2022 Town Hall meeting on hot and cold QCD
Massachusetts Institute of Technology
Sep 23-25, 2022

Quantum Information Science for QCD Research

Zohreh Davoudi
University of Maryland, College Park

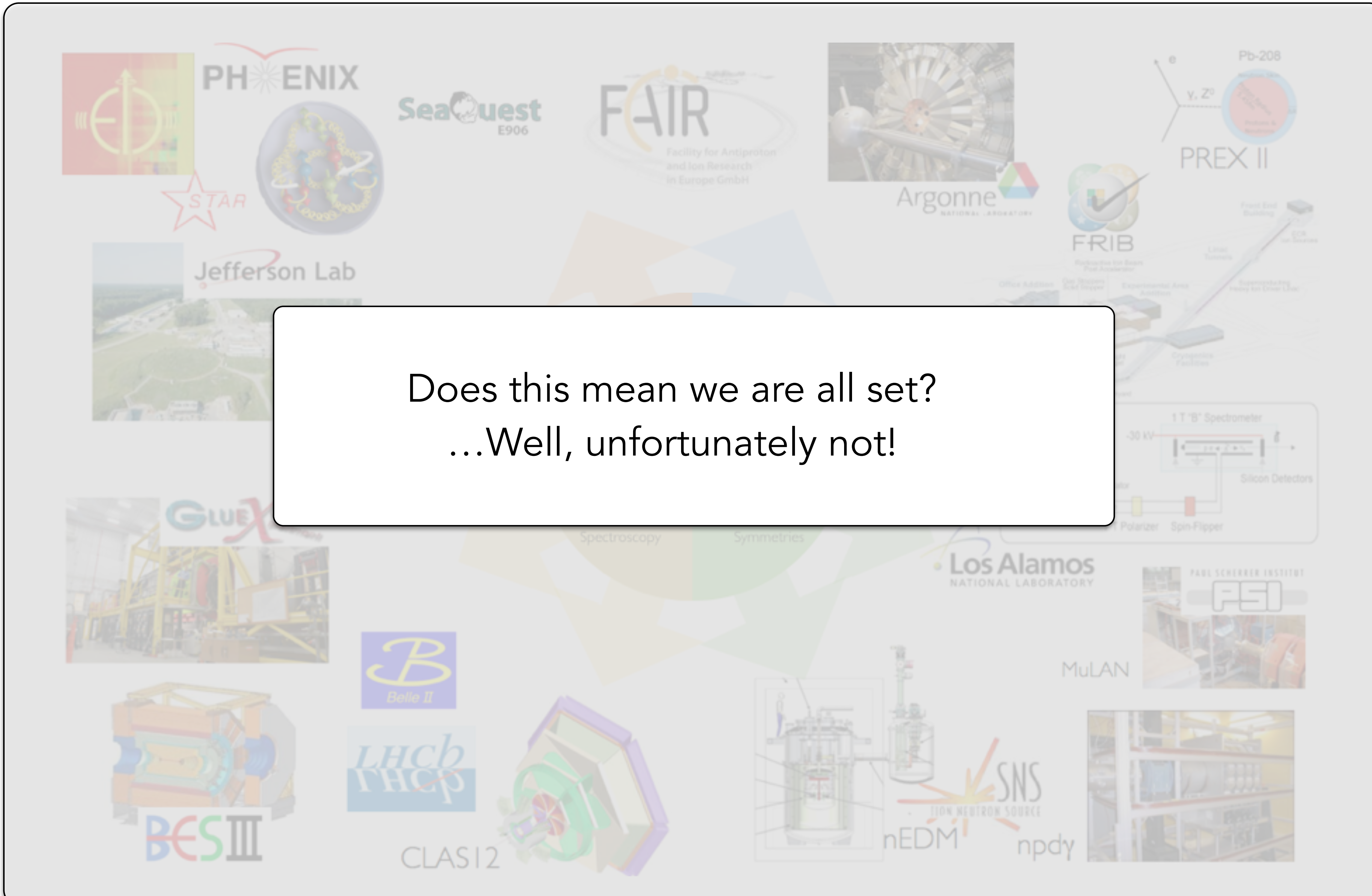
[PART I]
WHY QUANTUM COMPUTING FOR THE NP/QCD RESEARCH?

LATTICE QCD HAS CARRIED OUT A SUCCESSFUL PROGRAM THAT SUPPORTS A BROAD EXPERIMENTAL PROGRAM IN NP.

See Martha Constantinou's great overview on day 1.

Slide content courtesy of Martin Savage.

LATTICE QCD HAS CARRIED OUT A SUCCESSFUL PROGRAM THAT SUPPORTS A BROAD EXPERIMENTAL PROGRAM IN NP.



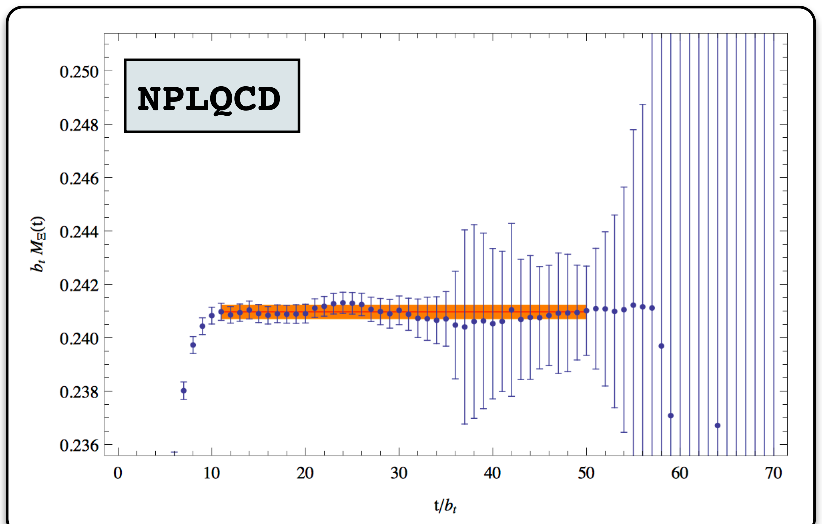
Does this mean we are all set?

…Well, unfortunately not!

Slide content courtesy of Martin Savage.

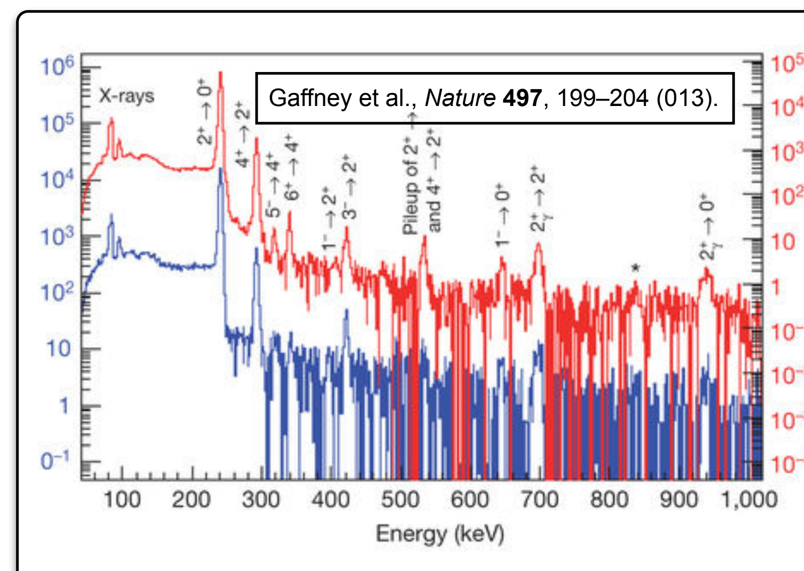
THREE FEATURES MAKE LATTICE QCD CALCULATIONS OF NUCLEI HARD:

i) The complexity of systems grows factorially with the number of quarks.



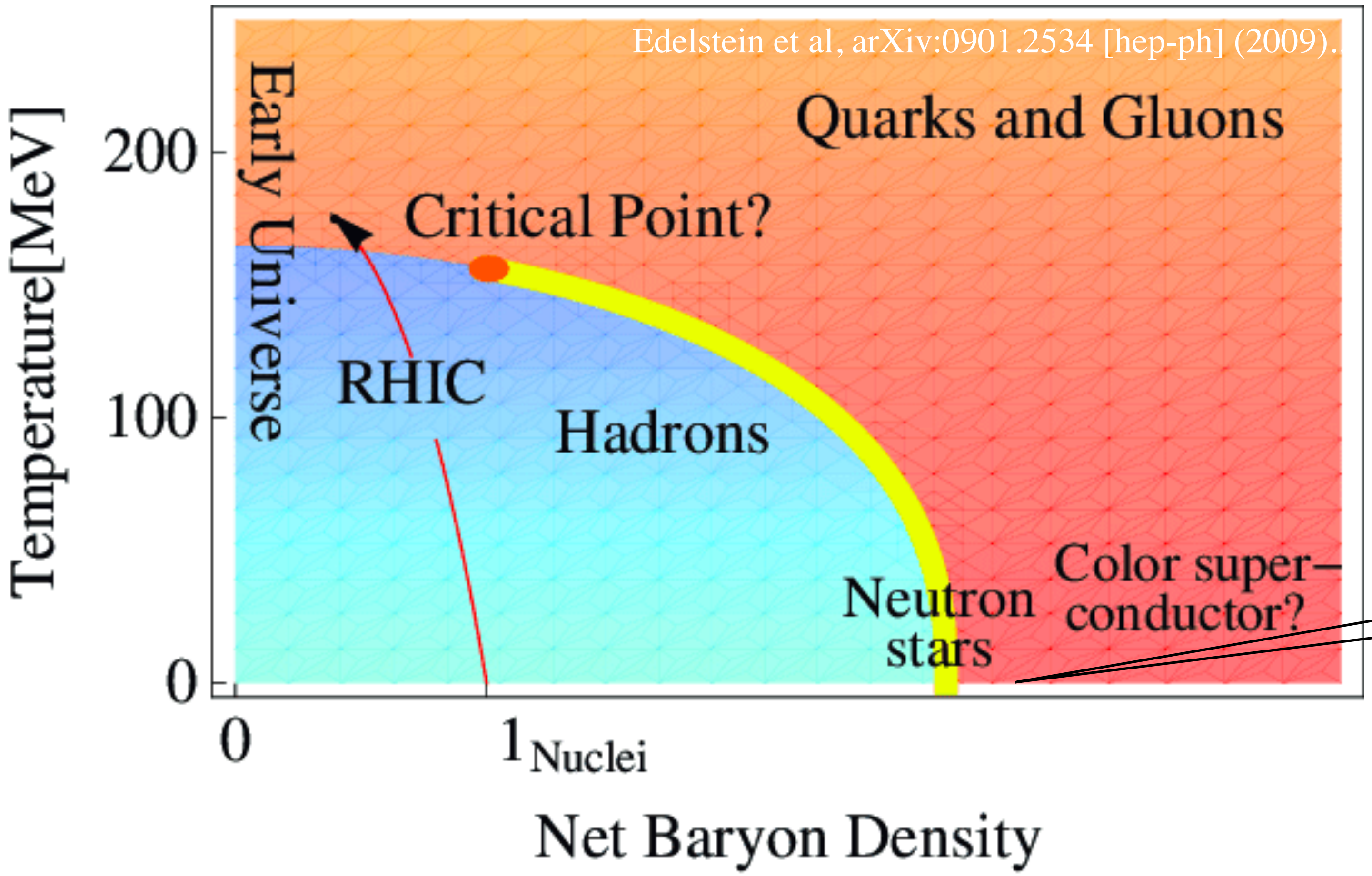
ii) There is a severe signal-to-noise degradation in Euclidean nuclear correlators.

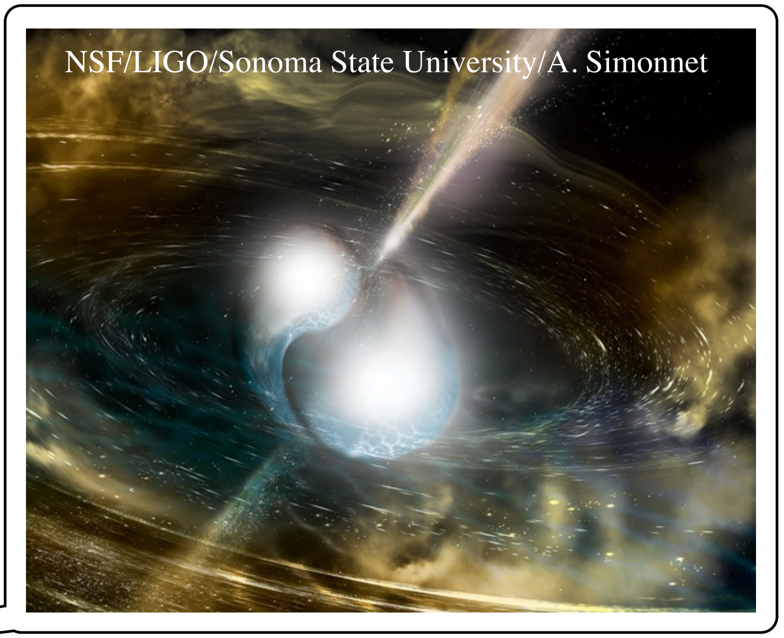
iii) Excitation energies of nuclei are much smaller than the QCD scale.



ADDITIONALLY THE SIGN PROBLEM FORBIDS:

i) Studies dense matter such as interior of neutron stars and phase diagram of QCD





