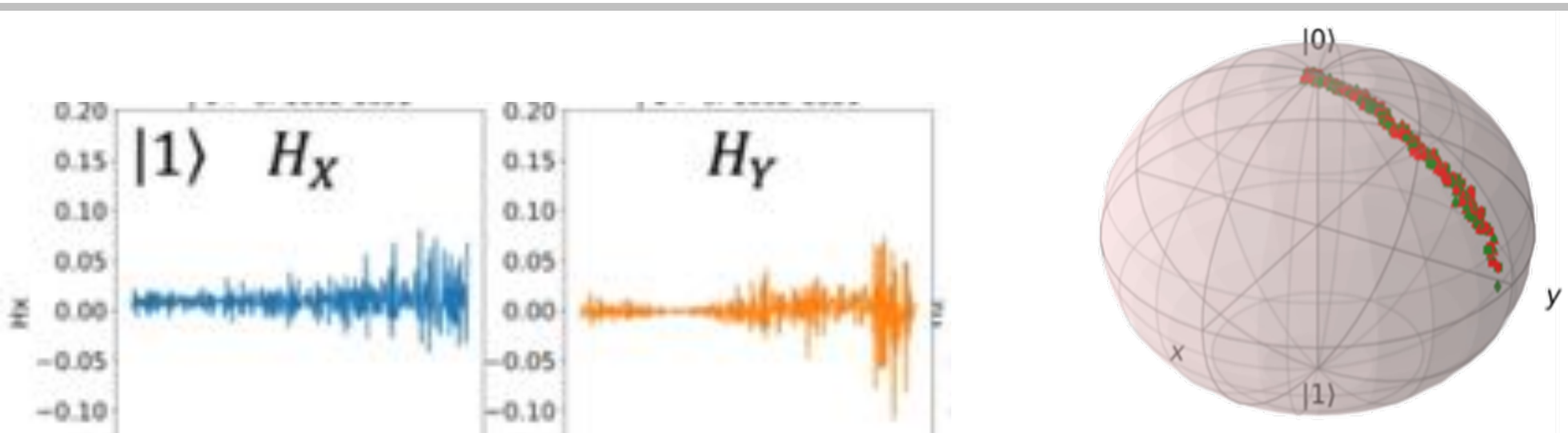
$$\dot{\rho}(t) = i[H(t), \rho(t)] + \sum_i \mathcal{L}_i[\rho(t)],$$

$$H(t) = h_x(t)\sigma_x + h_y(t)\sigma_y + h_z(t)\sigma_z$$

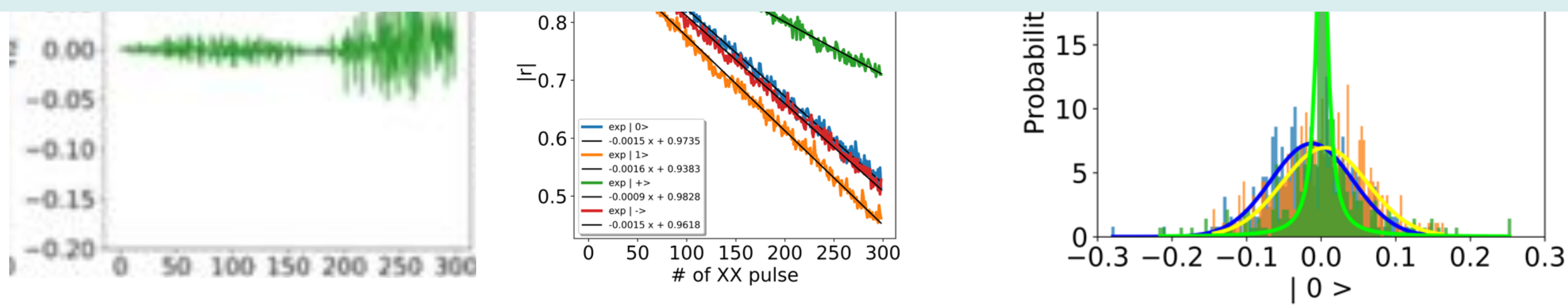
XX gate errors



Error Statistics (XX Gates)



We can extract the full details of noise statistics → So What?



Detailed characterization of gate noise statistics on IBM Q → See Li-Chai Shi's poster (Poster #15)

Quantum Simulation of Open Quantum System Dynamics

Quantum Physics

[Submitted on 24 Jun 2021 (v1), last revised 16 Jul 2021 (this version, v2)]

Efficient Quantum Simulation of Open Quantum System Dynamics on Noisy Quantum Computers

Shin Sun, Li-Chai Shih, Yuan-Chung Cheng

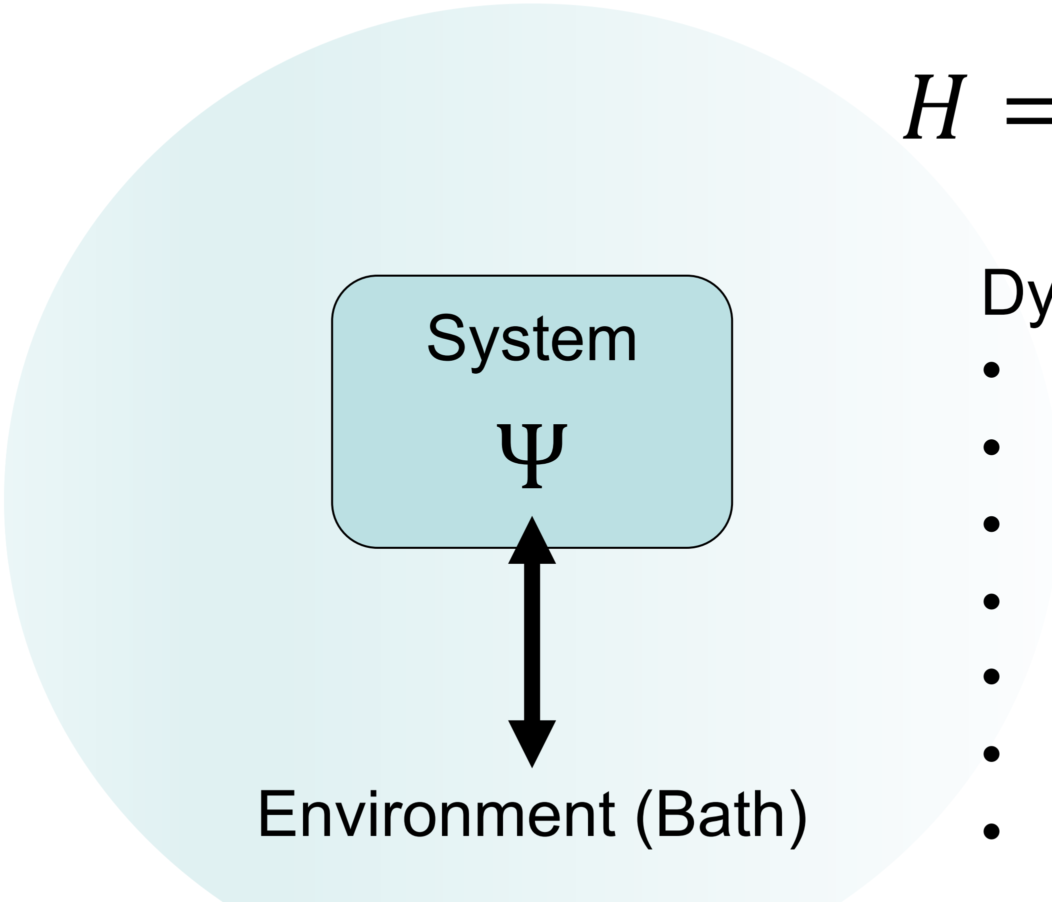
Quantum simulation represents the most promising quantum application to demonstrate quantum advantage on near-term noisy intermediate-scale quantum (NISQ) computers, yet available quantum simulation algorithms are prone to errors and thus difficult to be realized. Herein, we propose a novel scheme to utilize intrinsic gate errors of NISQ devices to enable controllable simulation of open quantum system dynamics without ancillary qubits or explicit bath engineering, thus turning unwanted quantum noises into useful quantum resources. Specifically, we simulate energy transfer process in a photosynthetic dimer system on IBM-Q cloud. By employing designed decoherence-inducing gates, we show that quantum dissipative dynamics can be simulated efficiently across coherent-to-incoherent regimes with results comparable to those of the numerically-exact classical method. Moreover, we demonstrate a calibration routine that enables consistent and predictive simulations of open-quantum system dynamics in the intermediate coupling regime. This work provides a new direction for quantum advantage in the NISQ era.