Path integral formulation…

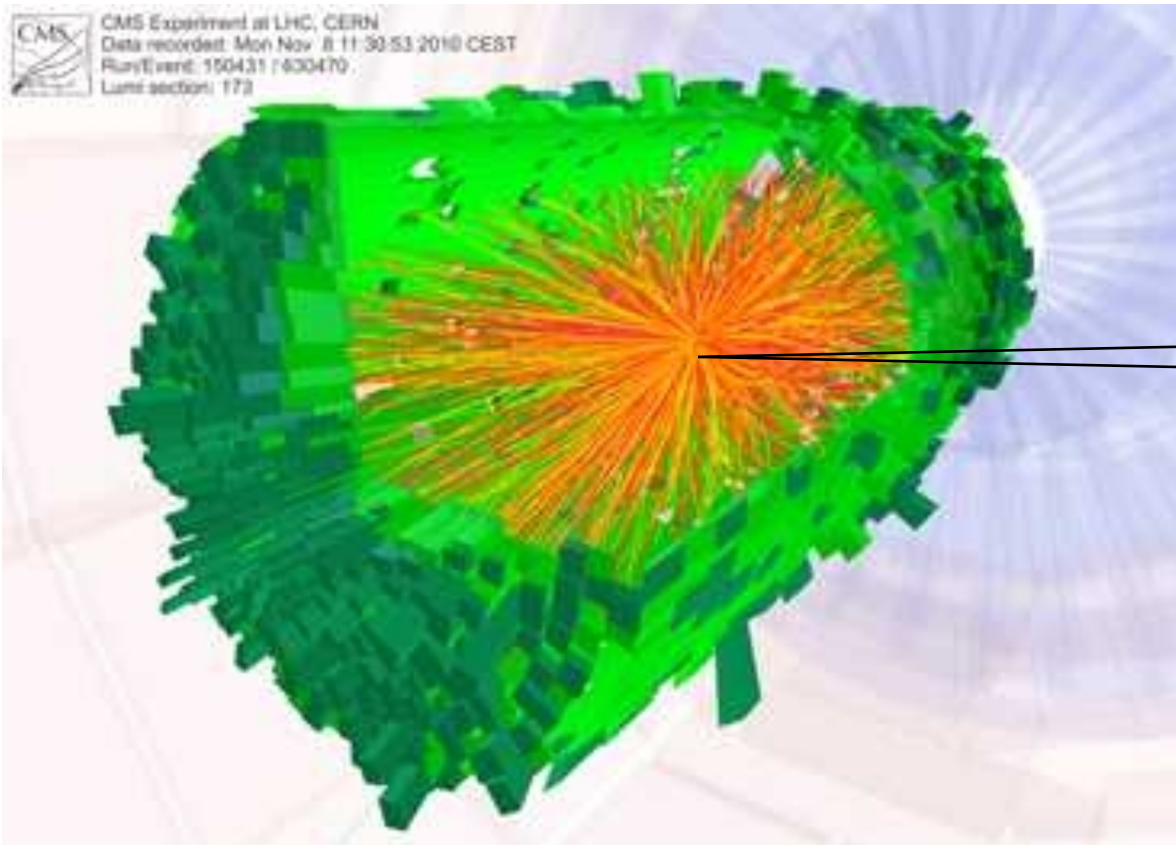
$$e^{-S[U,q,\bar{q}]}$$

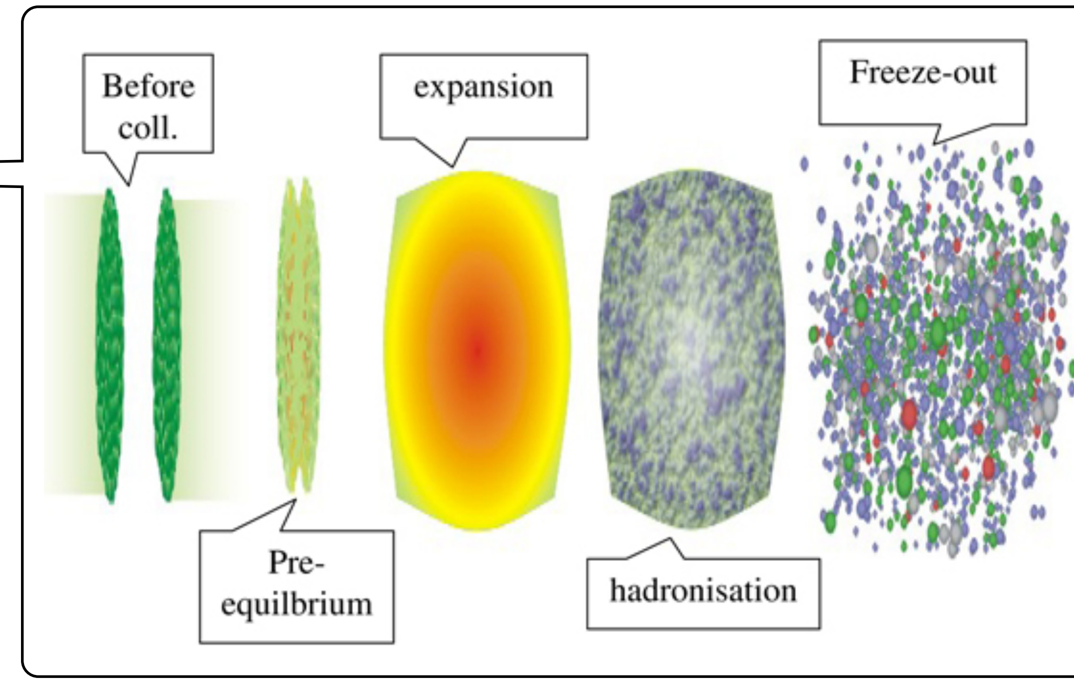
…with a complex action:

$$\mathcal{L}_{\rm QCD} \to \mathcal{L}_{\rm QCD} - i\mu \sum_f \bar{q}_f \gamma^0 q_f$$

ADDITIONALLY THE SIGN PROBLEM FORBIDS:

ii) Real-time dynamics of matter in heavy-ion collisions or after Big Bang…





…and a wealth of dynamical response functions, transport properties, parton distribution functions, and non-equilibrium physics of QCD.

Path integral formulation:

$$e^{iS[U,q\bar{q}]}$$

Hamiltonian evolution:

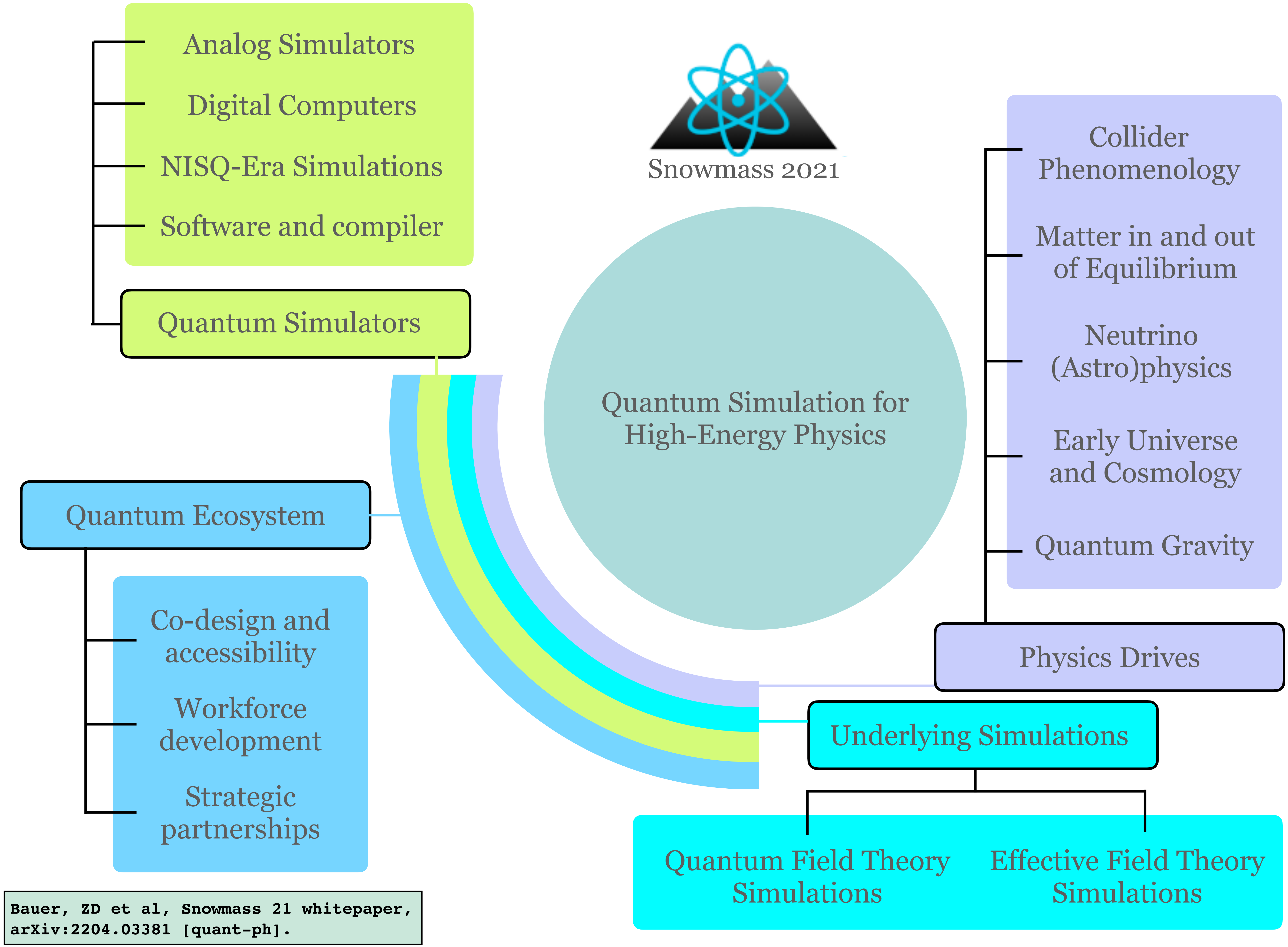
$$U(t) = e^{-iHt}$$

INTRACTABLE PROBLEMS IN HIGH ENERGY PHYSICS ARE IDENTIFIED IN THE SNOWMASS PROCESS…

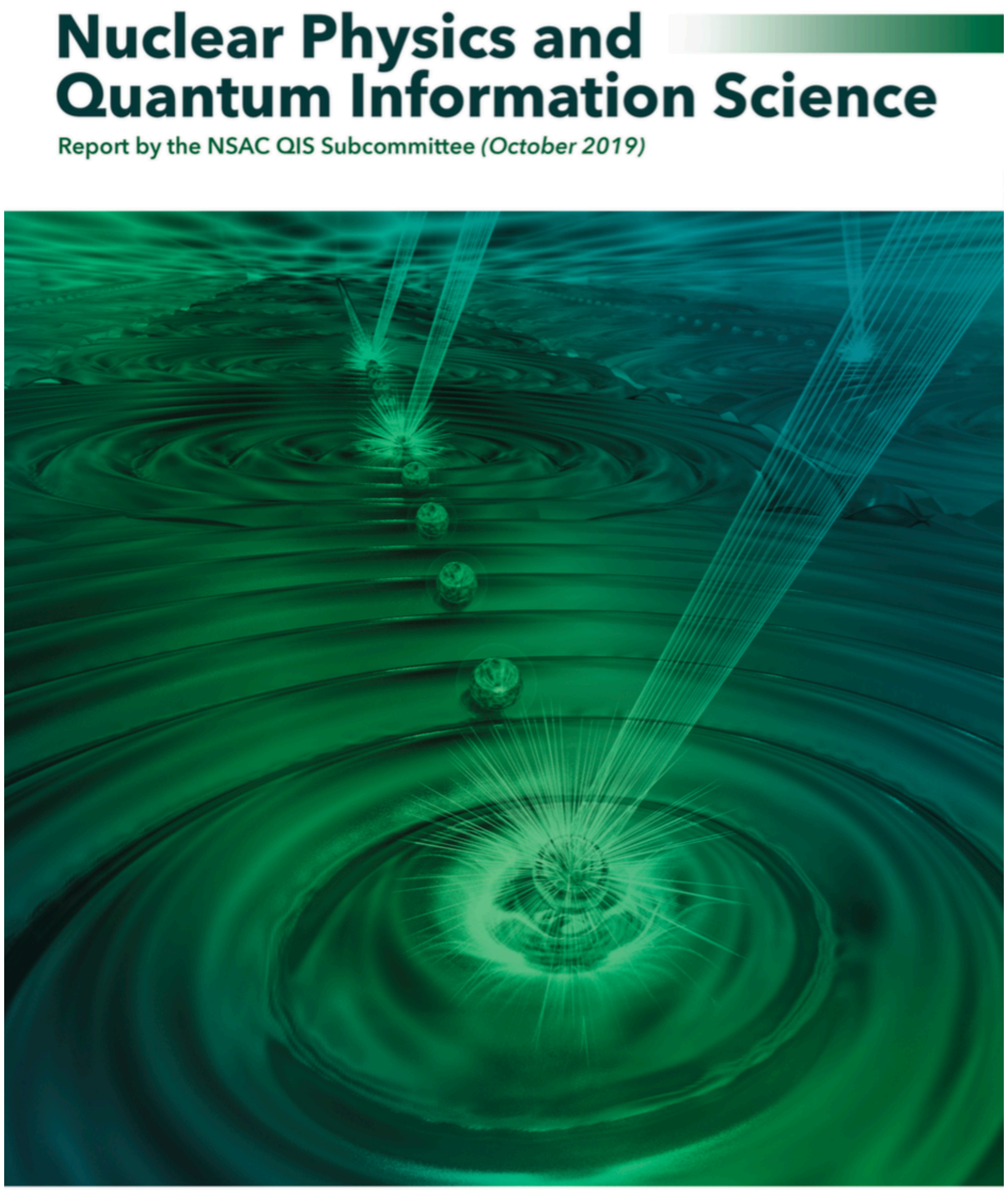
- Collider Phenomenology
- Matter in and out of Equilibrium
- Neutrino (Astro)physics
- Early Universe and Cosmology
- Quantum Gravity

Physics Drives

Bauer, ZD et al, Snowmass 21 whitepaper,
arXiv:2204.03381 [quant-ph].


Analog Simulators
Digital Computers
NISQ-Era Simulations
Software and compiler
Quantum Simulators
Snowmass 2021
Quantum Simulation for High-Energy Physics
Collider Phenomenology
Matter in and out of Equilibrium
Neutrino (Astro)physics
Early Universe and Cosmology
Quantum Gravity
Physics Drives
Quantum Ecosystem
Co-design and accessibility
Workforce development
Strategic partnerships
Underlying Simulations
Quantum Field Theory Simulations
Effective Field Theory Simulations
Bauer, ZD et al, Snowmass 21 whitepaper, arXiv:2204.03381 [quant-ph].

SIMILAR STUDIES IN NUCLEAR PHYSICS: PAST AND UPCOMING…



[Recommendation 1A]
Quantum Computing and Simulation in Nuclear Physics

[Recommendation 1B]
Quantum Sensing in Nuclear Physics

[Recommendation 2]
Exploratory Techniques and Technologies in Combined NP and QIS

[Recommendation 3]
A Quantum-Ready Nuclear Physics Workforce

A meeting planned later in the Fall to discuss opportunities in QIS for NP, to provide input to the Long-Range Planning process.

Organizers: Joe Carlson and Martin Savage

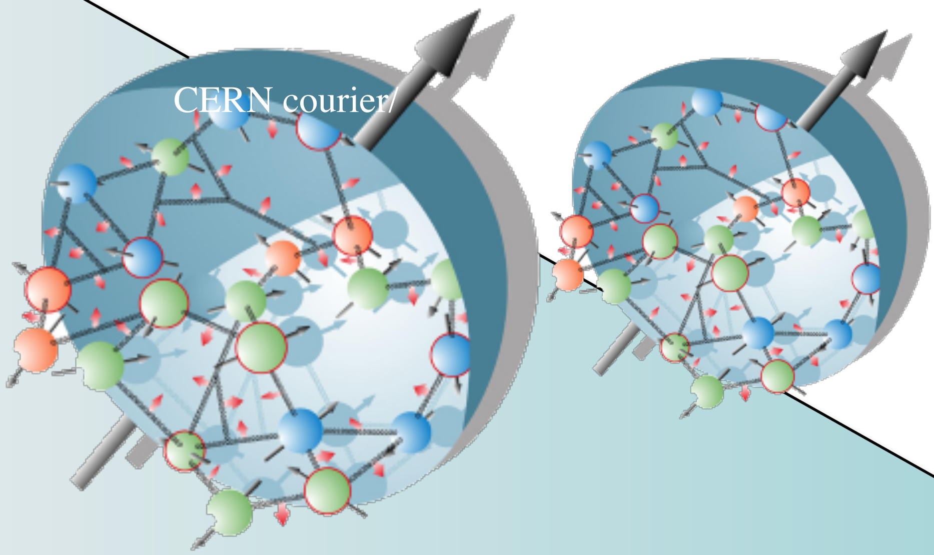
Beck, Savage et al, NSAC subcommittee report on QIS (2019).

[PART II]
WHAT HAS TO BE DEVELOPED IN THE COMING YEARS?

A RANGE OF QUANTUM SIMULATORS WITH VARING CAPACITY AND CAPABILITY

- Atomic systems (trapped ions, cold atoms, Rydbergs)
- Condensed matter systems (superconducting circuits, dopants in semiconductors such as in Silicon, NV centers in diamond)
- Laser-cooled polar molecules
- Optical systems (cavity quantum electrodynamics)

HOW SIMILAR TO QUANTUM-CHEMISTRY AND MATERIAL SIMULATIONS?

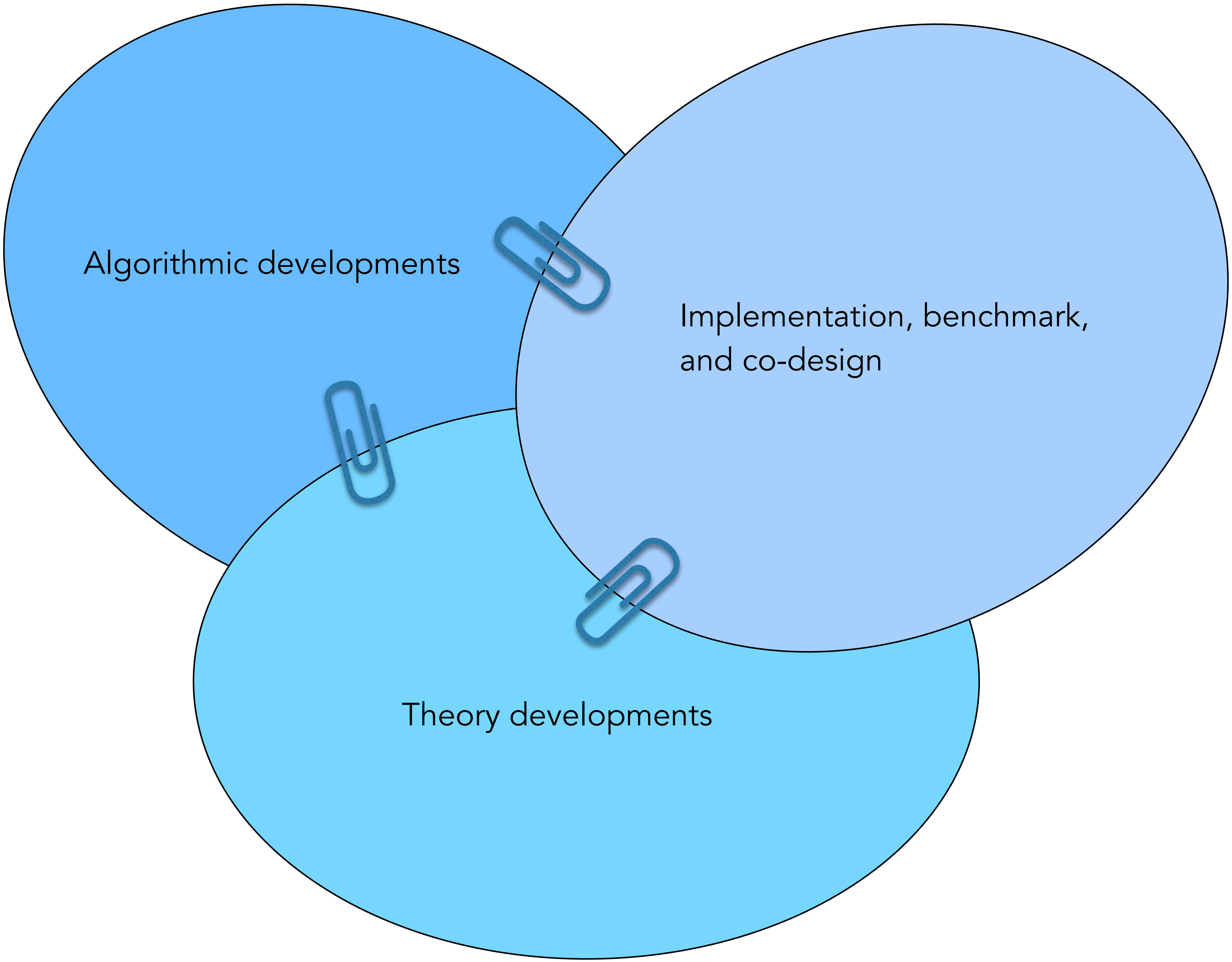


Starting from the Standard Model

Both bosonic and fermionic DOF are dynamical and coupled, exhibit both global and local (gauge) symmetries, relativistic hence particle number not conserved, vacuum state nontrivial in strongly interacting theories.

Attempts to cast QFT problems in a language closer to quantum chemistry and NR simulations: Kreshchuk, Kirby, Goldstein, Beauchemin, Love, arXiv:2002.04016 [quant-ph], Kreshchuk, Jia, Kirby, Goldstein, Vary, Love, Entropy 2021, 23, 597, Liu, Xin, arXiv:2004.13234 [hep-th], Barata , Mueller, Tarasov, Venugopalan (2020)

QUANTUM SIMULATION OF QUANTUM FIELD THEORIES: A MULTI-PRONG EFFORT



How to formulate QCD in the Hamiltonian language?

What are the efficient formulations? Which bases will be most optimal toward the continuum limit?

How to preserve the symmetries? How much should we care to retain gauge invariance?

How to quantify systematics such as finite volume, discretization, boson truncation, time digitization, etc?

Theory developments

MANY HAMILTONIAN FORMULATIONS OF GAUGE THEORIES EXIST, BUT WHICH ONE TO PICK?

Gauge-field theories (Abelian and non-Abelian):

Group-element representation
Zohar et al; Lamm et al

Prepotential formulation
Mathur, Raychowdhury et al

Loop-String-Hadron basis
Raychowdhury and Stryker

Link models, qubitization
Chandrasekharan, Wiese et al, Alexandru, Bedaque, et al.

Fermionic basis
Hamer et al; Martinez et al; Banuls et al

Bosonic basis
Cirac and Zohar

Light-front quantization
Kreshchuk, Love, Goldstien, Vary et al.; Ortega at al

Local irreducible representations
Byrnes and Yamamoto;
Ciavarella, Klco, and Savage

Manifold lattices
Buser et al

Dual plaquette (magnetic) basis
Bender, Zohar et al; Kaplan and Styker; Unmuth-Yockey; Hasse et al; Bauer and Grabowska

Spin-dual representation
Mathur et al

Scalar field theory

Field basis
Jordan, Lee, and Preskill

Continuous-variable basis
Pooser, Siopsis et al

Harmonic-oscillator basis
Klco and Savage

Single-particle basis
Barata , Mueller, Tarasov, and Venugopalan.

Algorithmic developments
[Digital]

- Near- and far-term algorithms with bounded errors and resource requirement for gauge theories?
- Can given formulation/encoding reduce qubit and gate resources?
- Should we develop gauge-invariant simulation algorithms?
- How do we do state preparation and compute observables like scattering amplitudes?

Algorithmic developments
[Analog]

Can practical proposals for current hardware be developed?

Can we simulate higher-dimensional gauge theories?

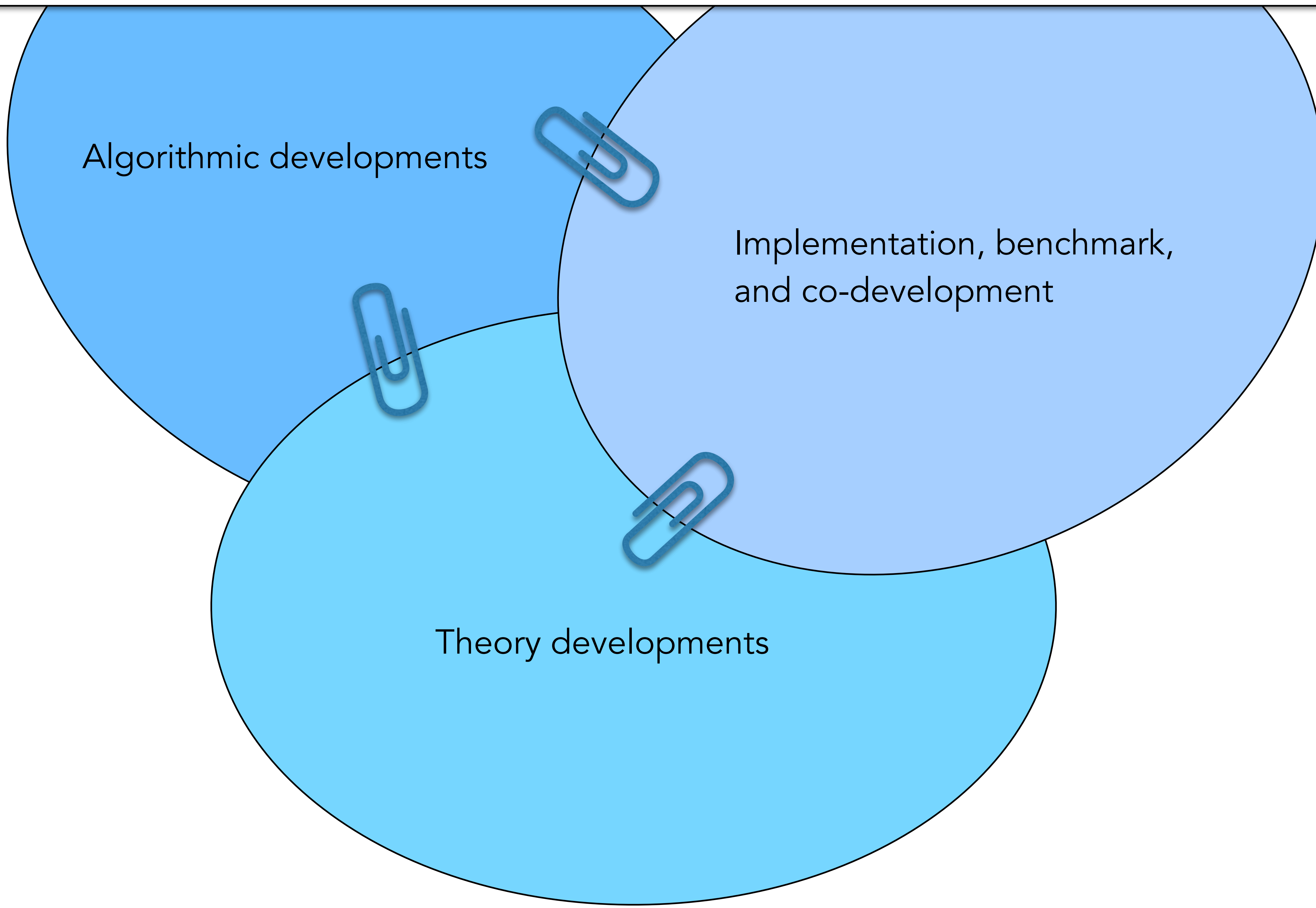
Can non-Abelian gauge theories be realized in an analog simulator?

Can we robustly bound the errors in the analog simulation? What quantities are more robust to errors?

Implementation, benchmark, and co-design

- What is the capability limit of the hardware for gauge-theory simulations so far?
- What is the nature of noise in hardware and how can it best be mitigated?
- Can we co-design dedicated systems for gauge-theory simulations?
- Can digital and analog ideas be combined to facilitate simulations of field theories?

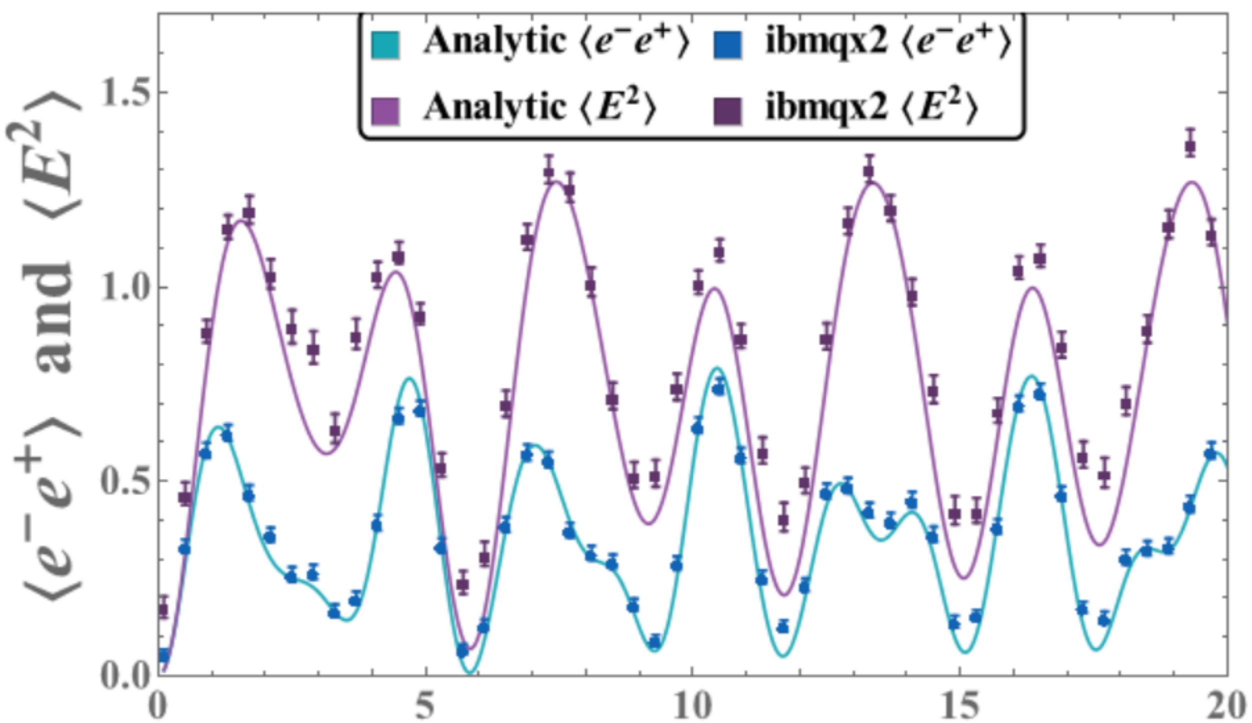
We've got a long way to go to get to **QCD** but we know what to do! If one thing we learned from the successful conventional lattice-QCD program is that **theory/algorithm/experiment** collaborations will be the key. It is even more important in the quantum-computing era since our computers are themselves physical systems!



[PART III]
EXAMPLES SHOWCASING PROGRESS IN A RANGE OF QCD-INSPIRED PROBLEMS…

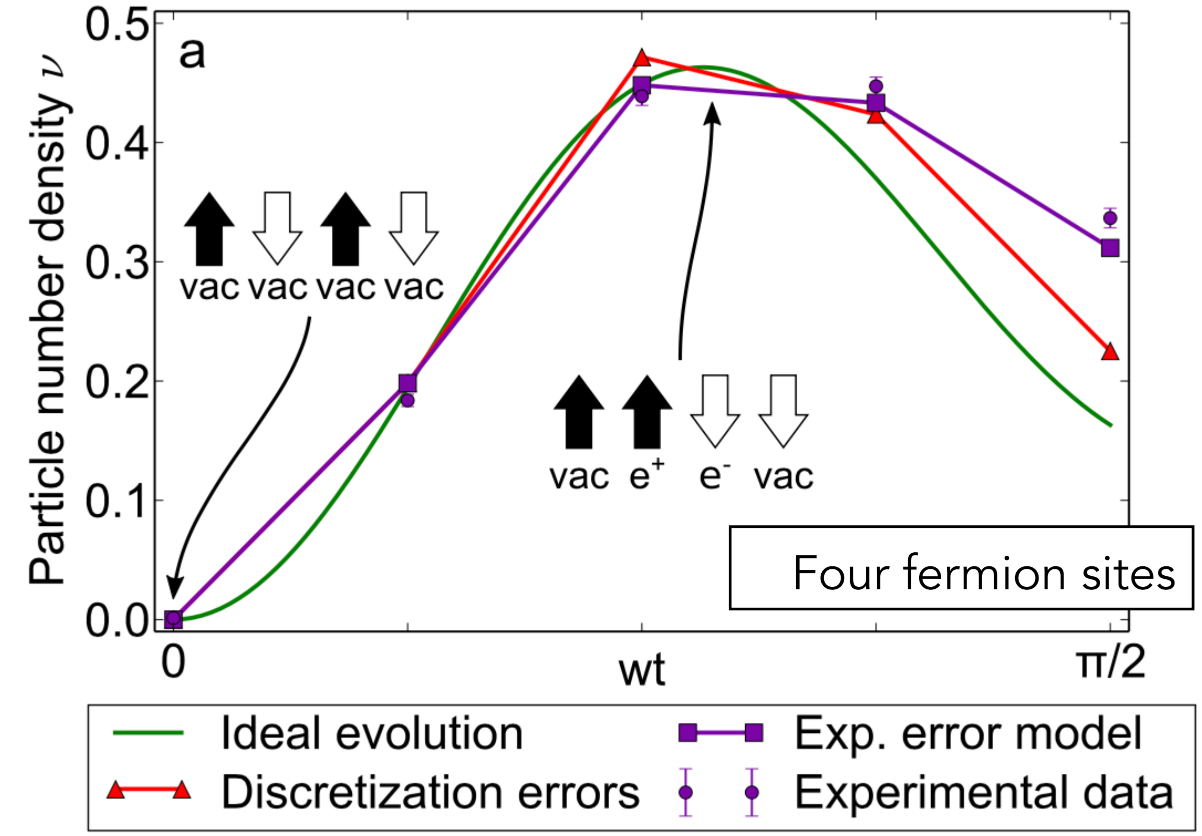
DIGITAL COMPUTATIONS OF ABELIAN LGTs

Klco, Savage, et al, Phys. Rev. A 98, 032331 (2018).