Subjects: **Quantum Physics (quant-ph)**
Cite as: arXiv:2106.12882 **[quant-ph]**
(or arXiv:2106.12882v2 **[quant-ph]** for this version)

Submission history

From: Shin Sun [view email]
[v1] Thu, 24 Jun 2021 10:37:37 UTC (2,512 KB)
[v2] Fri, 16 Jul 2021 13:05:02 UTC (2,512 KB)

Open Quantum System Dynamics



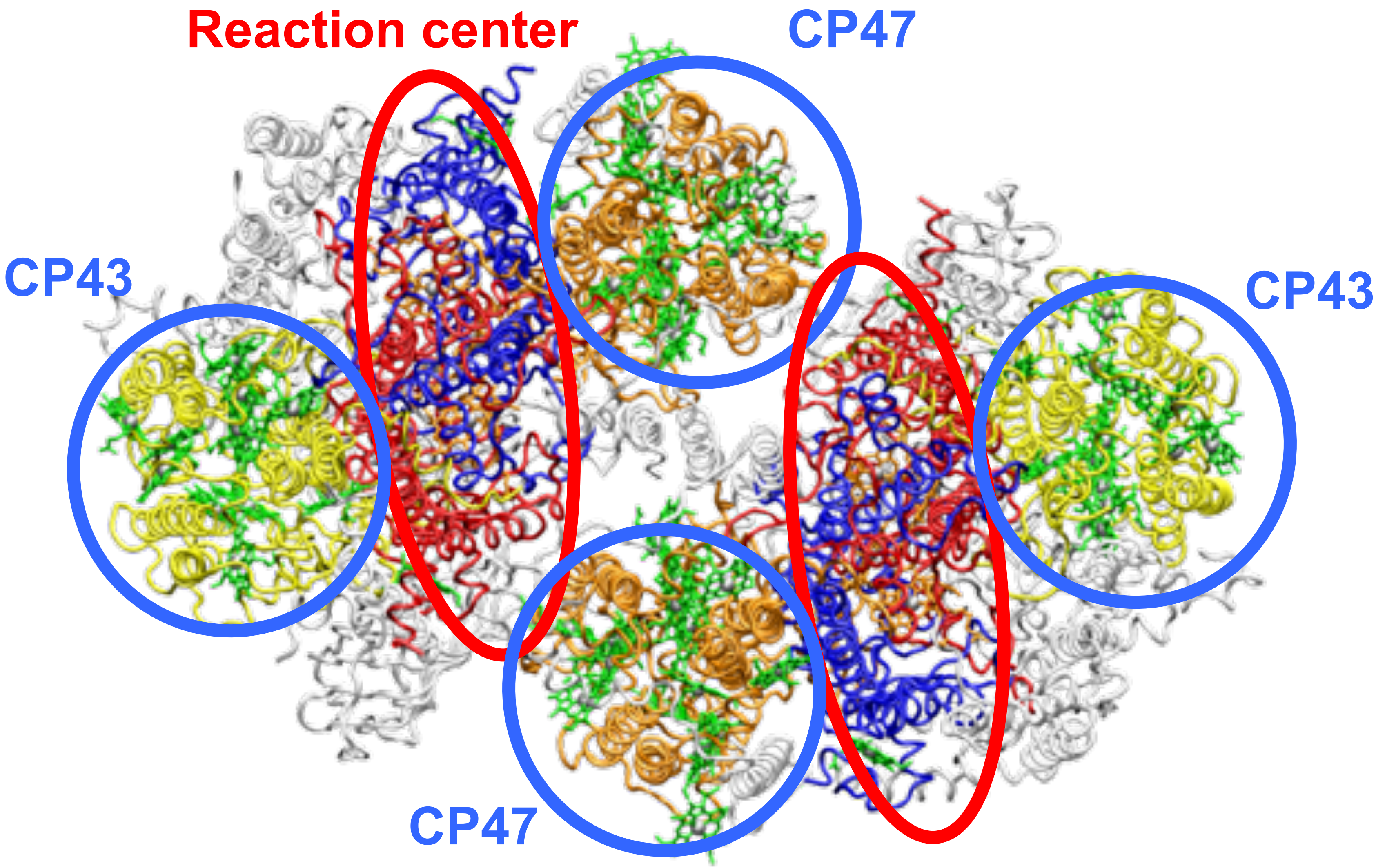
$$H = H_S + H_B + H_{SB}$$

Dynamical phenomena:

- Relaxation
- Internal conversion
- Decoherence/dephasing
- Population transfer
- Energy transfer
- Electron transfer
- …

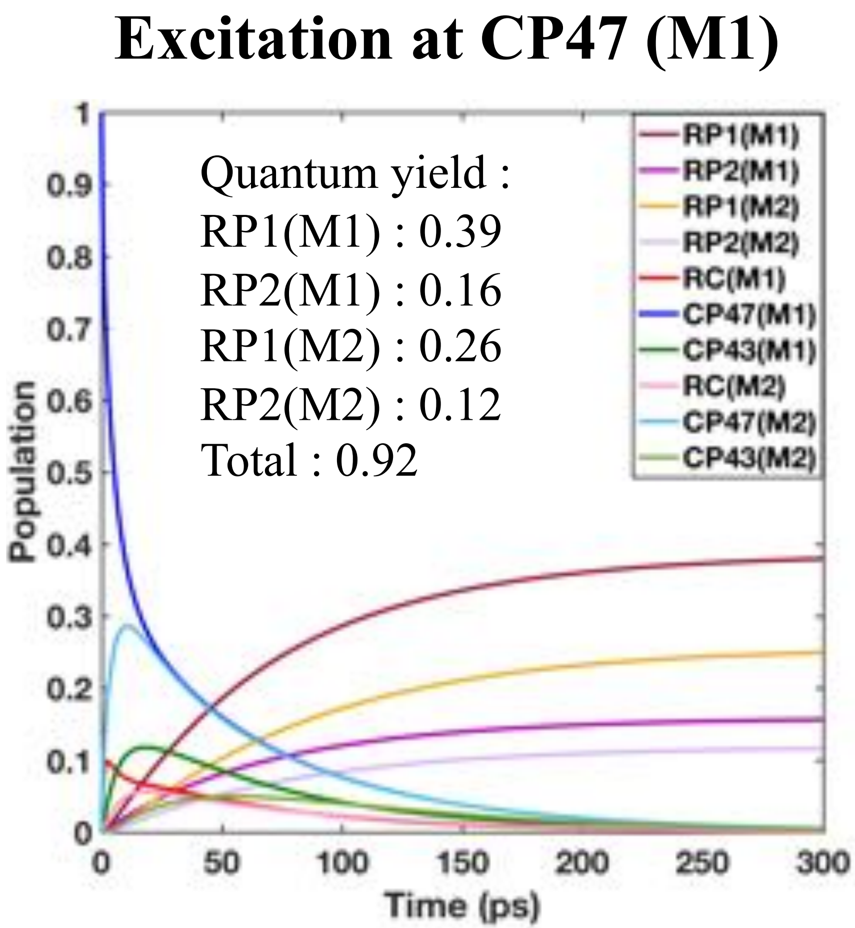
Open quantum system dynamics play critical roles in a broad array of chemical and physical processes!!