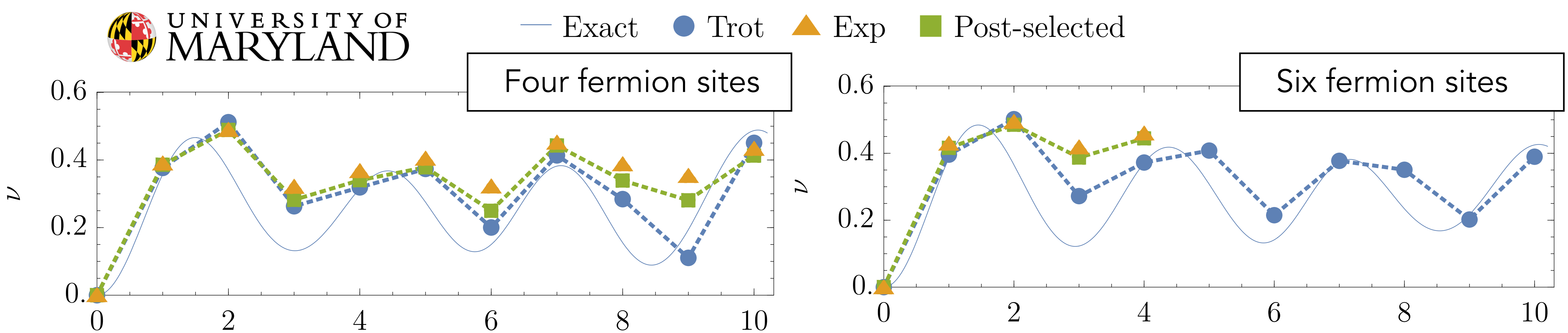


A hybrid classical-quantum approach allows a 2-qubit reduction of 4-qubit simulation.

Martinez et al, Nature 534, 516 EP (2016).



UNIVERSITY OF MARYLAND

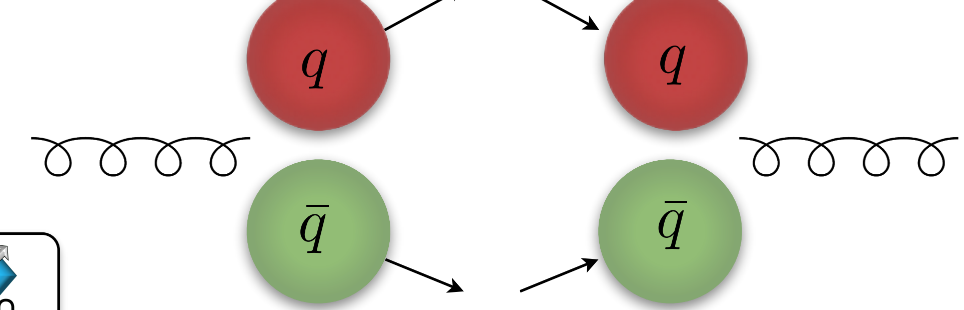


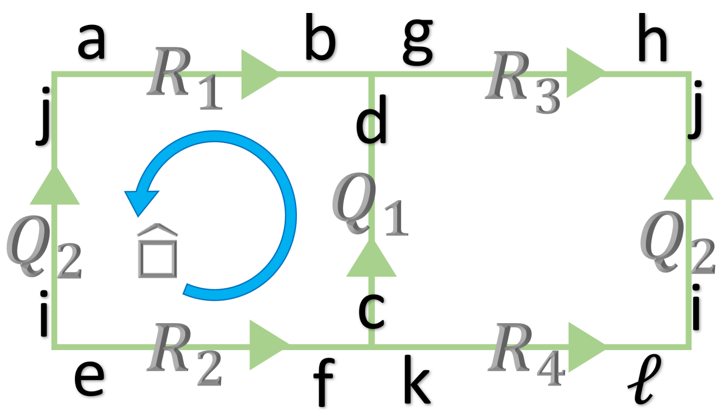
80 entangling gates!

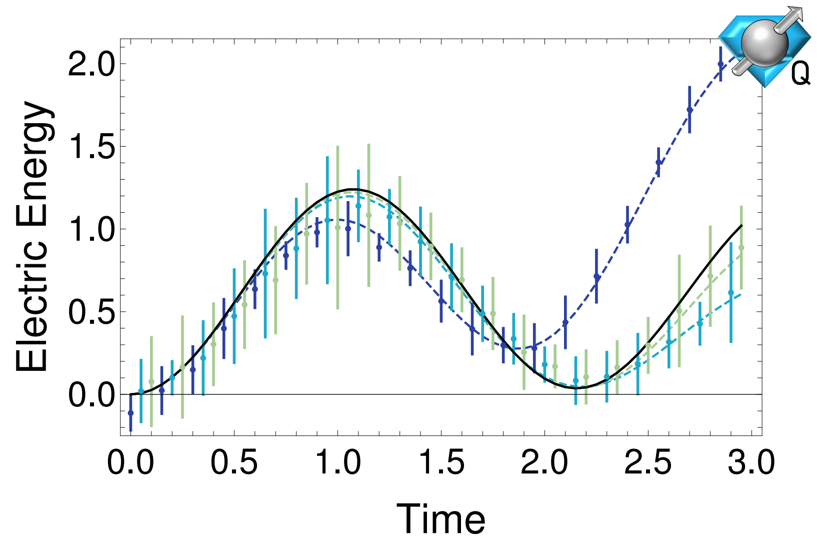
90 entangling gates!

Nguyen, Tran, Zhu, Green, Huerta Alderete, ZD, Linke, *PRX Quantum* 3 (2022) 2, 020324.

DIGITAL COMPUTATIONS OF NON-ABELIAN LGTs



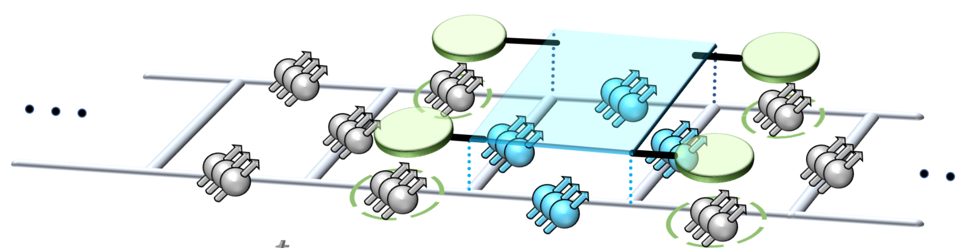


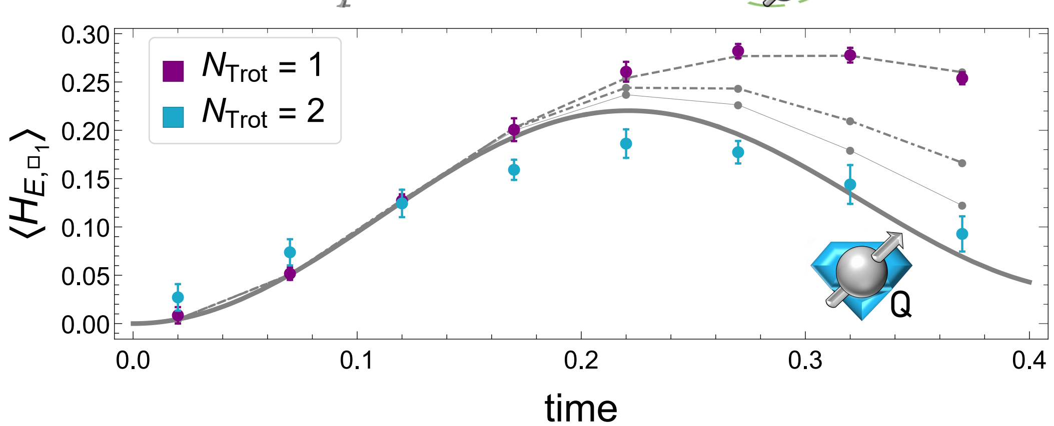


Real-time dynamic of pure SU(3) with global irrupts on IBM

Ciavarella, Klco, and Savage, Phys. Rev. D 103, 094501 (2021).

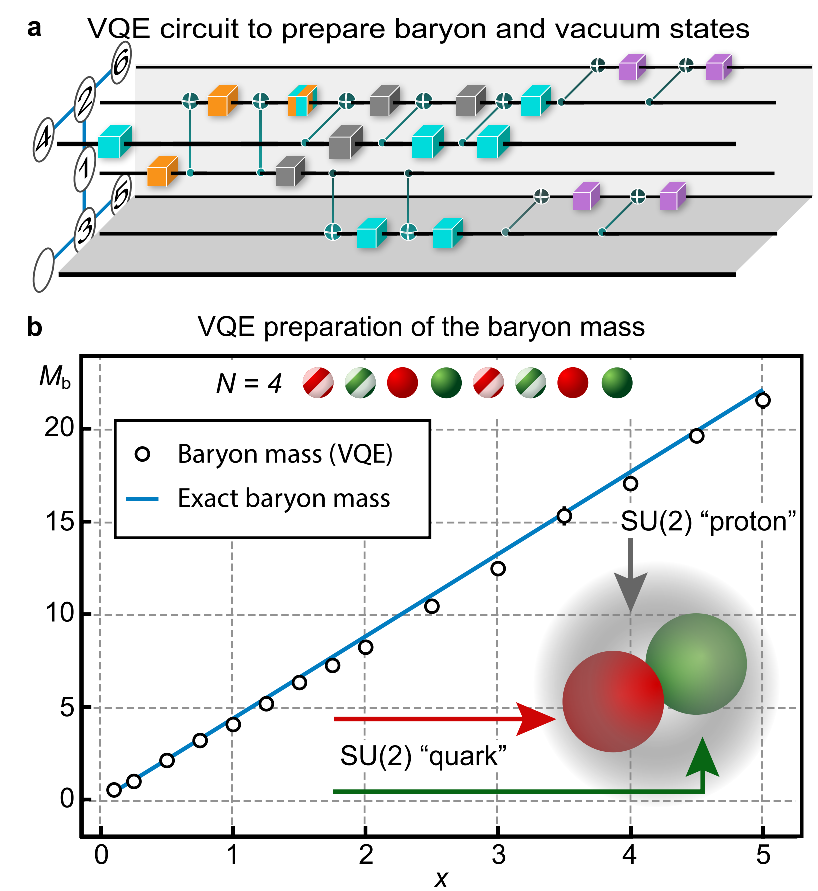
Real-time dynamic of pure SU(2) with global irreps on IBM





Klco, Savage, and Stryker, Phys. Rev. D 101, 074512 (2020).

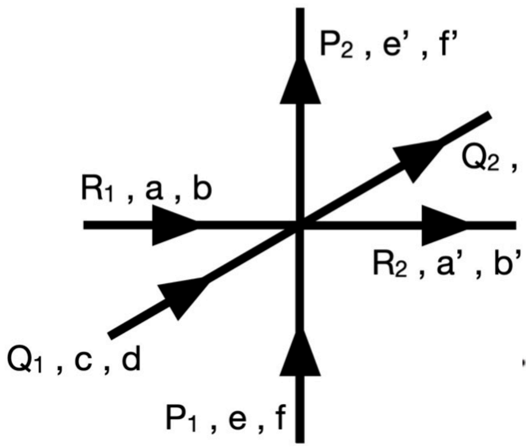
Low-lying spectrum of SU(2) with matter in 1+1 D on IBM

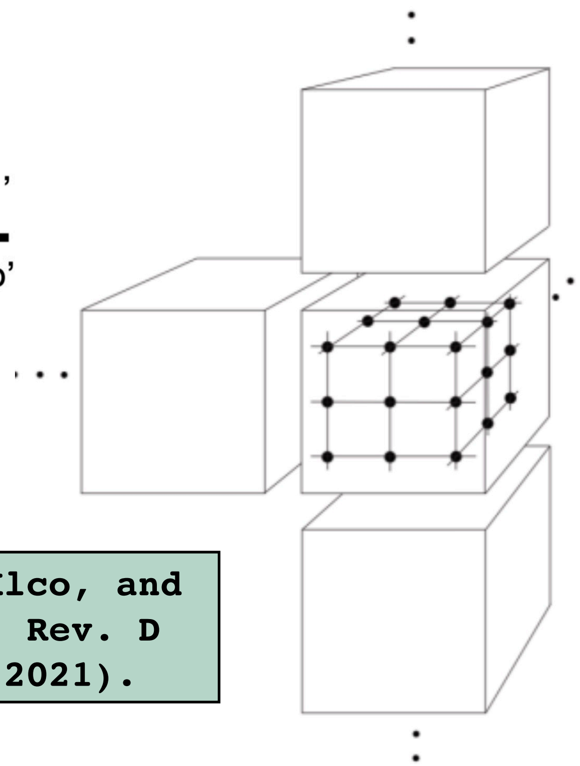


Atas et al, Nature Communications 12, 6499 (2021). SU(3) example: Atas et al: arXiv:2207.03473 [quant-ph].

See also studies on D-wave annealers: Rahman et al, Phys. Rev. D 104, 034501 (2021), Illa and Savage, arXiv:2202.12340 [quant-ph], Farrel et al, arXiv:2207.01731 [quant-ph].

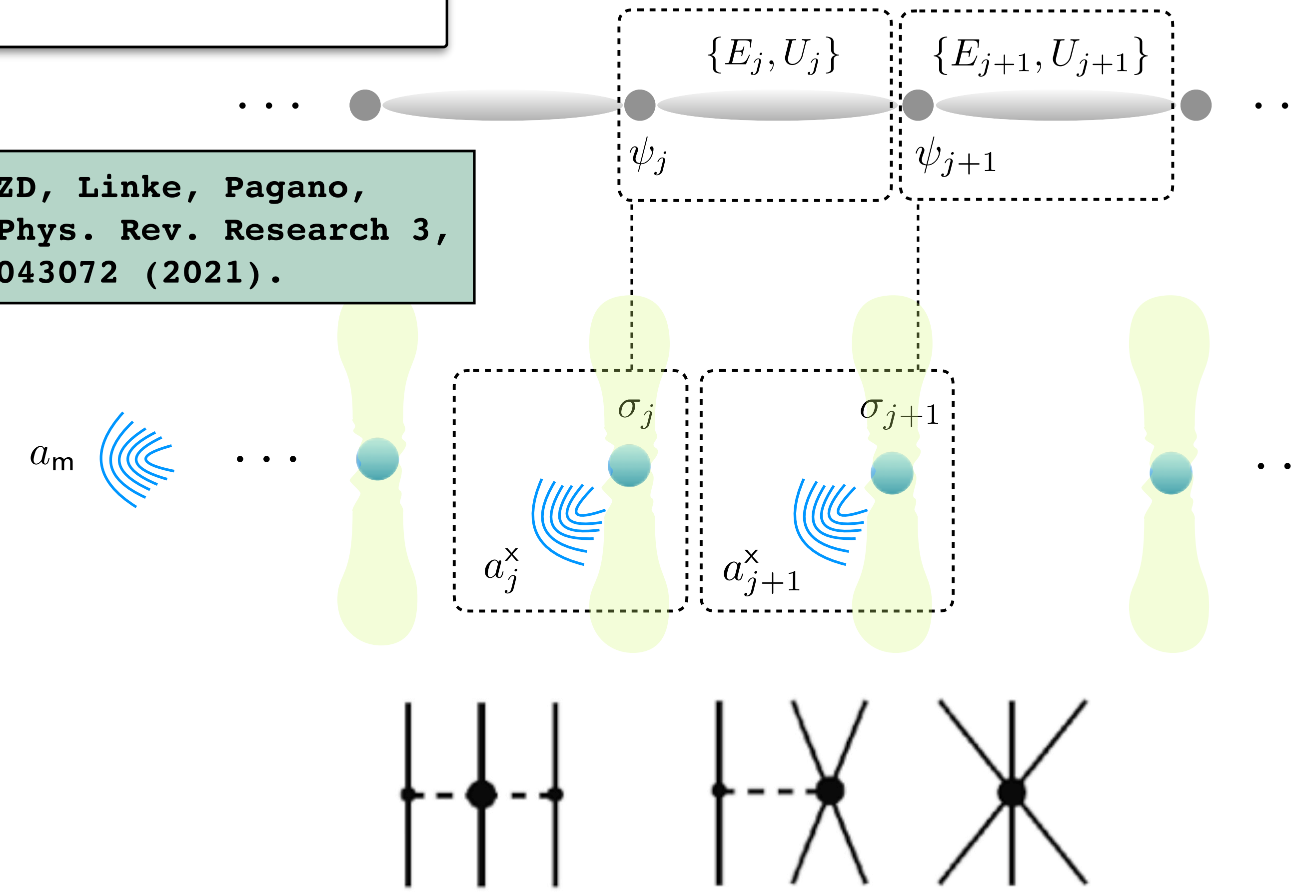
SOME CO-DESIGN EXAMPLES: MULTI-DIMENSIONAL LOCAL HILBERT SPACES AND MULTI-MODE INTERACTIONS