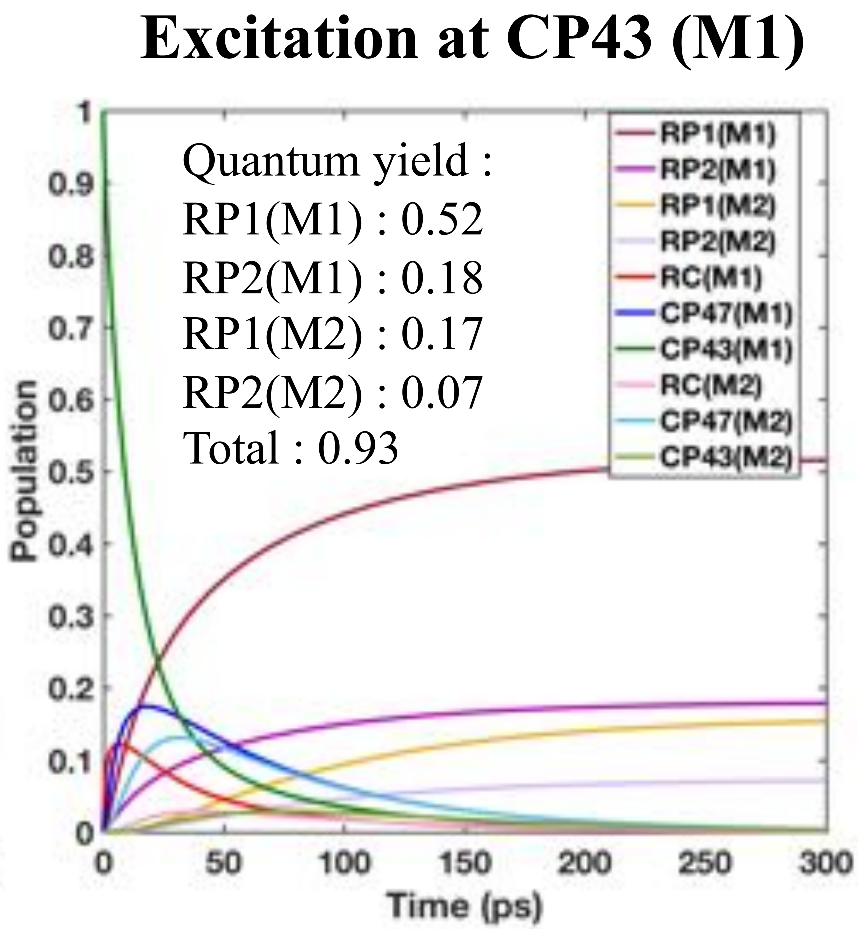
Photosystem II Core Complex (PSII)



Dimer structure with 70 chlorophylls and 4 pheophytins

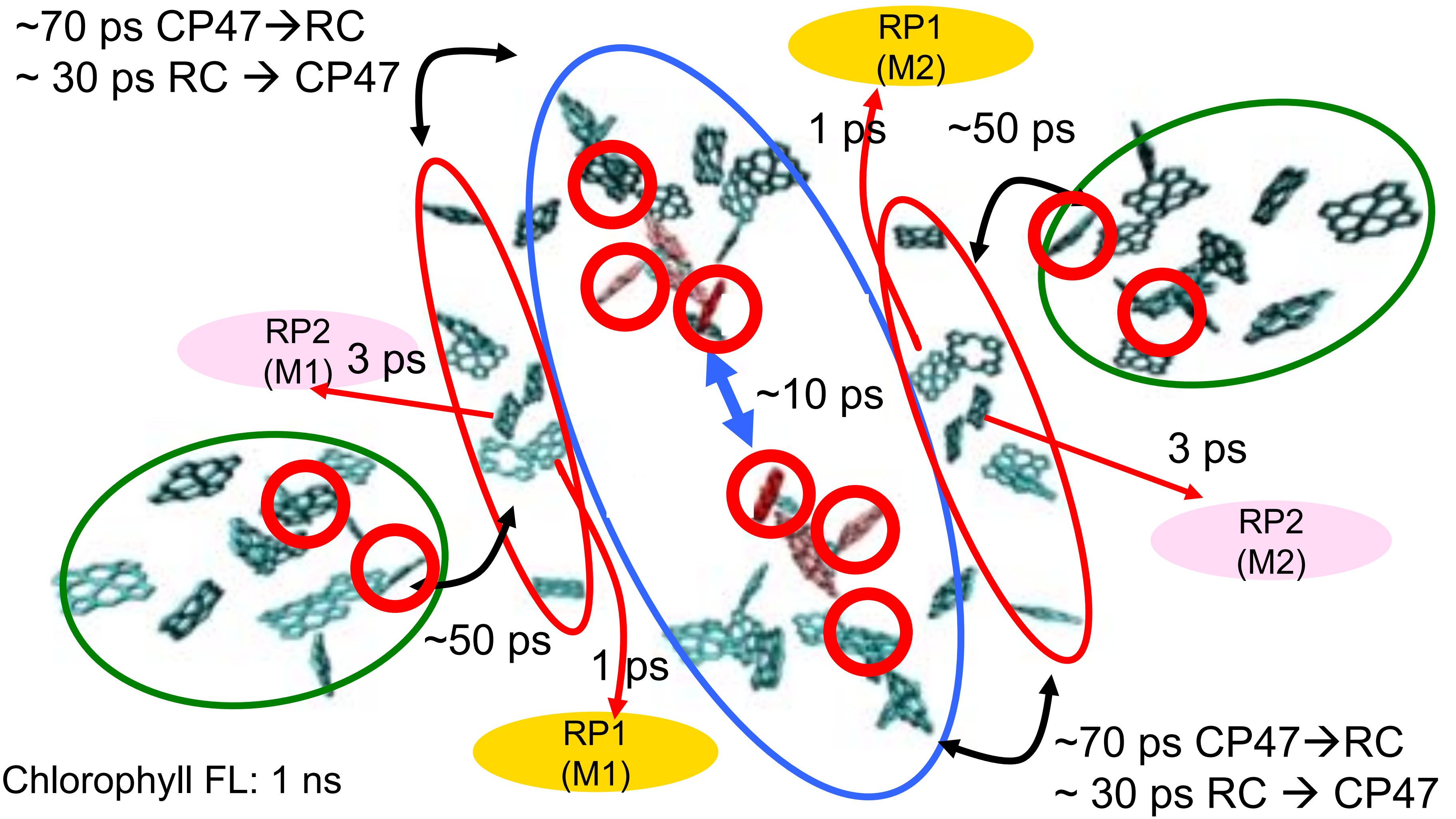
Dynamics of Light Harvesting (Dimer)





- Energy flows to both RCs mediated by CP47
- Light harvesting is reversible and the antennas are connected

Energy Transfer Network in PSII Dimer



- Part of the energy flows to CP47 and shared by both RCs
- Energy transfer "hot spots" can be identified

Open Quantum System Dynamics

- Dissipative quantum dynamics of open quantum systems are crucial in a broad range of physical and/or chemical phenomena in complex systems, such as photosynthetic light harvesting. In this research we aim to turn nowadays NISQ devices into useful tools for quantum simulation of open quantum systems.
- Simulation of dissipative quantum system is difficult for classical computers in the intermediate noise-strength regime -- Non-Markovian dynamics, non-perturbative effects, quantum coherence…

$$\partial_t \rho_{\rm rel} = \mathcal{P} L \rho_{\rm rel} + \int_0^t dt' \mathcal{K}(t') \rho_{\rm rel}(t - t')$$

Simulating Light Harvesting on a NMR QC

npj | Quantum Information

www.nature.com/npjqi

ARTICLE OPEN

Efficient quantum simulation of photosynthetic light harvesting

Bi-Xue Wang[1], Ming-Jie Tao[1,2], Qing Ai[2,3], Tao Xin[1], Neill Lambert[3], Dong Ruan[1], Yuan-Chung Cheng[4], Franco Nori[3,5], Fu-Guo Deng[2,6] and Gui-Lu Long[1,7,8,9,10]

Near-unity energy transfer efficiency has been widely observed in natural photosynthetic complexes. This phenomenon has

principles for efficient artificial light harvesting.

npj Quantum Information (2018)4:52 ; doi:10.1038/s41534-018-0102-2

Not scalable because the requirement to simulating environment noise explicitly can not be fulfilled on nowadays NISQ devices!

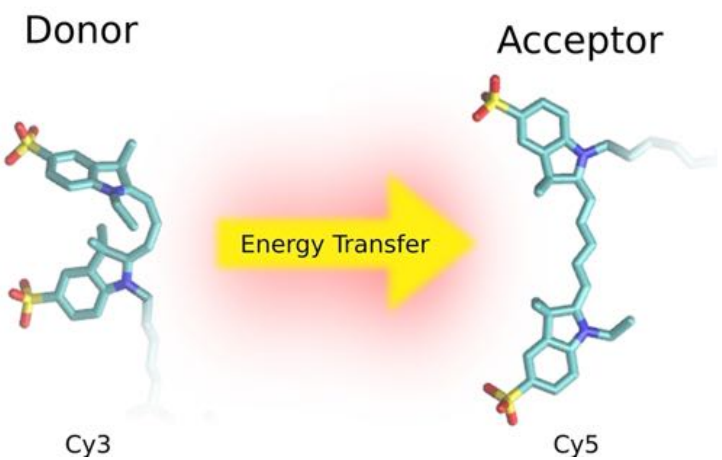
NISQ Devices

- Available near-term quantum computers (e.g. IBM-Q) are NISQ devices
- **NISQ** = Noisy Intermediate-Scale Quantum Computer
- Simulating a close quantum system on a NISQ device is prone to error due to both coherent and incoherent noises – effects required in simulating open quantum systems

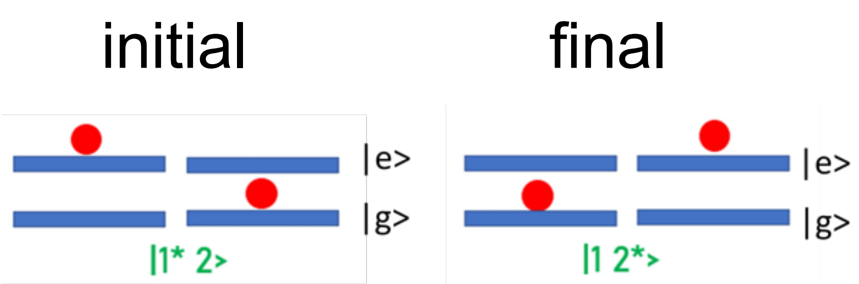
"Can we utilize intrinsic noises in a QC to simulate open quantum system dynamics?"