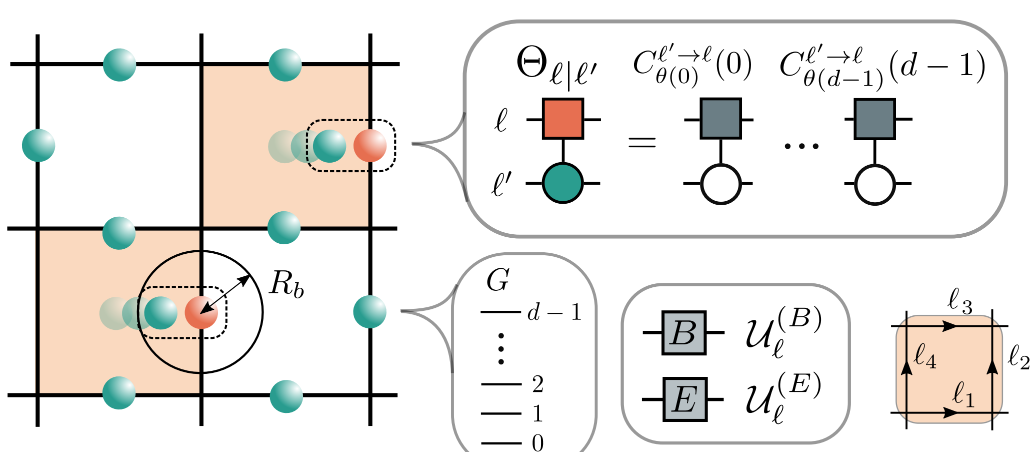




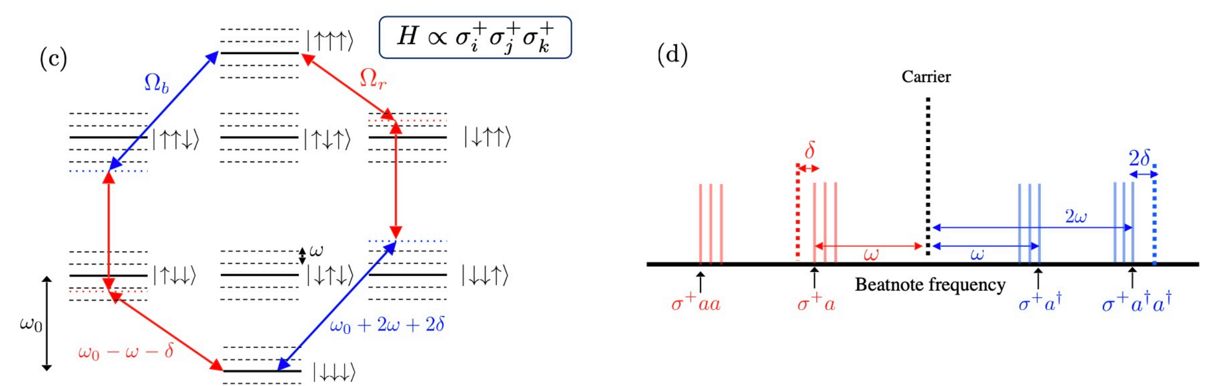
Ciavarella, Klco, and Savage, Phys. Rev. D 103, 094501 (2021).

ZD, Linke, Pagano, Phys. Rev. Research 3, 043072 (2021).



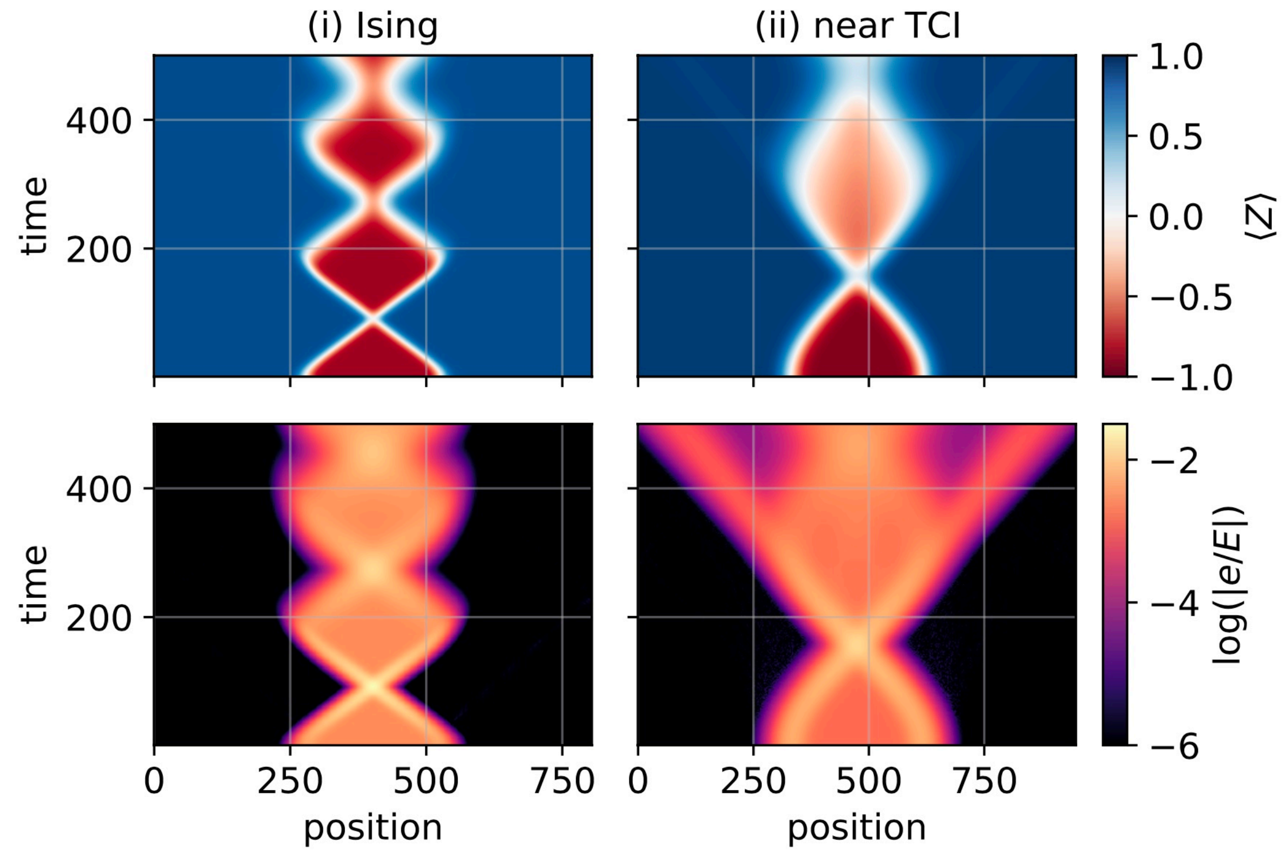


González-Cuadra, Zache, Carrasco, Kraus, Zoller, arXiv:2203.15541 [quant-ph].

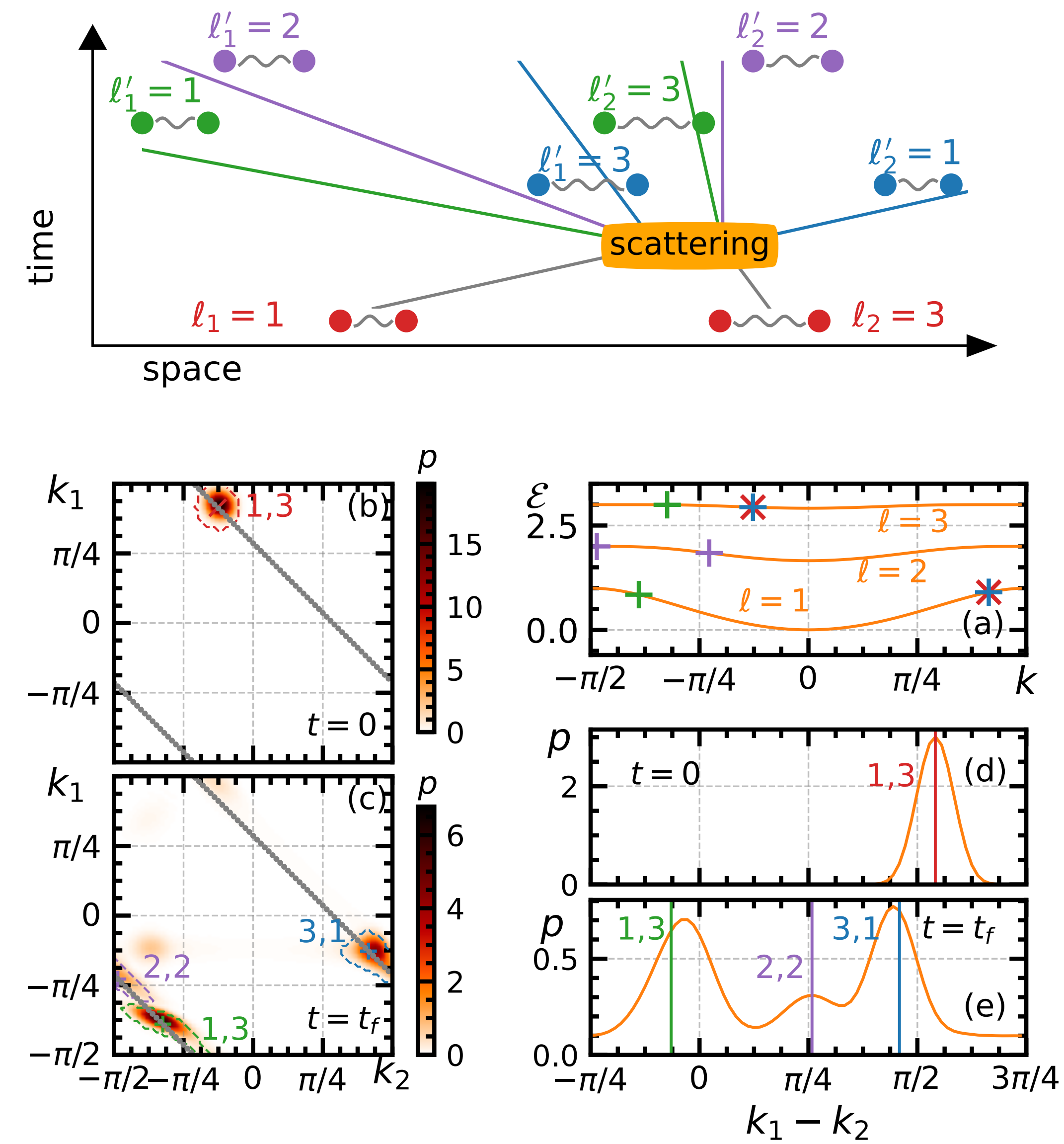


Andrade, ZD, Grass, Hafezi, Pagano, Seif, arXiv:2108.01022 [quant-ph], Bermudez et al, Pays.Rev.A79, 060303 R (2009), Katz, Centina, Monroe, arXiv:2202.04230 [quant-ph].

FIRST STEPS TOWARD COLLISION PROCESSES
— NUMERICAL SIMULATIONS —

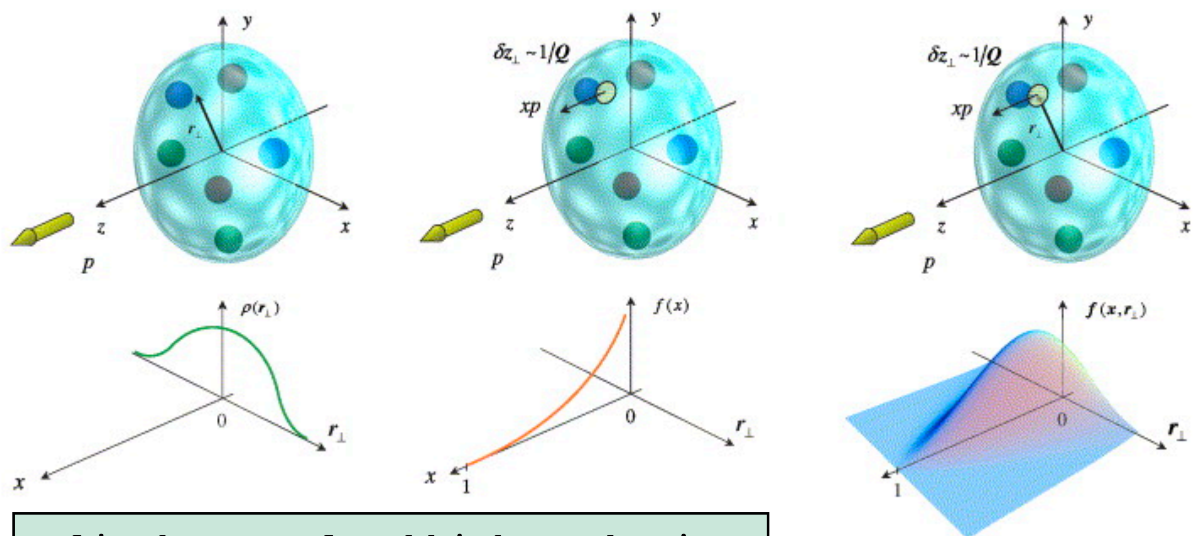


Ashley Milsted, Liu, John Preskill, and Vidal, PRX Quantum 3 (2022) 2, 020316.



Surace, Lerose, New J. Phys. 23 (2021) 062001.

PARTON DISTRIBUTION FUNCTIONS, DECAY AMPLITUDES



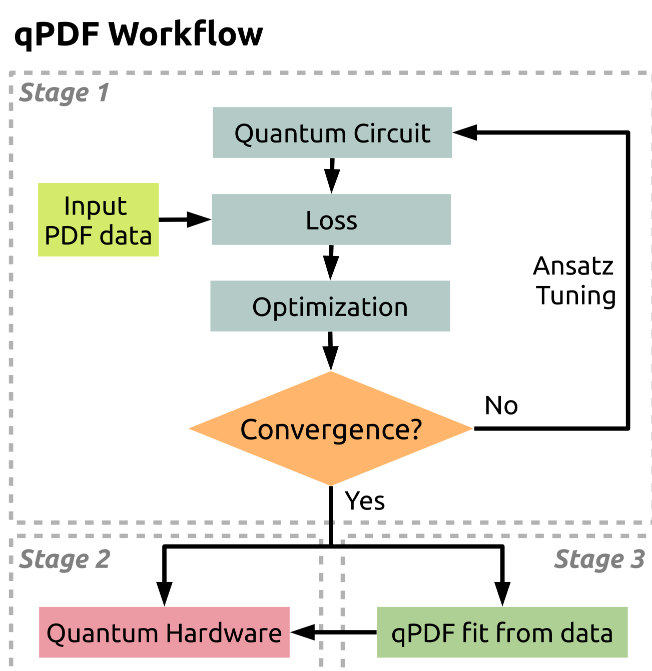
Belitskya, Radyushkinbc, Physics Reports 418 (2005), 1-387.

Either calculate PDFs directly since non-equal time amplitudes are possible on quantum computers…

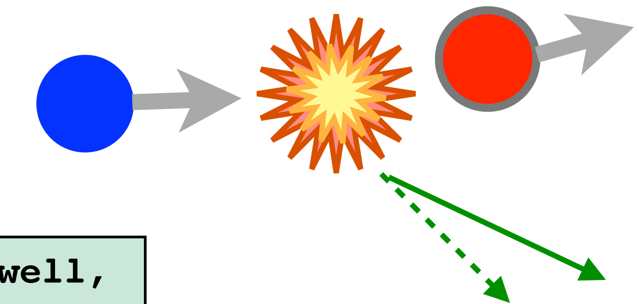
Mueller, Tarasov, and Raju Venugopalan, PRD 102, 016007 (2020), Lamm, Lawrence, and Yamauchi, Phys. Rev. Res. 2, 013272 (2020), Echevarria, Egusquiza, Rico, and G Schnell, PRD 104, 014512 (2021).