Model Energy Transfer System

- We adopt the simplest energy transfer system, a unbiased exciton dimer as our model system, and encode the exciton occupation in qubit working basis.



An essential step in photosynthetic light harvesting



$$H = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = a_1^{+} a_2 + a_1 a_2^{+}$$

(simplest symmetric dimer case)

Picture adapted from Wallace B, Atzberger PJ (2017) Förster resonance energy transfer: Role of diffusion of fluorophore orientation and separation in observed shifts of FRET efficiency. PLOS ONE 12(5)

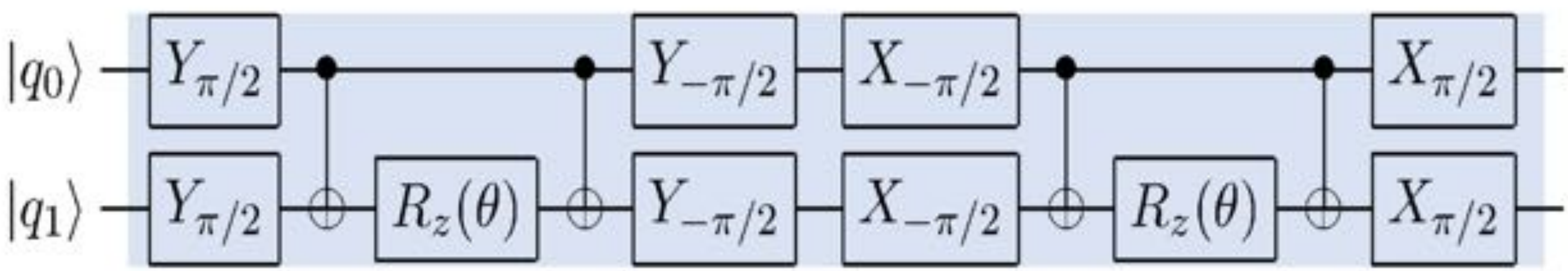
Model Energy Transfer System

Encode the exciton occupation in qubit working basis.

Jordan–Wigner representation:

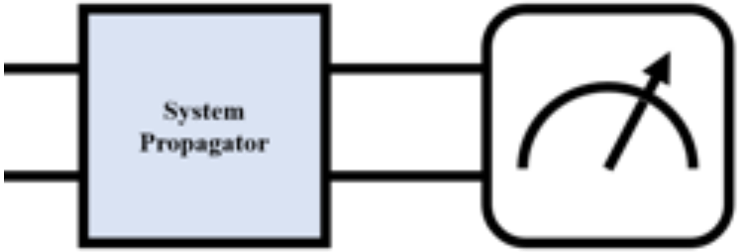
$$a_n^+ = \frac{1}{2}(X_n - iY_n) \qquad a_n = \frac{1}{2}(X_n + iY_n)$$

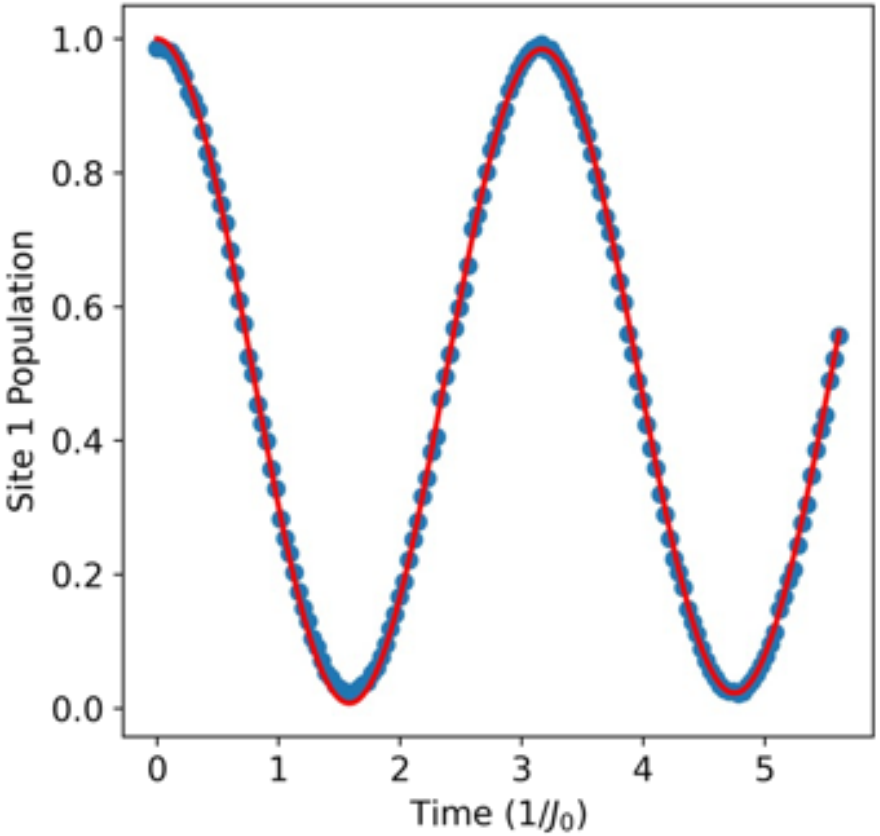
Quantum Circuit for Unitary Time Evolution (θ=t):



Picture adapted from Wallace B, Atzberger PJ (2017) Förster resonance energy transfer: Role of diffusion of fluorophore orientation and separation in observed shifts of FRET efficiency. PLOS ONE 12(5)

Coherent Evolution

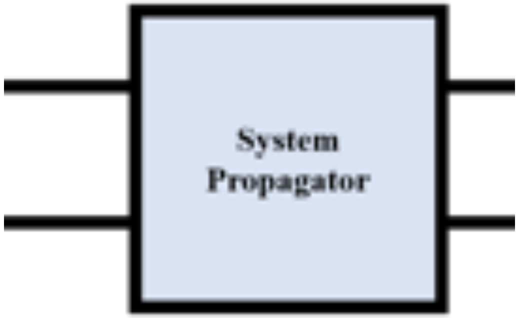




Rabi oscillation nicely described on IBM-Q:

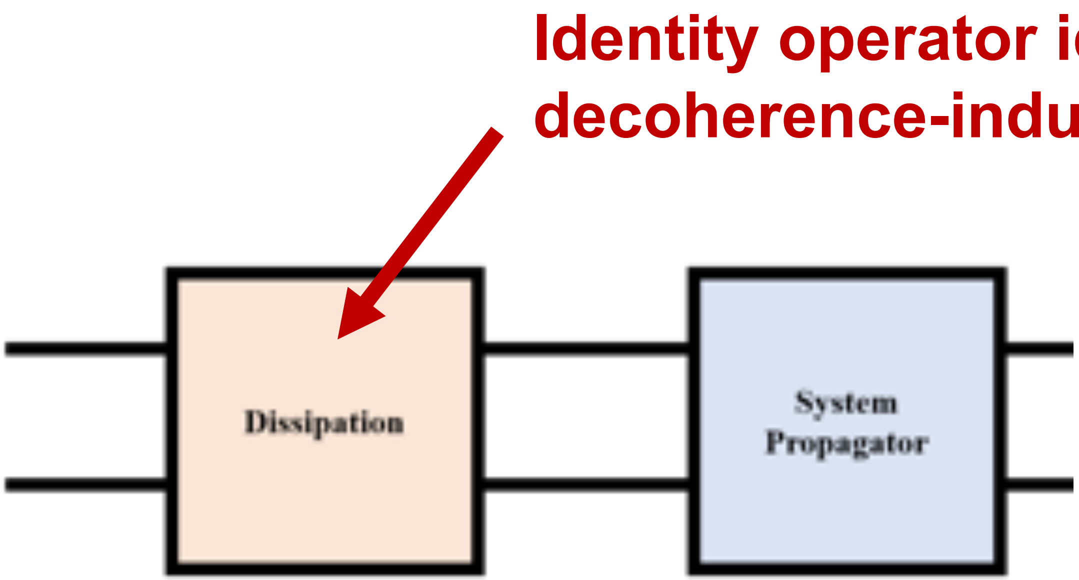
- If the population is intermediately renormalized within the one-exciton manifold
- Leakage errors can be easily mitigated and do not affect the coherence in the one-exciton space
- Errors limit the length of the quantum simulation

Introducing Dissipative Dynamics



Introducing Dissipative Dynamics

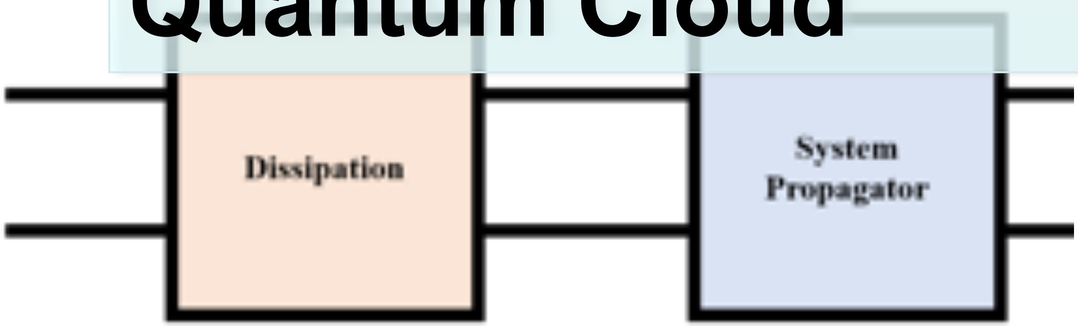
- To introduce desired noises, we append to the system propagator a pulse sequence which contracted to identity ideally but make the system decohere due to gate imperfection – **decoherence-inducing gate sequence**.



Introducing Dissipative Dynamics

- To introduce desired noises, we append to the system propagator a pulse sequence which contracted to identity ideally but make the system decohere due to gate imperfection – **decoherence-inducing gate sequence**.
- The number of pulses per simulation time corresponds to the system-bath coupling strength.

Carry out calculations on real quantum computers – IBM-Q Quantum Cloud

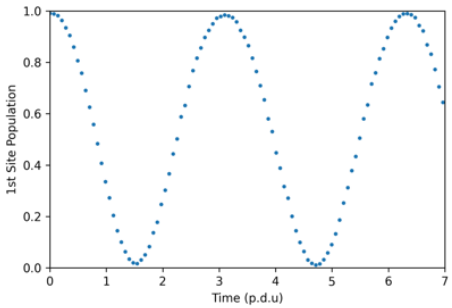


Pulses tested:

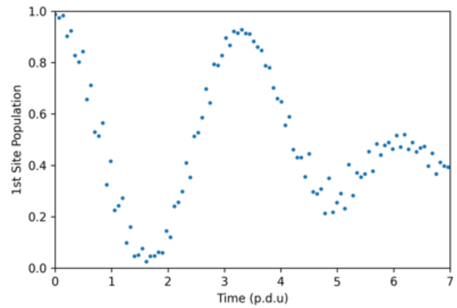
1. XX
2. (XZXZZ)(XZXZZ)
3. (SWAP)(SWAP)

Energy Transfer Dynamics : X^2

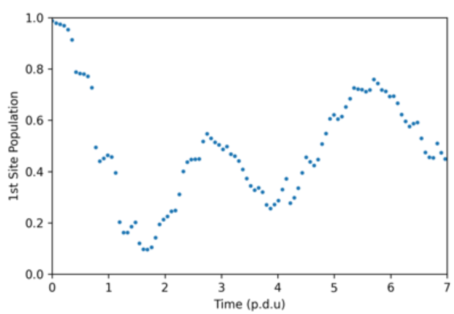
#pulses /Δt = 0



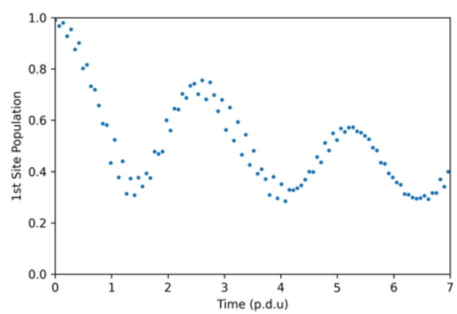
#pulses /Δt = 20



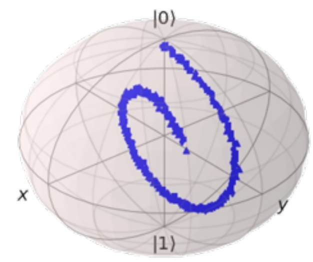
#pulses /Δt = 40

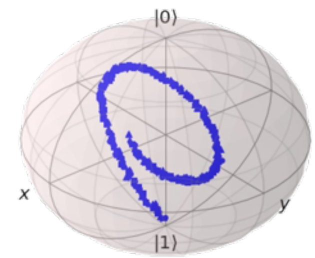


#pulses /Δt = 70



X^2 Bloch Sphere Dynamics





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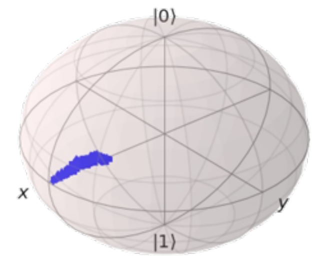
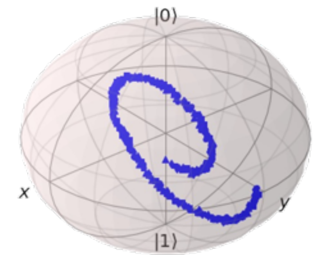


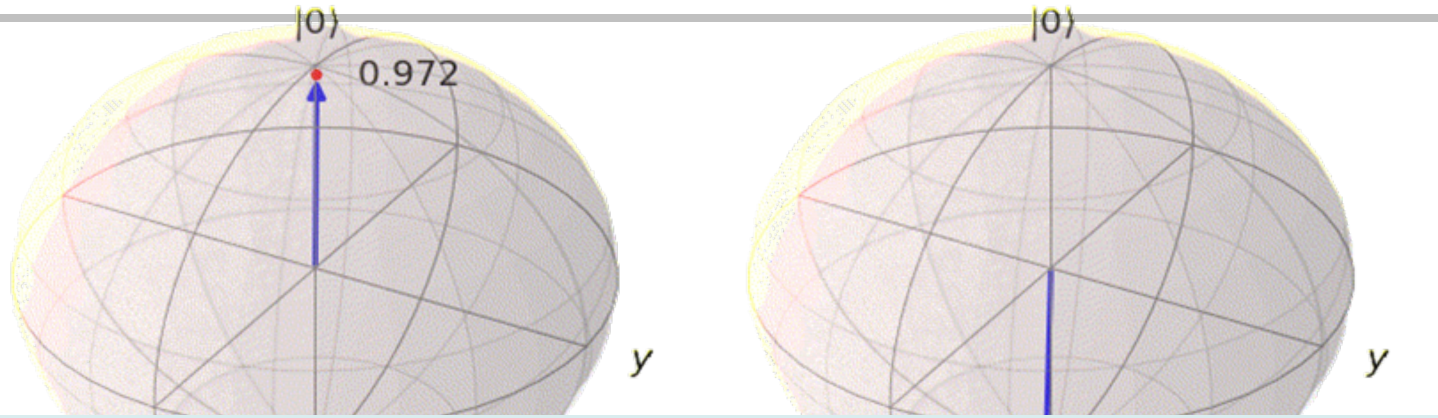


The simplest pulse results in unphysical dissipative dynamics.