…or expedite global fitting of PDFs with variational quantum eigensolvers…

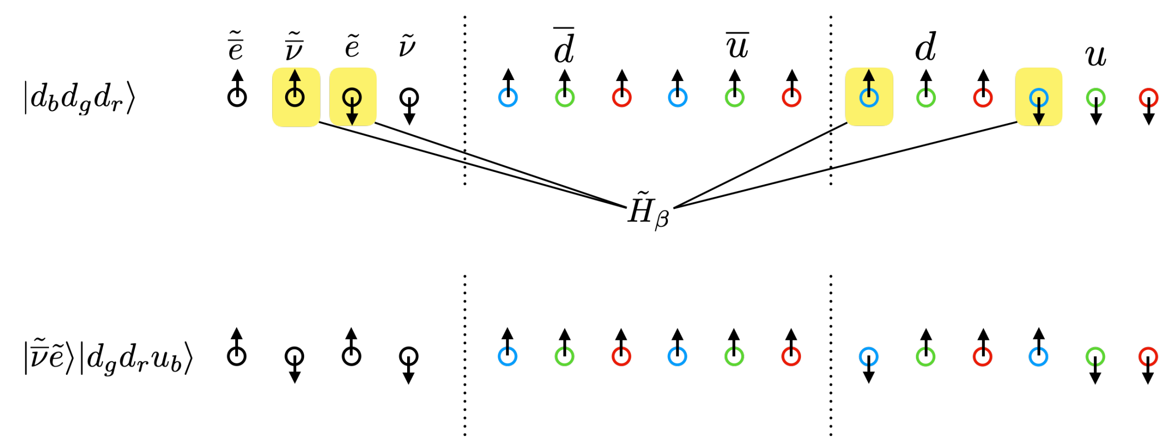
Perez-Salinas, Cruz-Martinez, Alhajri, and Carrazza , PRD 103, 034027 (2021), Qian, Basili, Pal, Luecke, and Vary, arXiv:2112.01927 (2021).

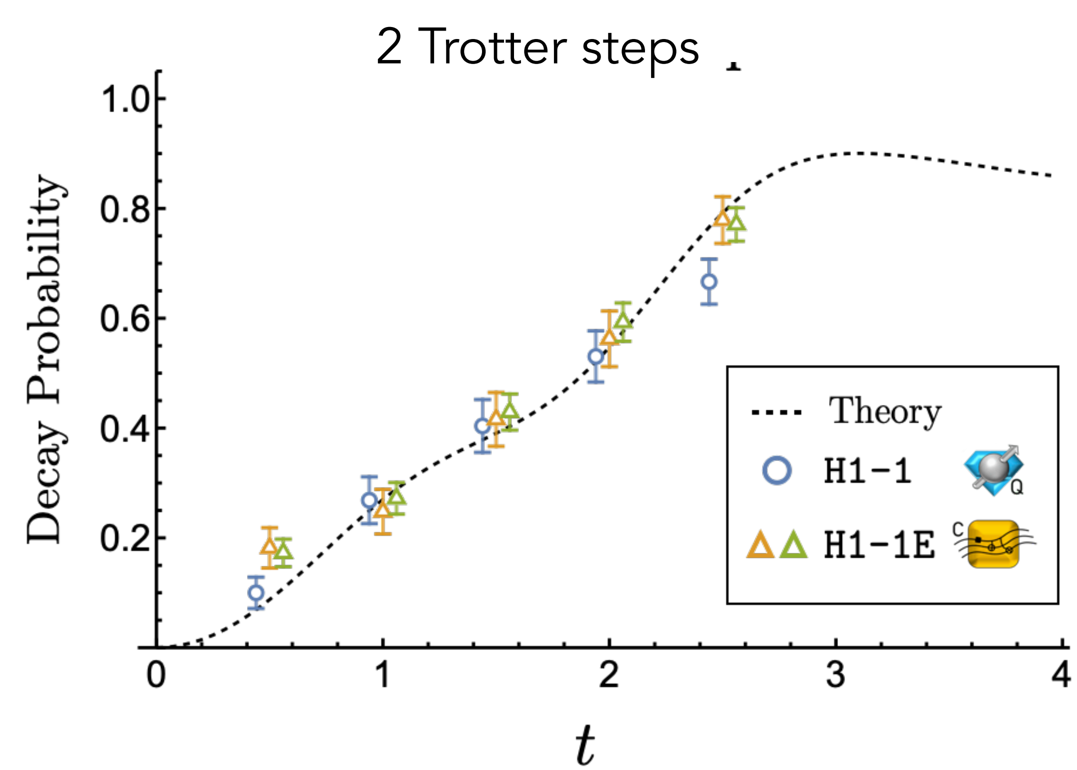


Quantum computing β decay in 1+1 QCD



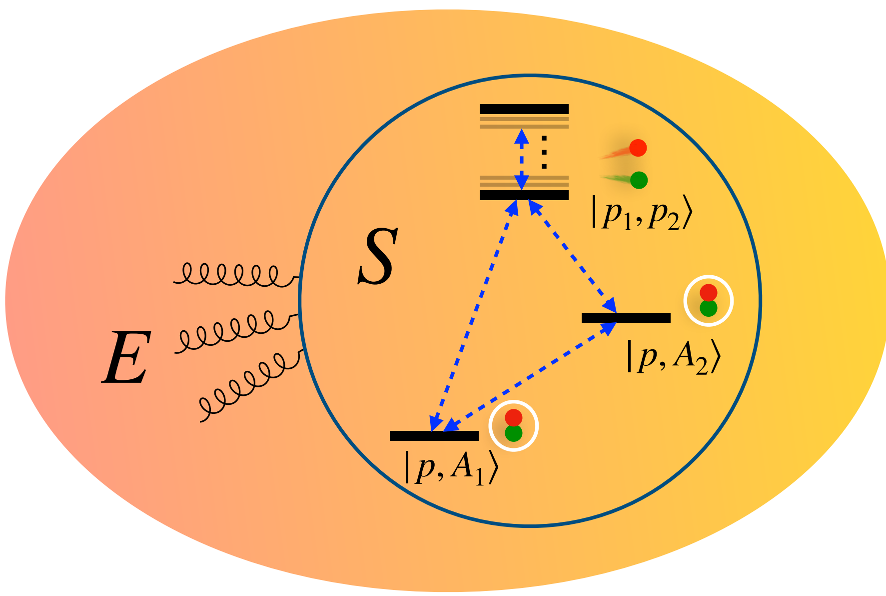
Farrell, Chernyshev, Powell, Zemlevskiy, Illa, and Savage, arXiv:2209.10781 [quant-ph].

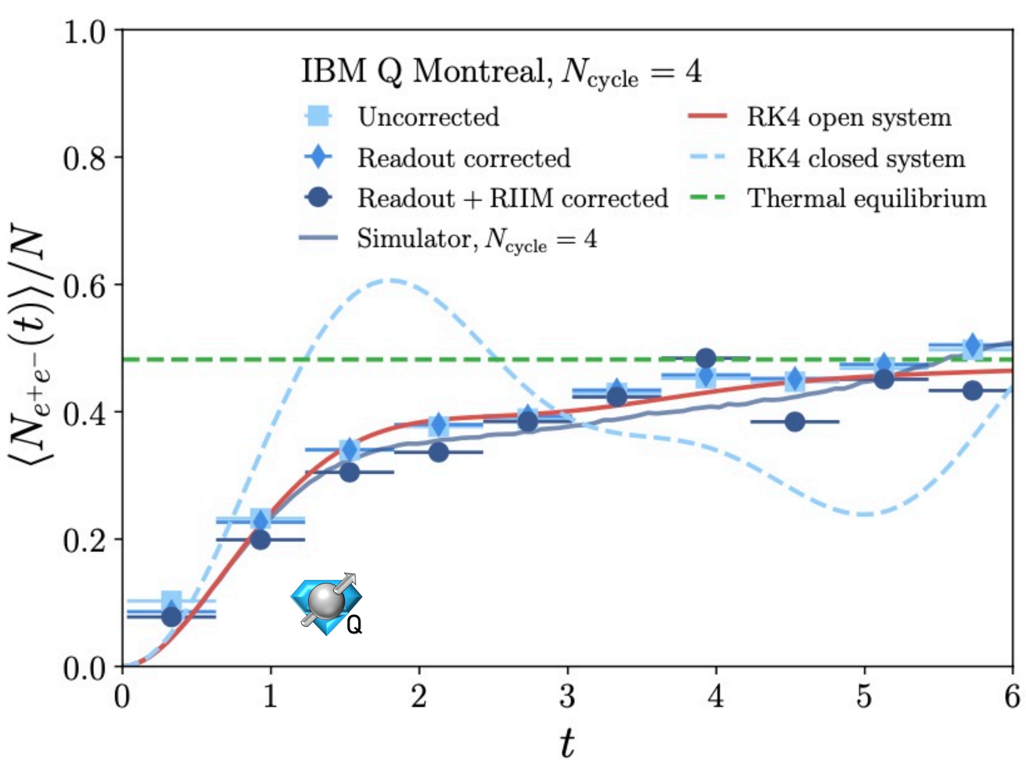




PROBES OF QUARK-GLUON PLASMA AND PHASES OF QCD

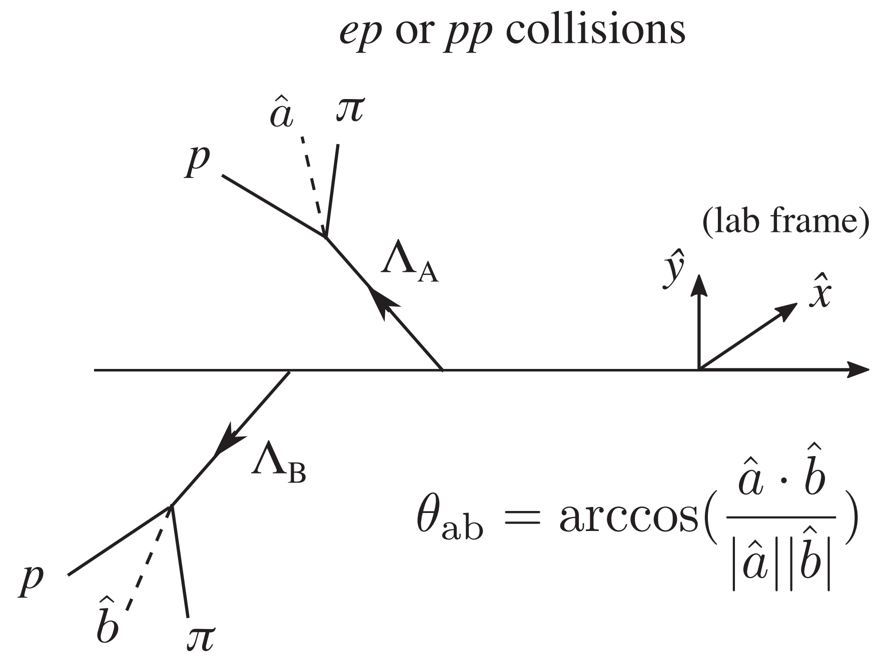
Open quantum system dynamics:
$q\bar{q}$ moving in medium



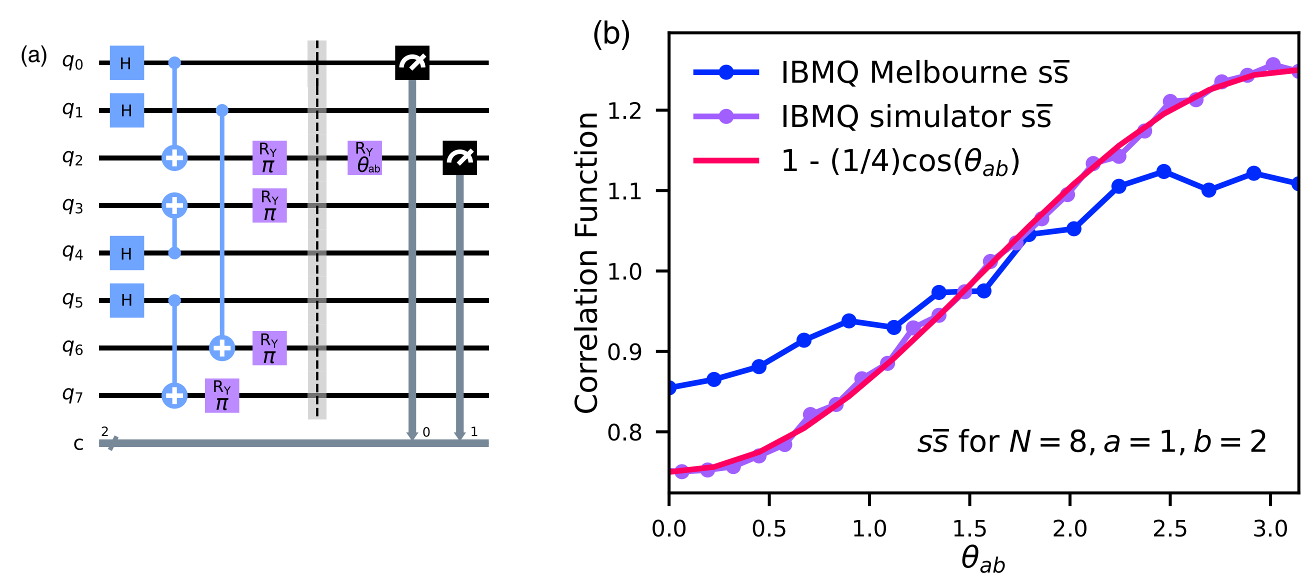


de Jong, Metcal, Mulligan, Ploskon, Ringer, and, Yao, *Phys.Rev.D* 104 (2021) 5, 051501.

Λ and $\bar{\Lambda}$ spin correlations provide novel insights into quantum features of many-body parton dynamics.



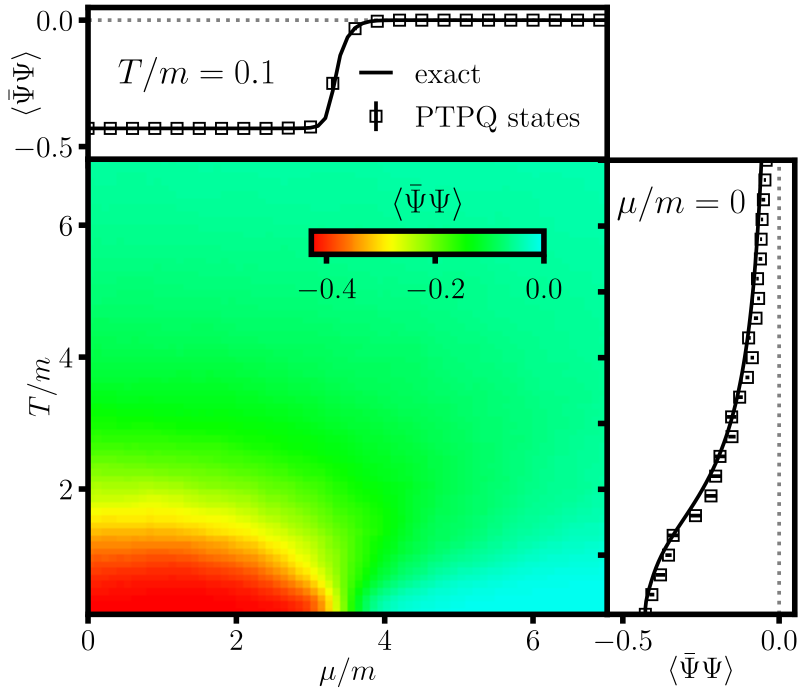
Quantum simulating a simple model of hadronization originating from QCD strings:



Gong, Parida, Tu, and Venugopalan, *Phys.Rev.D* 106 (2022) 3, L031501.