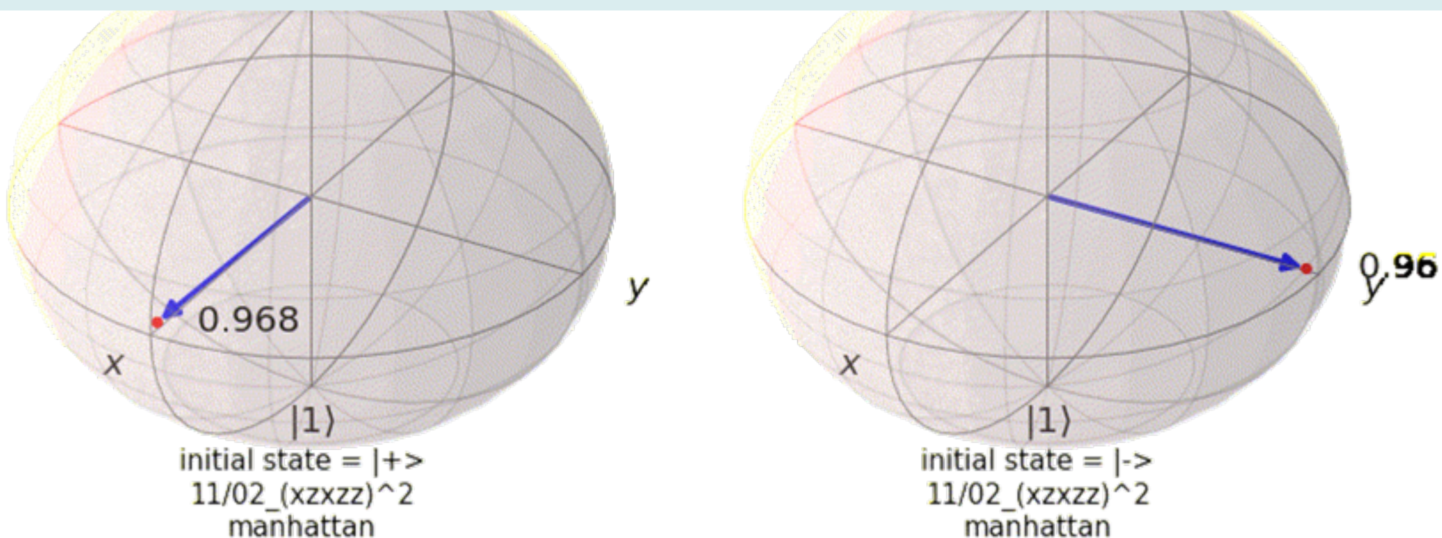
All experiments executed on ibmq_manhattan

Can’t just use any identity sequences!

300 $(XZXZZ)^2$ Steps (on manhattan, 11/02)

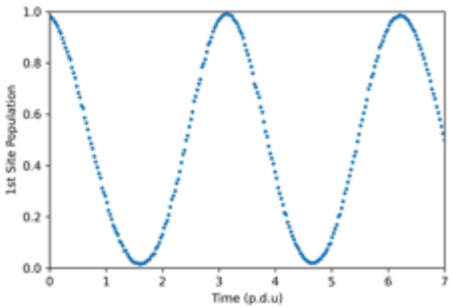


$(XZXZZ)^2$ produces well-behaved depolarization noises → a proper decoherence-inducing gate sequence from the principle of dynamical decoupling.

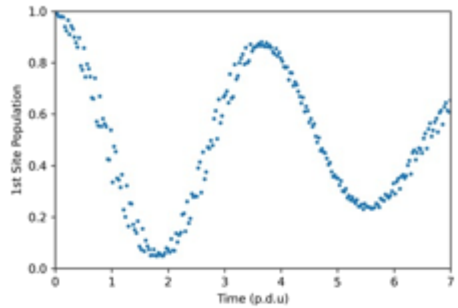


Energy Transfer Dynamics : $(XZXZZ)^2$

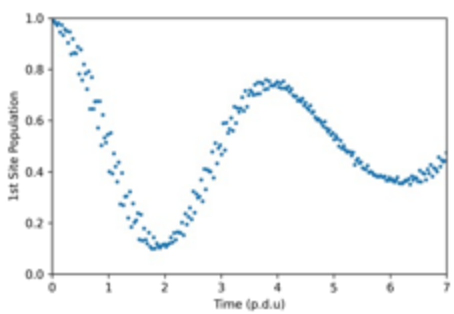
#pulses /Δt = 0



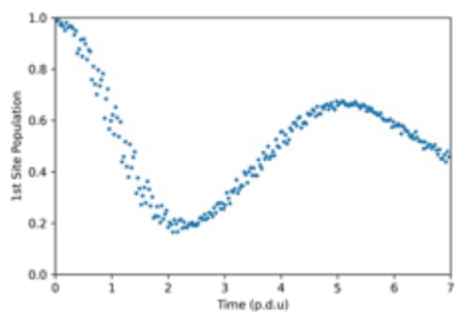
#pulses /Δt = 25



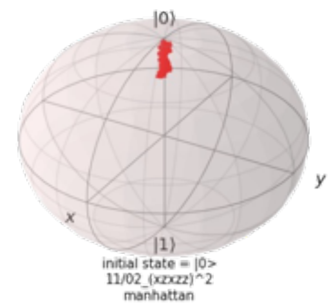
#pulses /Δt = 35



#pulses /Δt = 55



$(XZXZZ)^2$ Bloch Sphere Dynamics



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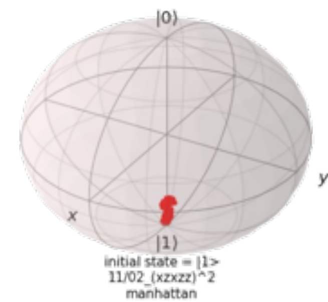

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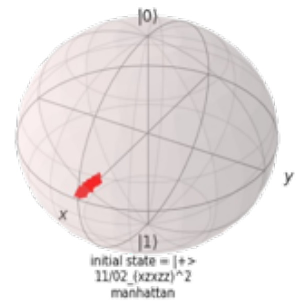
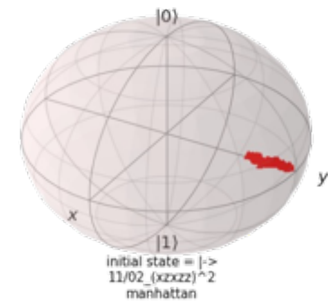


|+>



|->

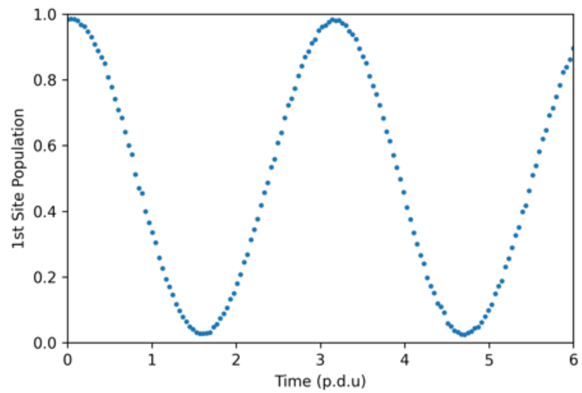
$(XZXZZ)^2$ sequence results in consistent coherent dissipative quantum dynamics – dynamical decoupling of unwanted noises.