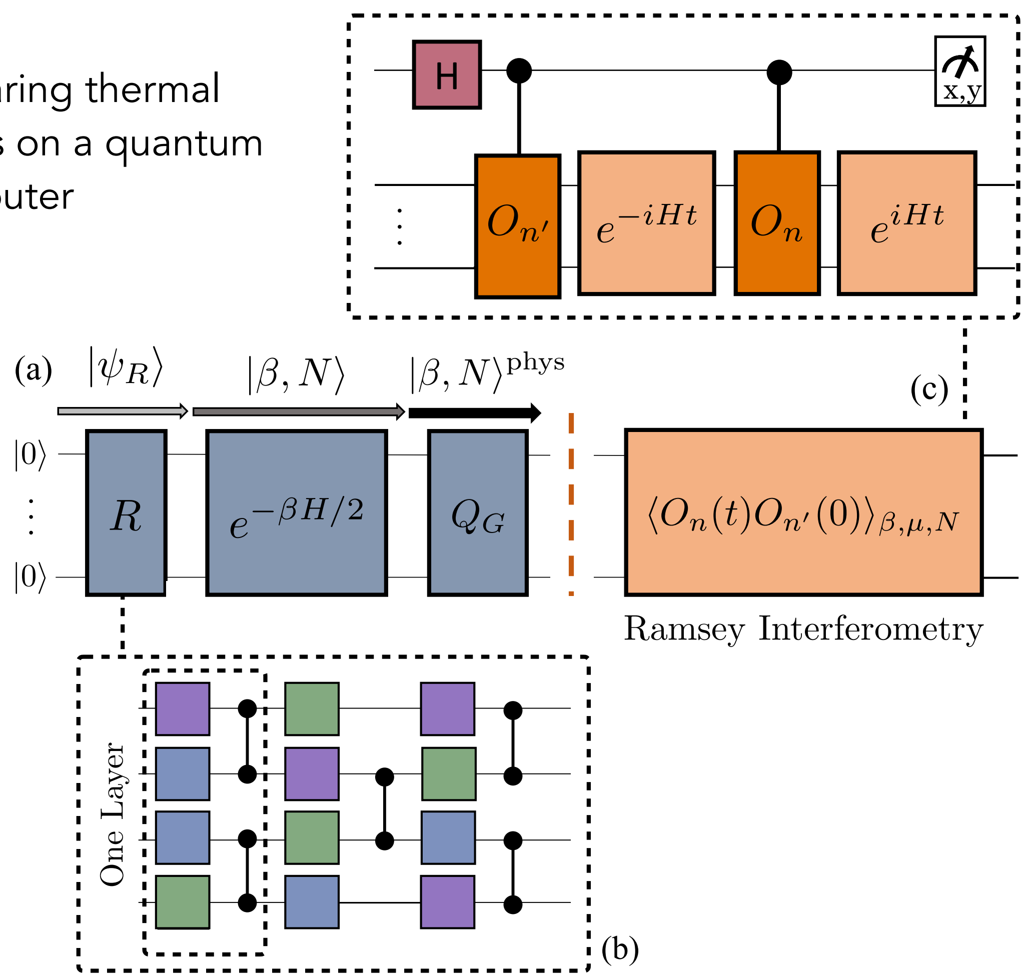
FINITE TEMPERATURE AND FINTIE DENSITY PHASE DIAGRAM

Toward Quantum Computing Phase Diagrams of Gauge Theories with Thermal Pure Quantum States, ZD, Mueller, Powers, arXiv:2208.13112 [hep-lat] (2022).

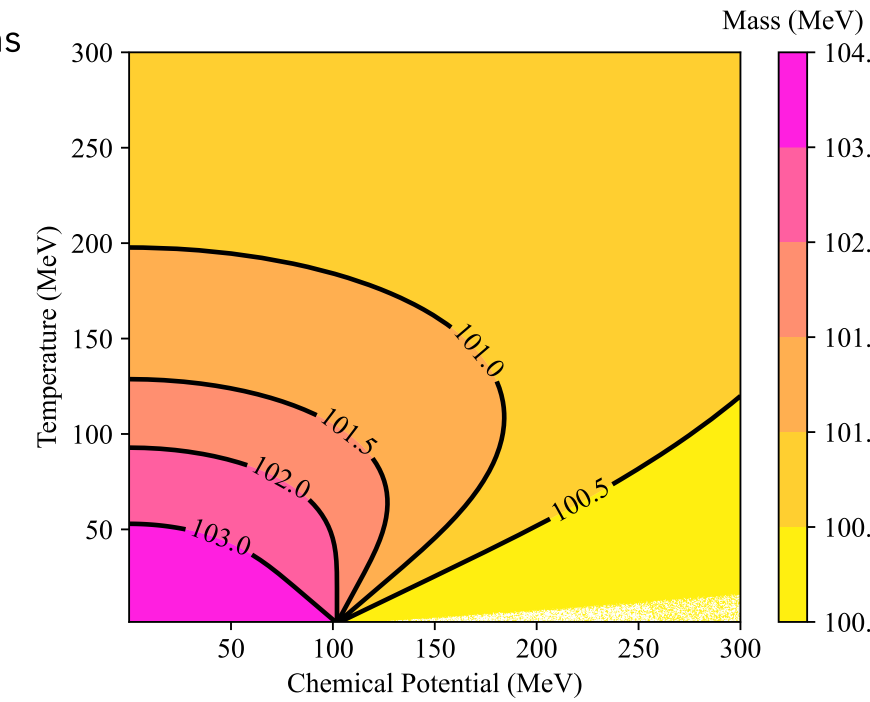


Phase diagram of Z_2^{1+1} with fermions

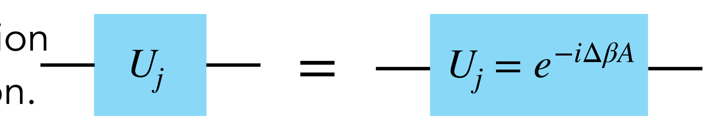
Preparing thermal states on a quantum computer

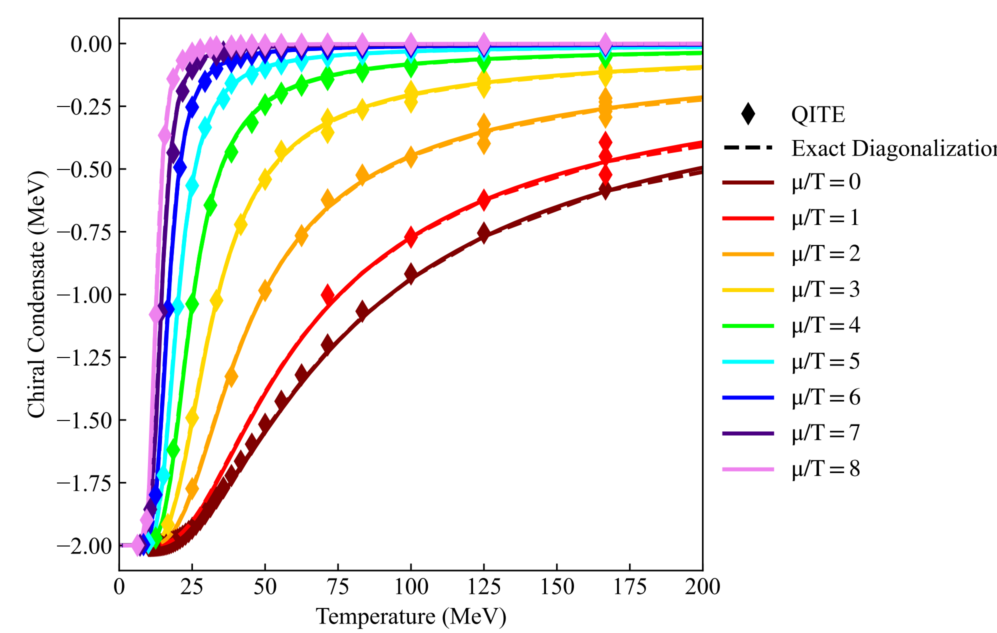


Explorations within NJL model



Approximating imaginary-time evolution with real-time evolution.



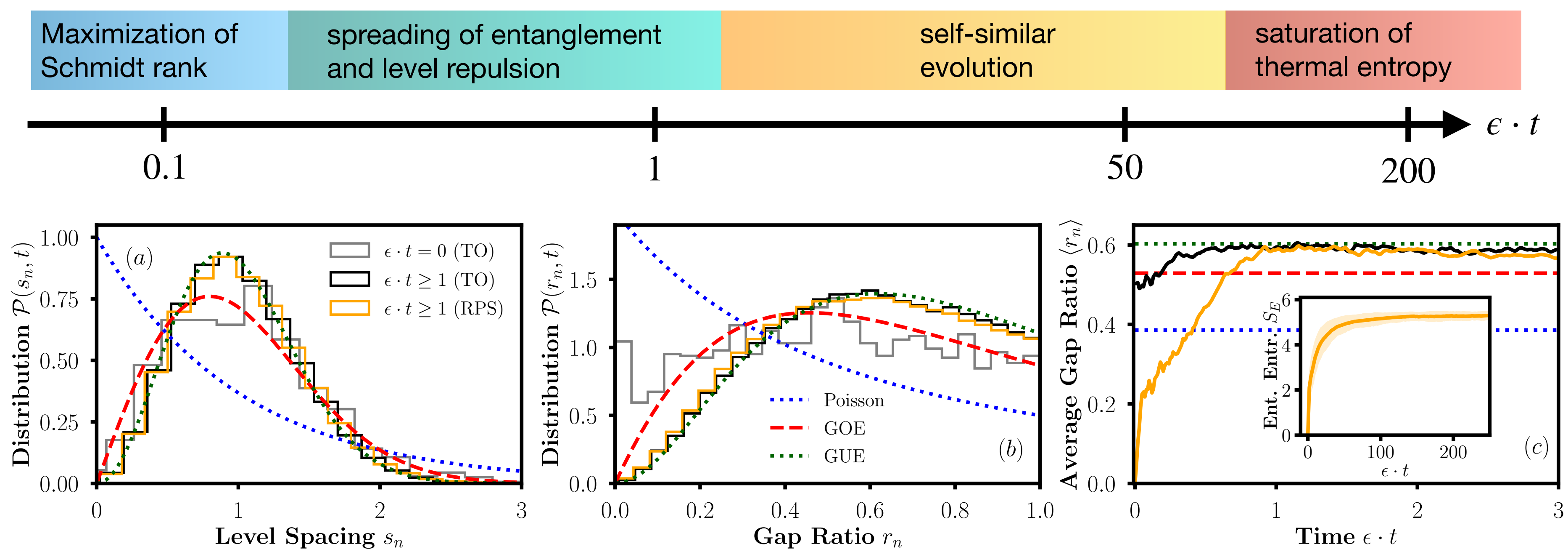


Quantum Simulation of Chiral Phase Transitions, Czajkaa, Kang, Ma , Zhaoa, *JHEP* 08 (2022) 209.

EMERGING UNDERSTANDING OF THERMALIZATION IN SIMPLE GAUGE THEORIES

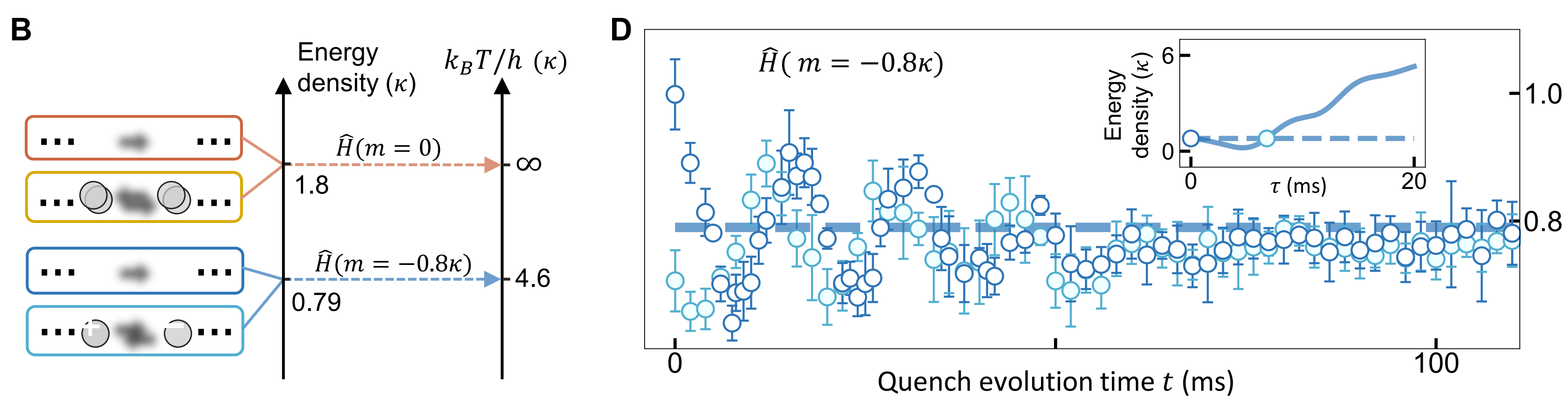
Numerical study of Z_2 LGT in 2+1 D

Mueller, Zache, Ott, Phys. Rev. Lett. 129, 011601 (2022).



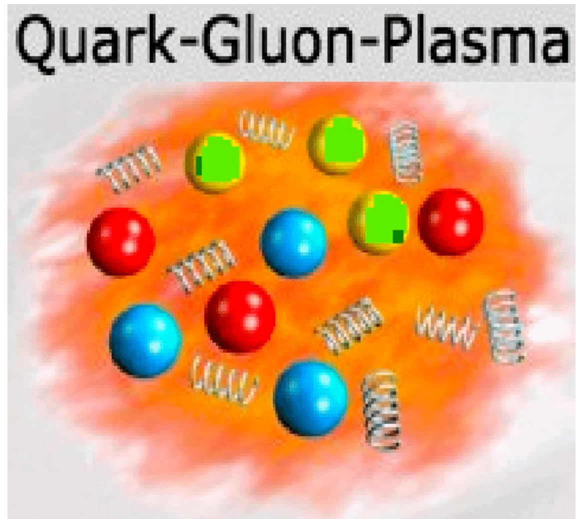
Quantum Link Model in a 70-site analog simulator

Zhou et al, Science 377 (2022) 6603.



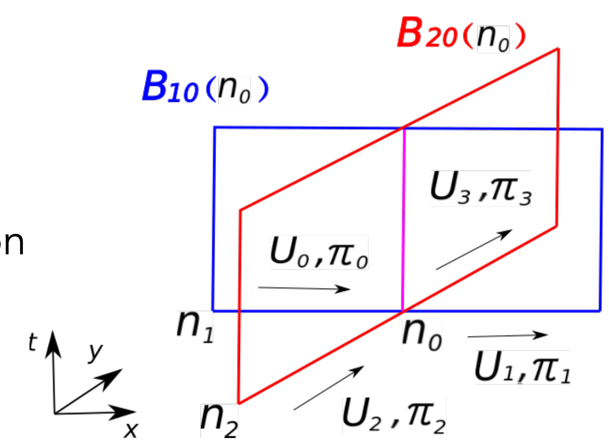
TRANSPORT AND NON-EQUILIBRIUM PROPERTIES

Transport coefficients from real-time correlators of energy momentum tensor

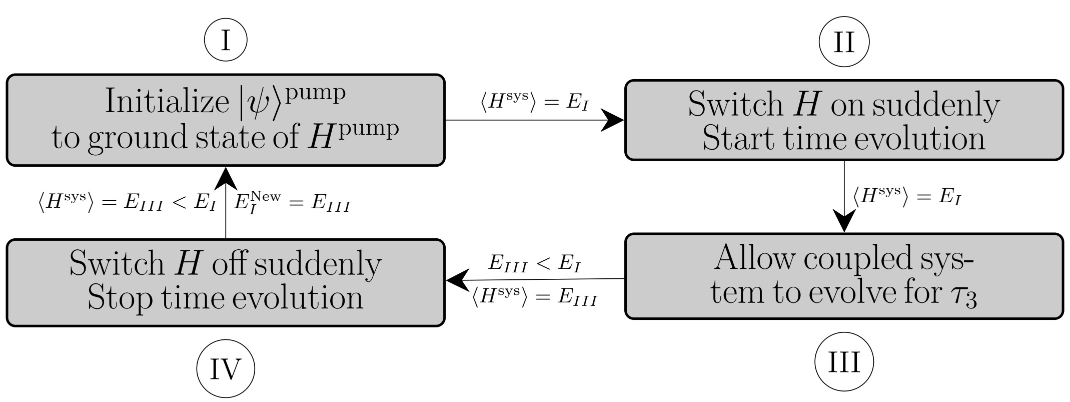


Cohen, Lamm, Lawrence, and Yamauchi, Phys. Rev. D 104, 094514 (2021).