All experiments executed on ibmq _manhattan

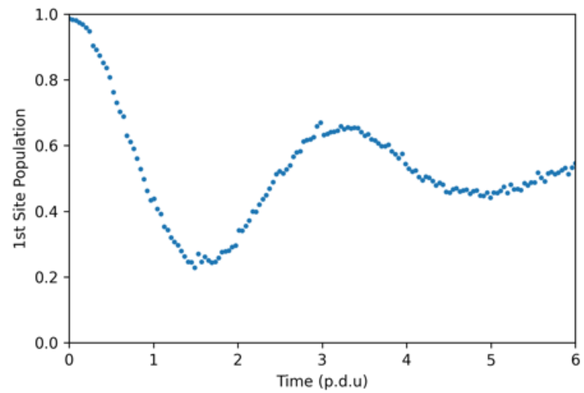
Energy Transfer Dynamics : $(SWAP)^2$

All the experiments are executed on ibmq_paris

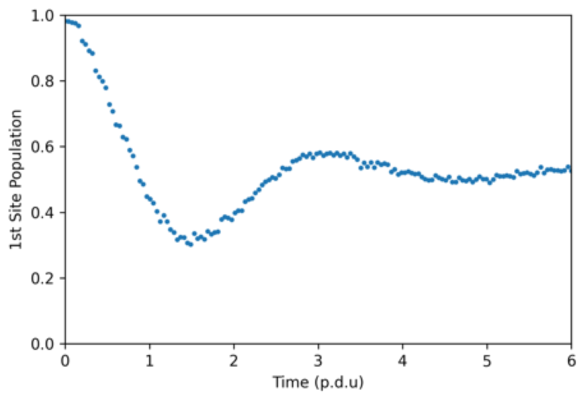
#pulses /Δt = 0



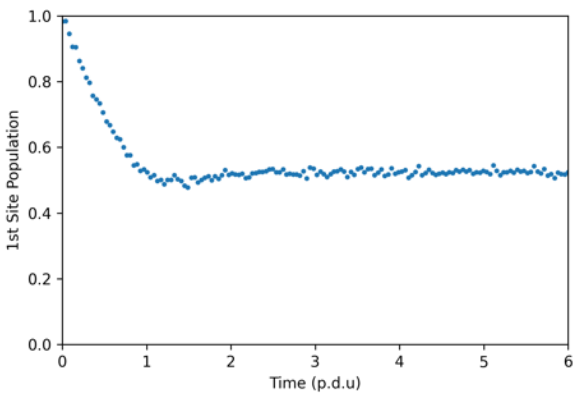
#pulses /Δt = 4



#pulses /Δt = 6



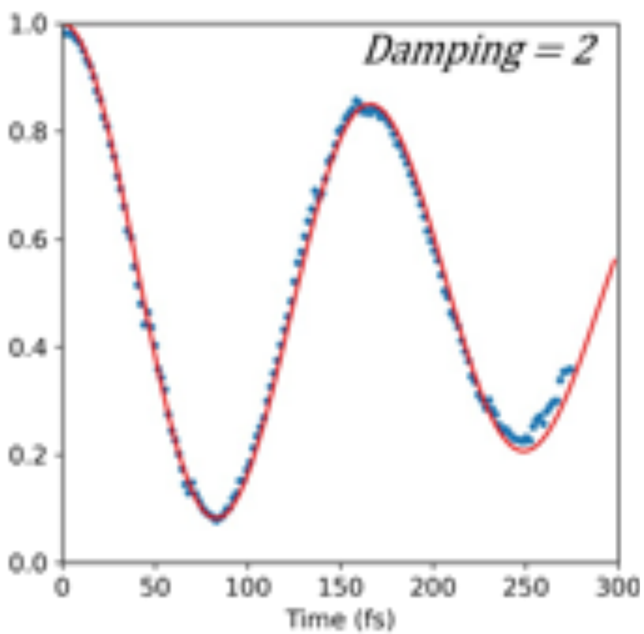
#pulses /Δt = 18



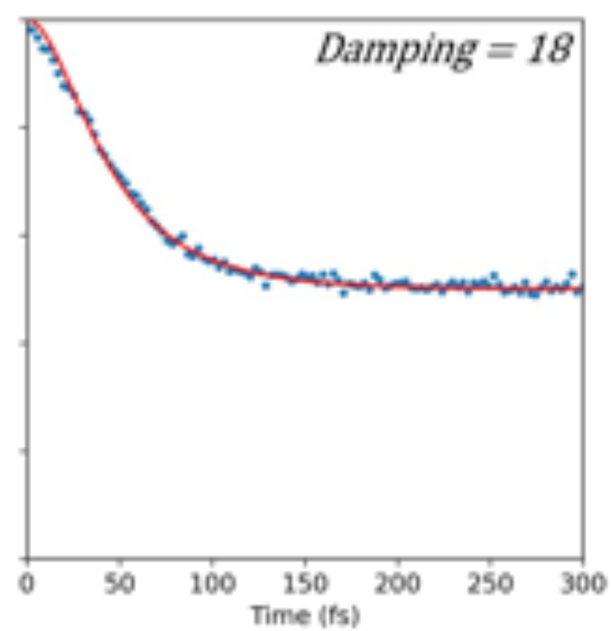
The $SWAP^2$ pulses produce consistent dynamics, demonstrating the **coherent-to-incoherent transition** with increasing system-bath coupling strength.

Compared to HEOM Calculations

- To validate the simulated dissipative dynamics, we compared the NISQ simulations to dynamics obtained using **hierarchical equation of motion** (HEOM) method – a numerically exact but expansive method
- Quantum simulations agree well with HEOM results in both the coherent and incoherent EET limits

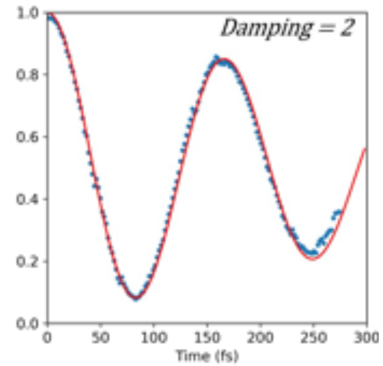


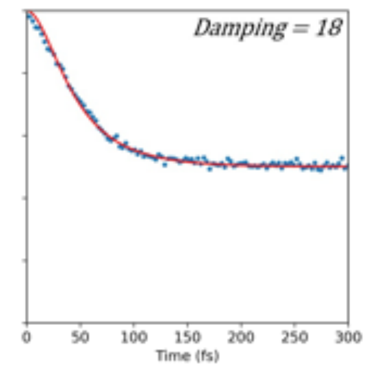
Coherent EET



Incoherent EET

Fitted HEOM Parameters

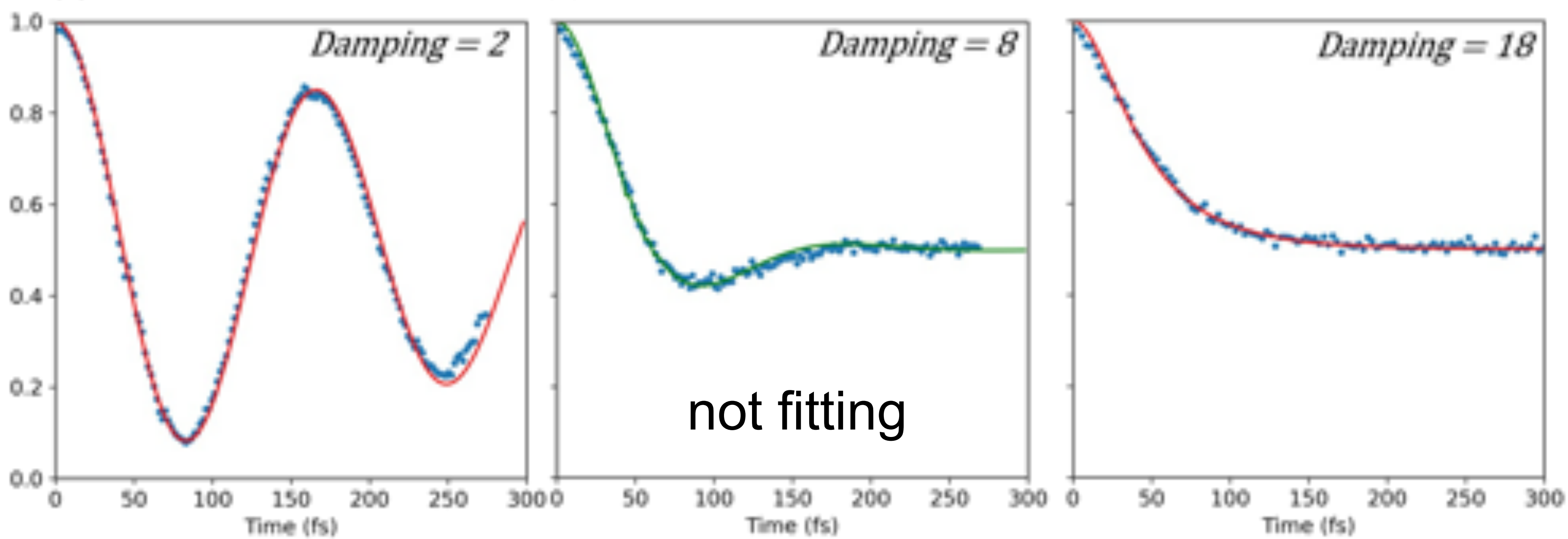




	Underdamped	**intermediate**	Overdamped
Damping coefficient	2	8 ?	18
Excitonic coupling	$100\ cm^{-1}$	↓	$100\ cm^{-1}$
Cutoff frequency	$100\ ps^{-1}$		$100\ ps^{-1}$
Reorganization energy	$15\ cm^{-1}$	95 cm^{-1}	$227\ cm^{-1}$
Hierarchy truncation	8		8
Temperature	300 K		300 K