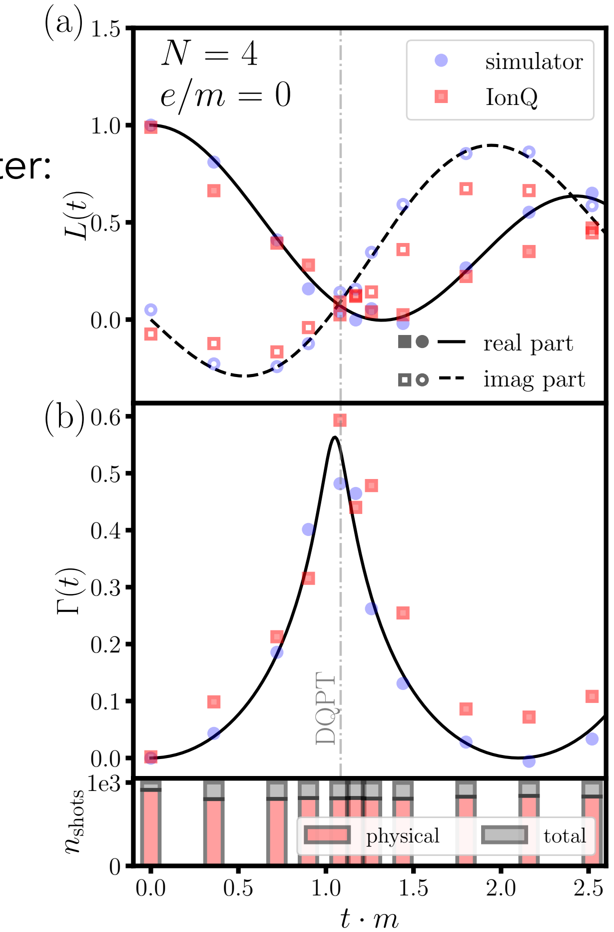
How to define energy-momentum tensor in Hamiltonian formulation

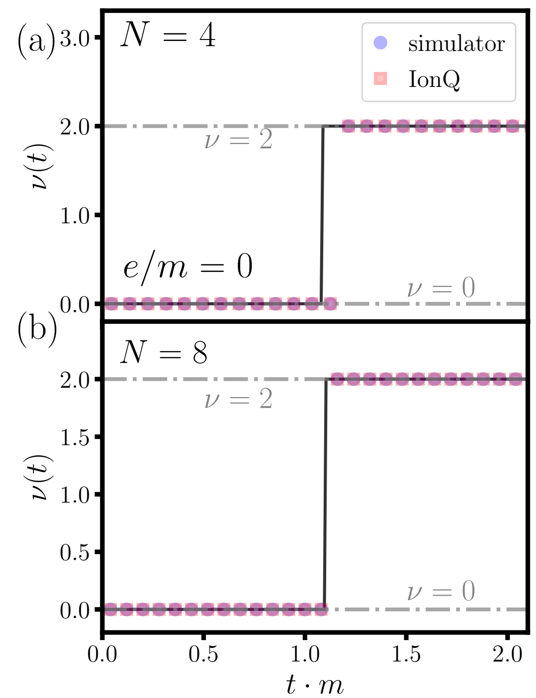


How to prepare a proton state? [Generally not developed sufficiently.]

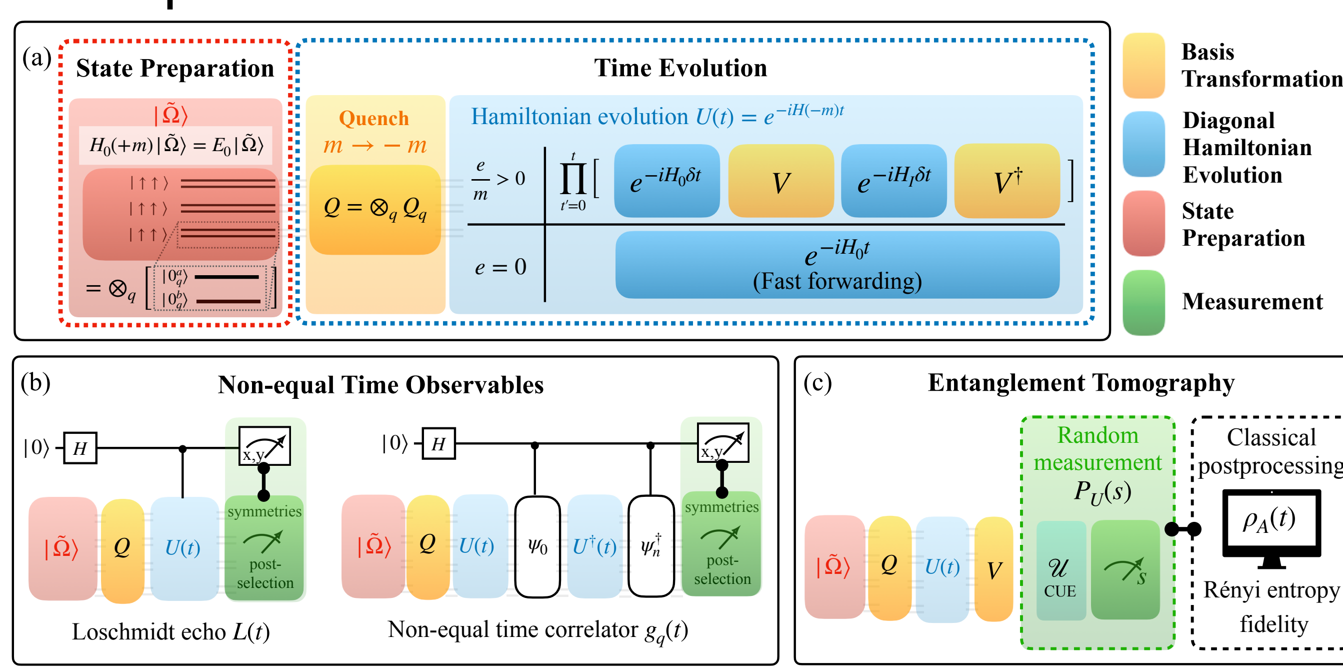


A dynamical phase transition and topological order in lattice Schwinger model with an IonQ quantum computer:



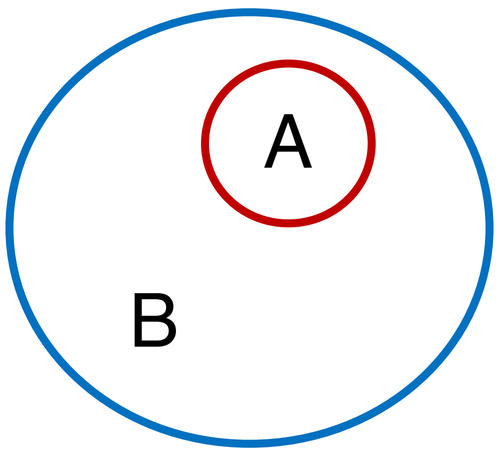


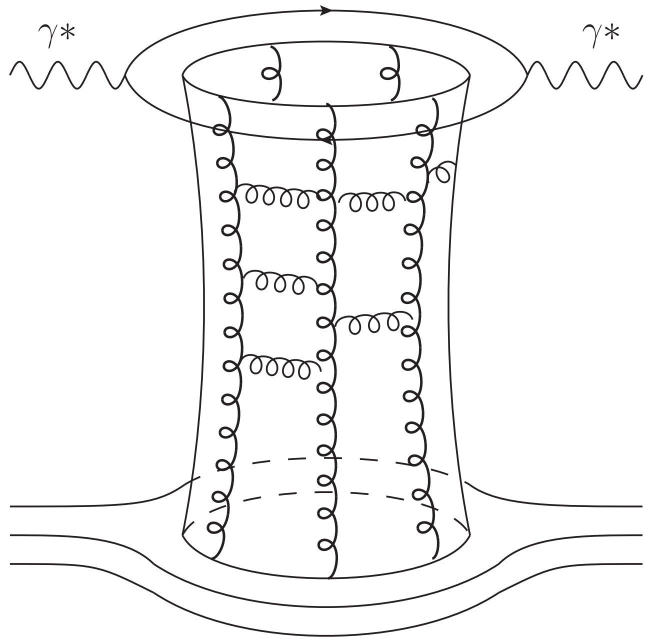
Mueller, Carolan, Connelly, Dumitrescu, ZD, Mueller, Yeter-Aydeniz, to be released (2022).



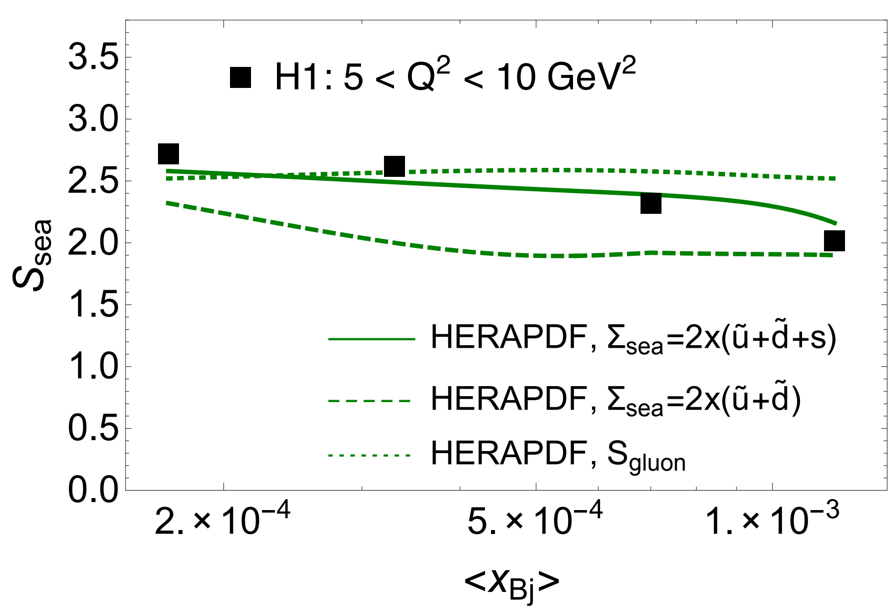
QUANTUM ENTANGLEMENT IN HIGH- AND LOW-ENERGY NUCLEAR PHYSICS

Deep inelastic scattering as a probe of entanglement?



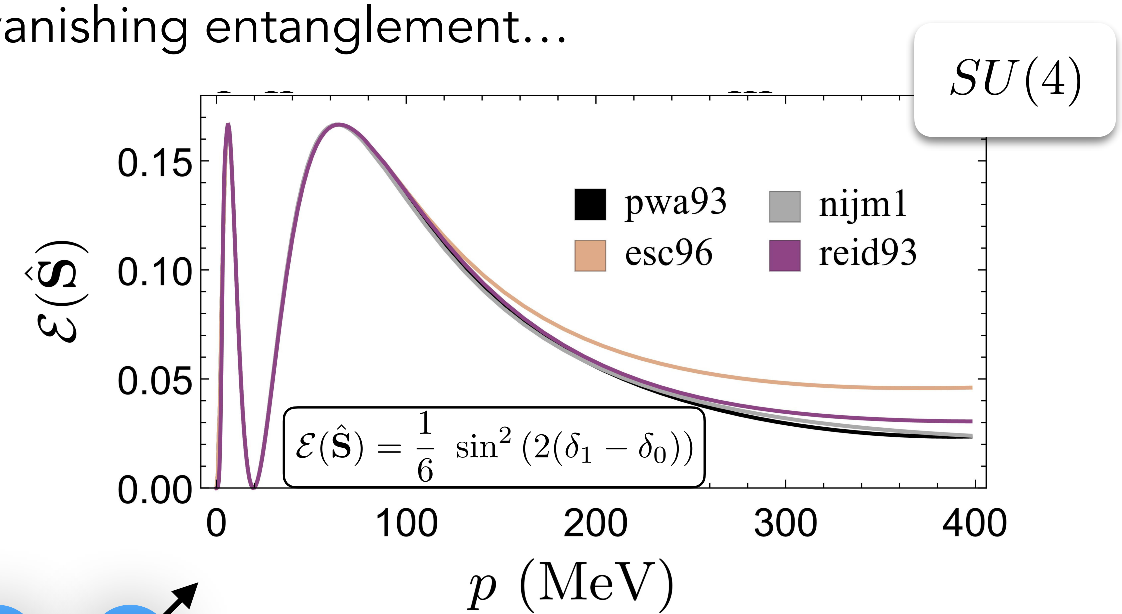


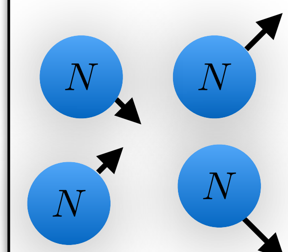
Entropy of hadrons derived from PDFs can be related to entanglement entropy.



Kharzeev and Levin,, Phys. Rev. D 95, 114008 (2017), Zhang, Hao, Kharzeev, and Korepin, Phys. Rev. D 105, 014002 (2022).

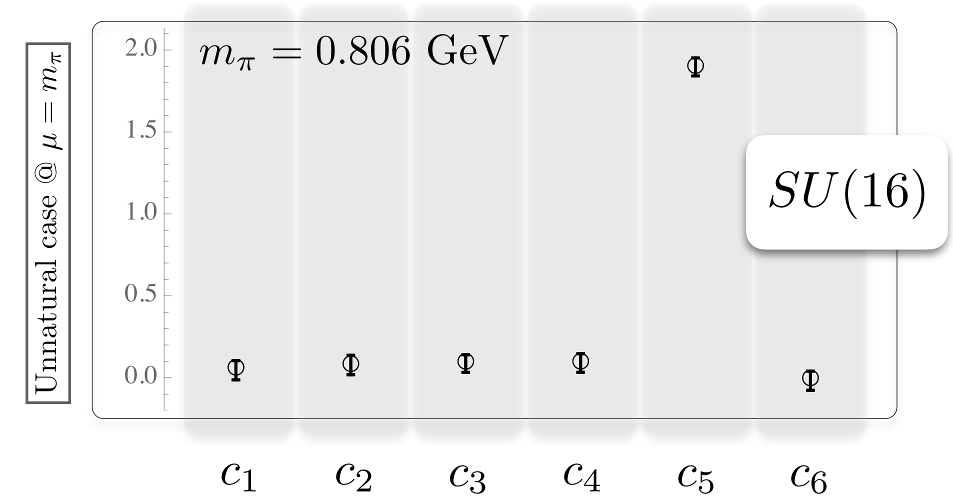
NN interactions at low energies are consistent with vanishing entanglement…

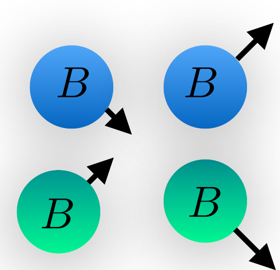




Beane, Kaplan, Klco and Savage, Phys. Rev. Lett. 122, 102001 (2019)

…as are low-energy BB interactions as obtained with lattice QCD.





Wagman, Winter, Chang, ZD, Detmold, Orginos, Savage, Shanahan (NPLQCD), Phys. Rev. D 96, 114510 (2017)

[FINALLY]
THOUGHTS AND REMARKS FOR THE LRP PROCESS…

Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

Organized by:

Alessandro Lovato – Joe Carlson (LANL), Phiala Shanahan (MIT), Bronson Messer (ORNL)
Witold Nazarewicz (FRIB/MSU), Amber Boehnlein (JLab), Peter Petreczky (BNL)
Robert Edwards (JLab), David Dean (JLab)

Workshop Resolution

High-performance computing is essential to advance nuclear physics on the experimental and theory frontiers. Increased investments in computational nuclear physics will facilitate discoveries and capitalize on previous progress. Thus, we recommend a targeted program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML.

The key elements of this program are to:

1) Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies, such as quantum computing, and other opportunities.

2) Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the nuclear physics community through educational and training activities.

3) Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross-disciplinary collaborations in high-performance computing and AI/ML.

4) Expand access to computational hardware through dedicated and high-performance computing resources.

Remarks collected on QC for NP at the Computational NP Workshop:

- Both QC and QC-inspired classical computations have the potential to address the NP science drives.
- Among areas of promise over the next decade are the exploration of prototype models with QCD-like features and identification of the right set of questions which are robust to errors so to acquire qualitative new understandings even with NISQ-era quantum technologies.
- Cross-cutting research involving collaboration with hardware developers and other domain scientists is essential. Quantum circuit design/algorithms/methodology requires collaboration with QIS, CS, and other domain sciences. Need to utilizes lattice QCD and other NP-centric techniques.
- Quantum information tools need to find their way into QCD simulations, classically and quantumly. The role of entanglement in NP need to be explored further.
- QC-inspired algorithms and state-of-the-art Hamiltonian-simulation strategies such as tensor networks need to be developed further. Need to take full advantage of HPC and new quantum-hardware emulators. HPC will be essential for pre/post-processing and hybrid classical-quantum computations.
- Need access to quantum devices dedicated to the NP program. Collaboration across NP will be valuable (through SciDAC-type programs).

THANK YOU