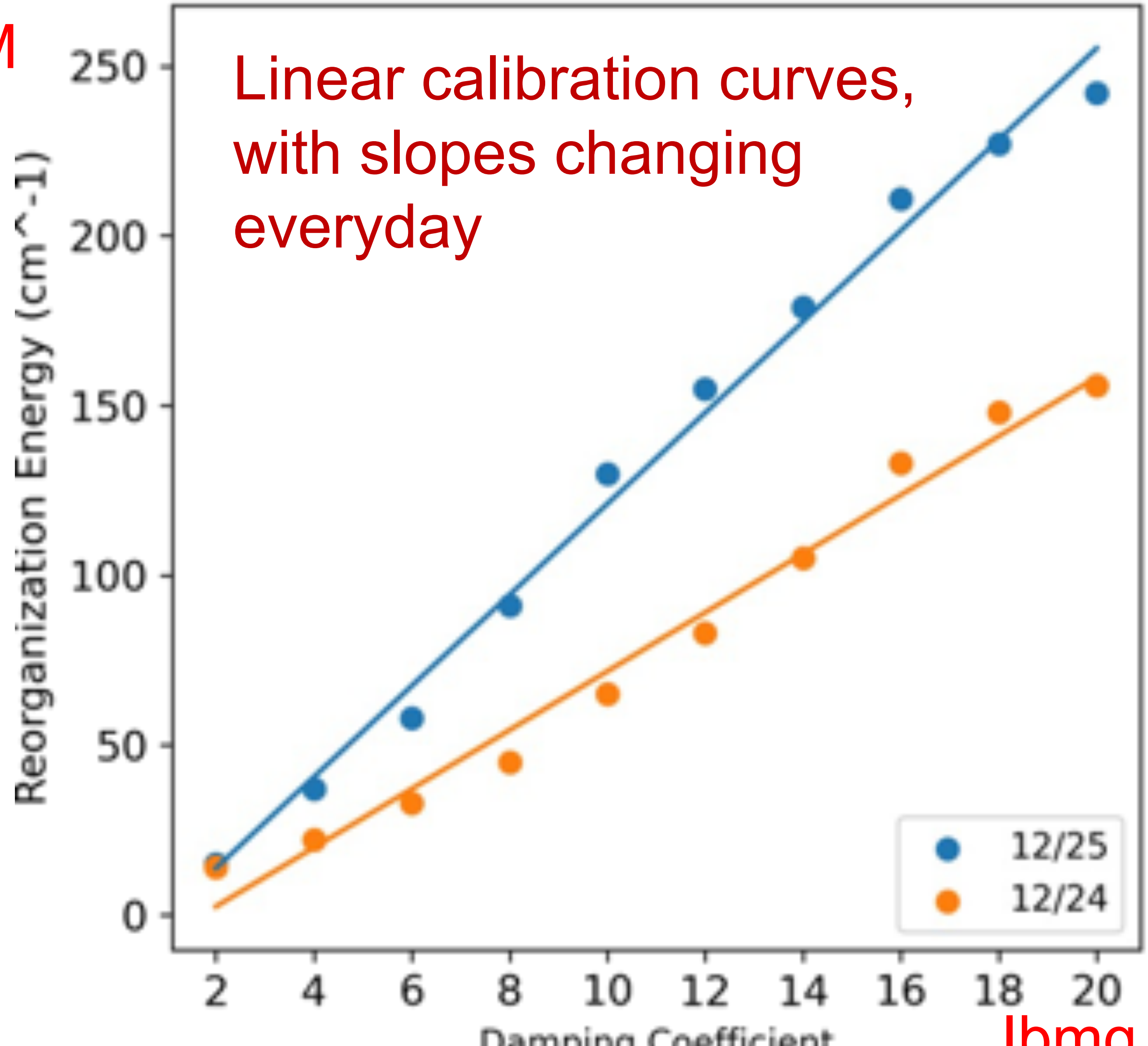
Prediction of Dynamics at the Intermediate Coupling Regime

- Interpolation can be used to accurately simulate dynamics at any system-bath coupling strength!
- Pre-calibration by fitting to HEOM at weak- and strong-coupling limits allows accurate ***prediction*** of energy transfer dynamics in the most difficult **intermediate-coupling regime**.



Simulations on Different Days

HEOM fitting



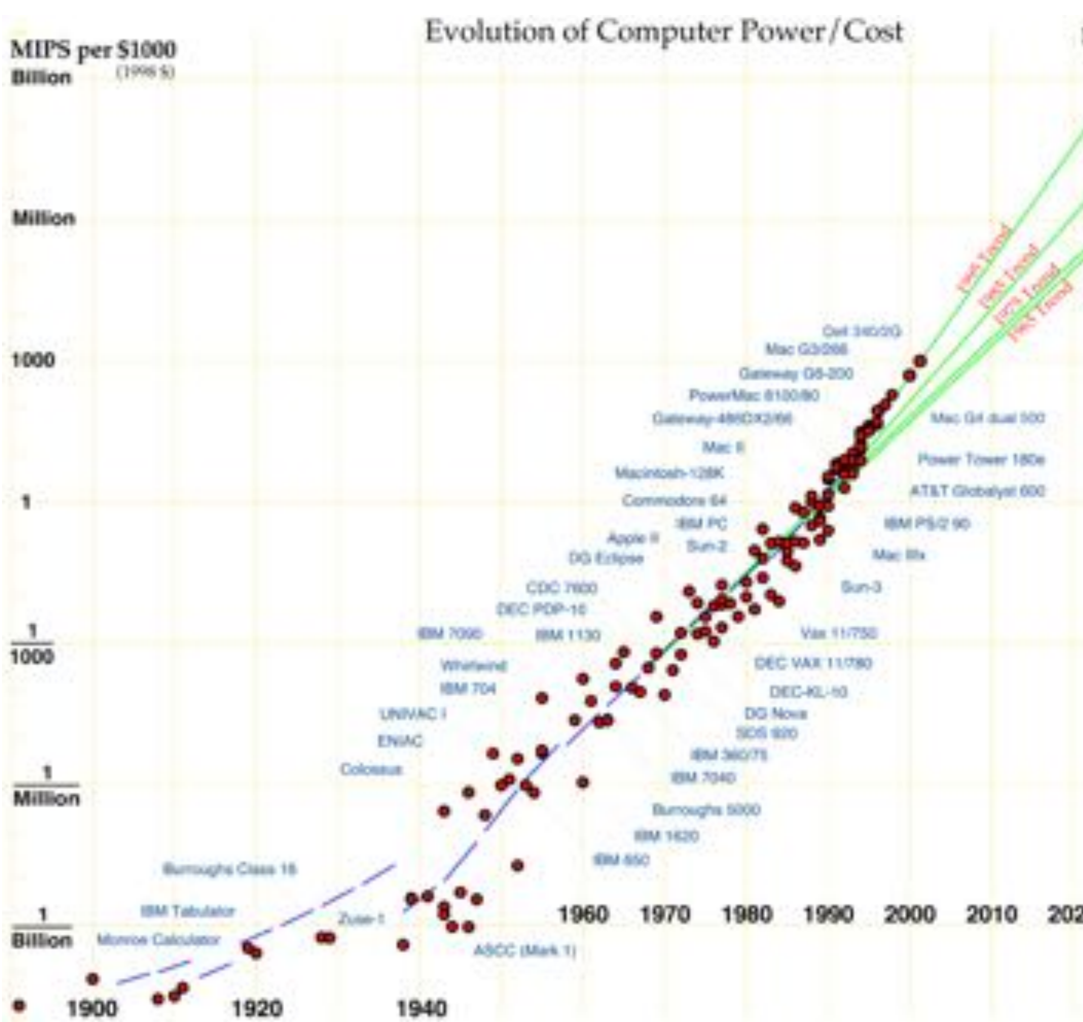
Ibmq_paris

Concluding Remarks

- We have successfully simulated dissipative dynamics for symmetric dimer systems under different damping regime using intrinsic gate noises of NISQ devices -- without using additional ancilla qubits.
- The current IBM-Q platform does not offer enough stability for consistent quantitative simulation of dissipative quantum dynamics; however, by employing our designed hardware-specific pulse sequences, the consistency can be significantly improved.
- We combined quantum simulation on NISQ devices and numerical post-processing to extrapolate the dynamics to longer time scales and to achieve accuracy comparable to HEOM-level theories on classical computers – might be another path to demonstrate quantum advantage.

Concluding Remarks

- Development of quantum computers is clearly still in the “vacuum tube” era of computing (ENIAC @ 1945) – who could have foreseen how computing has changed our societies…
- We need revolutionary ideas and creative applications in order to fully realize the potential of quantum computing – chemical science & quantum simulations



http://www.epocalc.net/pages/comp_timeline.htm

Acknowledgements

IBM-Q Center @ NTU

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Thank You!!